Streamflow Estimation in

Ungauged Basins

Using Regionalization Methods

Streamflow Estimation in Ungauged Basins Using Regionalization Methods

By

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ABSTRACT

Considering the growing population of the earth and the decreasing water resources, the need for reliable and accurate estimation and prediction of streamflow time series is increasing. Due to the climate change and anthropogenic impacts on hydrologic systems, the estimation and prediction of streamflow time series remains a challenge and it is even more difficult for regions where watersheds are ungauged in terms of streamflow. The research presented in this dissertation, was scoped to develop a reliable and accurate methodology for daily streamflow prediction/estimation in ungauged watersheds. The study area in this research encompasses Ontario natural watersheds with various areas spread in different regions.

In this research work nonlinear data-driven methods such as Artificial Neural Networks (ANN) and conventional methods such as Inverse Distance Weighted (IDW) as well as their combination are investigated for different steps in streamflow regionalization. As such, Watershed classification prior to regionalization is investigated as an independent step in regionalization. Nonlinear classification techniques such as Nonlinear Principal Component Analysis (NLPCA) and Self-Organizing Maps (SOMs) are investigated for watershed classification and finally a methodology which combines watershed classification, streamflow regionalization and hydrologic model optimization is presented for reliable streamflow prediction in ungauged basins.

The results of this research demonstrated that a multi-model approach which combines the results of proposed individual models based on their performance for the gauged similar and close watersheds to the ungauged ones can be a reliable streamflow regionalization model for all watersheds in Ontario. Physical similarity and spatial proximity of watersheds was found to play an important role in similarity between the streamflow time series, hence, it was incorporated in all individual models. It was also shown that watershed classification can significantly improve the results of streamflow regionalization. Investigated nonlinear watershed classification techniques applicable to ungauged watersheds can capture the nonlinearity in watersheds physical and hydrological attributes and classify watersheds homogeneously. It was also found that the combination of watershed classification techniques, regionalization techniques and hydrologic models can impact the results of streamflow regionalization substantially. Furthermore, to evaluate the uncertainty associated with the predictions in ungauged watersheds, an ensemble modelling framework is proposed to generate ensemble predictions based on the proposed regionalization model.

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List of Abbreviations and Symbols

ANN	Artificial Neural Network
AR	Auto Regressive
ARMA	Auto Regressive Moving Average
BTOPMC	Block wise use of TOPMODEL with Muskingum-Cunge flow routing method
CDCD	Canadian Daily Climate Data
CNLPCA	Compact Non-Linear Principal Component Analysis
CPN or CPNN	Counter Propagation Neural Network
DB	Davies–Bouldin
EOF	Empirical Orthogonal Function
FDC	Flow Duration Curve
GA	Genetic Algorithm
GRNN	General Regression Neural Network
HBV	Hydrologiska Byråns Vattenbalansavdelning
IAHS	International Association of Hydrological Science
ICA	Independent Component Analysis
IDW-PS	Inverse Distance Weighted and Physical Similarity
IHACRES	Identification of unit Hydrographs And Component flows from Rainfall, Evaporation and Streamflow data
LZFPC	Lower-Zone Free Primary water storage Content
LZFSC	Lower-Zone Free Secondary water storage Content

LZTWC	Lower-Zone Tension Water storage Content
MAC-HBV	McMaster University Hydrologiska Byraºns Vattenbalansavdelning
MLP	Multilayer Perceptron
MLR	Multiple Linear Regression
MRA	Multiple Regression Analysis
NLPCA	Nonlinear Principal Component Analysis
NSGA II	Non-Sorted Genetic Algorithm II
NSE	Nash Sutcliffe Efficiency
PCA	Principal Component Analysis
PSO	Particle Swarm Optimization
PUB	Prediction in Ungauged Basins
SAC-SMA	Sacramento Soil Moisture Accounting
SCE	Shuffle Complex Efficiency
SOMs	Self-Organizing Maps
SRTM	Shuttle Radar Topography Mission
SWAT	Soil and Water Assessment Tool
VE	Volume Error
USGS	US Geological Survey
UZFWC	Upper-Zone Free Water storage Content
UZTWC	Upper-Zone Tension Water storage Content
Q_{obs}	Observed streamflow
Q_{sim}	Simulated streamflow

Declaration of Academic Achievement

This thesis was prepared in accordance with the guidelines of the McMaster School of Graduate Studies for sandwich thesis consisting of published papers and manuscripts under preparation for publication in peer-reviewed journals. Chapter 2 and 3 are published papers and chapter 4 is an under-review manuscript and chapter 5 is a submitted manuscript. As such, these chapters have been co-authored. The original contributions of the thesis author to each paper and the reasons for including them in the main body of this thesis are outlined below:

Chapter 2: Streamflow Prediction in Ungauged Basins: Review of Regionalization Methods by T.Razavi and P. Coulibaly, Journal of Hydrologic Engineering, 18(8), 958–975. (With permission from publisher)

T. Razavi has conducted an extensive literature review on daily streamflow regionalization studies specifically during the last two decades (1990- 2011). This review work was conducted in 2010-2011, and prepared as a manuscript for publication by T. Razavi in 2012 under the supervision and guidance of P. Coulibaly. It was reviewed and edited by P. Coulibaly. This paper should be included in the thesis because it presents an extensive review of daily streamflow regionalization studies with recent advances and future directions.

Chapter 3: Classification of Ontario Watersheds Based on Physical Attributes and Streamflow Series. by: T. Razavi and P. Coulibaly, Journal of Hydrology, 493, 81-94. (With permission from publisher)

The idea of using nonlinear principal component analysis for watershed classification came from a discussion with P. Coulibaly and was the basis for this paper. T. Razavi investigated this technique and other watershed classification techniques to improve streamflow regionalization. The modeling work was done by T. Razavi in the computer laboratory of P. Coulibaly during 2012-2013. The manuscript was prepared by T. Razavi and reviewed and edited by P. Coulibaly. This paper investigates one primary step of regionalization systematically and the results of this study were required for the next step of the research, therefore, it is included in the thesis.

Chapter 4: Evaluation of Continuous Streamflow Regionalization Using Classified and Unclassified Basins by T. Razavi and P. Coulibaly, Journal of Hydrology , Under review.

This research work was planned to be done after the research work in previous paper by T. Razavi and P. Coulibaly. The modeling and computational work was done by T. Razavi during 2012-2014 under the supervision and guidance of P. Coulibaly. The manuscript was then prepared by T. Razavi in 2013. It was reviewed and edited by P. Coulibaly. This study should be included in the thesis because it is in line with the research plan and investigates nonlinear regionalization techniques.

Chapter 5: Improving Daily Streamflow Regionalization by Multi-Model Combination , T. Razavi and P. Coulibaly, Submitted to Journal of Hydrologic Engineering.

The idea for developing the individual models for streamflow regionalization in this research work came from T. Razavi and later on the idea for developing the combination model came from P. Coulibaly. The computer modeling for this research work was completed in 2014. The manuscript was prepared by T. Razavi and reviewed and edited by P. Coulibaly in 2014.

Chapter 1 : Introduction

In this chapter a general background of the research along with some definitions are presented. It is then followed by problem statement and motivations of the research as well as research objectives. Finally, the thesis layout is presented.

1.1. Background

The total amount of water available to the earth is limited. The hydrologists need to know the quantity of that water to manage and maintain the existing water resources. A water budget or water balance can be developed to quantify the amount of total water available at different scales (e.g. watershed, region, and continent). Such water budget is a conceptualized hydrologic cycle illustrated in Figure 1-1 . This figure demonstrates the components of the hydrologic cycle which are important elements in water resources management. The main input to a hydrologic budget is precipitation (e.g. rain, snow, hail...). Some of the precipitation may be intercepted by vegetation such as trees and structural objects which will eventually return to the atmosphere by evaporation or reach the ground. Once precipitation reaches the ground, some of that may fill depression storage (water retained in puddles, ditches, and other depressions in the surface of the ground) some may infiltrate to the ground which will replenish soil moisture and groundwater reservoirs and some may become surface runoff which flow over the earth's surface to a minor channel such as gullies or flows to major stream/river. Water budget can be established for a region defined topographically (such as watersheds or drainage basin), politically (such as country or city) or chosen on some grounds (Viessman and Lewis 1995). Watersheds define surface water boundary and are drained by a system of connecting rivers/streams to a single outlet and hence they are understandable basis for establishing the water balance.

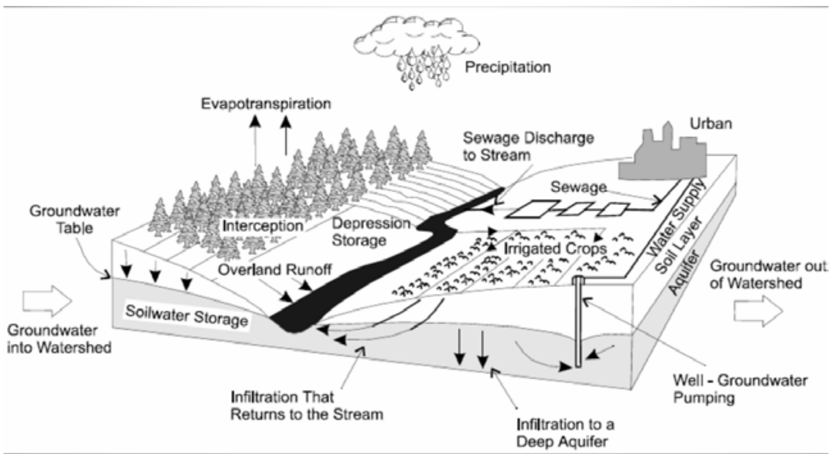

Figure 1-1 The hydrologic cycle

(Ontario stormwater Management Planning & Design Manual, 2003, Ontario Ministry of the Environment)

Surface runoff ultimately reaches the main stream of watershed and generates the streamflow. Streamflow is an important element in hydrologic cycle. Reliable and accurate prediction of streamflow plays an important role in watershed management since it is required for design of hydraulic infrastructures, watershed management plans, flood prediction, etc.

Rainfall-runoff (or hydrologic) models simulate the hydrologic cycle using watersheds physical and climatological characteristics. Therefore, hydrologic models are main tools for estimation/prediction of streamflow. Other less common options are data-driven techniques such as time series or regression models. Hydrologic models might be conceptual or physically based, lumped or distributed models. In general a hydrologic model needs a set of model parameters and meteorological inputs. Each of this information might be unknown or known imperfectly.

Ungauged basins

As explained earlier watershed or water catchment or drainage basin in hydrology is recognized as an area of land where surface water from precipitation or glaciers drains to a body of water such as stream, river or lake and finally converges to the outlet which is at the lowest elevation of the watershed. Ungauged basins are those without enough hydrological observations (or measurements). In other words, hydrometric stations are not available in ungauged basins or they became inactive. Sivapalan et al. (2003) defines ungauged basins as the ones with inadequate records (in terms of both data quantity and quality) of hydrological observations. For example, if the variable of interest has not been measured at the required resolution or for the length of period required for model calibration, the basin would be considered as ungauged with respect to that variable. Variables of interest can be any of hydrological variables such as precipitation, runoff, streamflow, etc.

Prediction in Ungauged basins and Regionalization

International Association of Hydrological Science (IAHS) dedicated a decade (2003-2012) to the challenging issue of Prediction in Ungauged Basins (PUB), and defined it as the prediction or forecasting of the hydrological responses of ungauged or poorly gauged basins and its associated uncertainty (Sivapalan et al. 2003). Different approaches can be used for hydrological predictions in ungauged basins. For example, measurements by remote sensing (e.g. satellites, radars) , application of physically-based hydrologic models where model parameters are specified using physical attributes of watersheds and extrapolation of hydrological information from gauged to ungauged basins. The two first options are less common due to low efficiency considering the high equipment, time and data requirements. Similarities between the watersheds are usually used to transfer information from gauged to ungauged locations. According to Kleeberg (1992), regionalization involves the transfer of information from one catchment (location) to another. In hydrology regionalization is usually recognized as the process of transferring hydrological information from gauged to ungauged basins (e.g. Wagener and Wheater 2006; Lamb and Calver 2002).

1.2. Problem Statement and Motivations

Water is vital for the life cycle and water resources on the earth are precious for human and aquatic ecoystems. The growing population of the earth, the increasing frequency and severity of flood and droughts worldwide, and the impact of human activities on the water resources highlights the need for better estimating and predicting the amount of available water on the earth for establishing a reliable water resources management system which includes water allocation, long-term planning, groundwater recharge, water supply and hydropower production, flood prediction, and design of hydraulic infrastructures such as spillways, culverts, dams.

While the importance of water availability and management is increasingly recognized, hydrological observation networks are declining (Mishra and Coulibaly 2009). In other words, hydrological measurements are not available in many river basins or watersheds in the world. For example, In the United States (US), approximately less than 25000 (10 %) river basins out of

250000 are gauged by US Geological Survey (USGS) (Geological Survey, 2009). According to Environment Canada currently there are over 2500 active hydrometric stations in Canada while over 5500 hydrometric stations are no longer active (http://www.ec.gc.ca/rhc-wsc), and many rivers remain ungauged (Coulibaly et al. 2013). In developing countries this issue is even worse. In any given region, in any part of the word , only a small fraction of the catchments have stream gauges and all other catchments have no stream gauge and therefore they are ungauged (Blöschl et al. 2013).

1.3. Objectives of the research

Considering the high number of ungauged basins over the world and the need for streamflow estimation /prediction, this research aims to develop an accurate and reliable tool for continuous streamflow regionalization in ungauged basins using regionalization methods. To achieve this objective the following goals were set to be achieved:

- Perform a comprehensive literature review on recent advances in streamflow regionalization.
- Investigate and propose a watershed classification methodology prior to regionalization
- Evaluate the efficiency of a systematic watershed classification prior to streamflow regionalization
- Evaluate and propose an efficient streamflow regionalization methodology with uncertainty estimate.

Each objective, achieved in Chapters 2, 3, 4 and 5, respectively, forms the basis of a paper that has been published or submitted for publication.

1.4. Thesis Layout

The first chapter of this Ph.D thesis presents a primary introduction of the research which clarifies the research motivations, objectives and layout. Chapter 2 presents an extensive literature review of previous streamflow regionalization studies. This review focuses on the studies during the last two decades (1990-2011) and covers the latest advances in the methodology along with hydrologic model optimization and uncertainty analysis. Chapter 3 proposes and evaluates novel watershed classification schemes prior to regionalization. In this chapter two reference classification based on streamflow time series are used to evaluate the performance of nonlinear classification techniques based on catchment attributes. In chapter 4, first the efficiency of watershed classification prior to streamflow regionalization is evaluated and then different combination of watershed classification, streamflow regionalization and hydrologic models are evaluated to identify best combinations for different watersheds. In chapter 5 four individual regionalization models for the study area are independently developed and improved, and combination of the four individual regionalization models for the region is developed which appears to be a reliable model for all watersheds of Ontario. In this chapter a framework for generation of ensemble streamflow prediction is proposed which can estimate the prediction uncertainty boundaries. Finally in chapter 6 conclusions and recommendations for future research are presented.

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Chapter 2 : Streamflow Prediction in Ungauged Basins: Review of Regionalization Methods

Summary of Paper I : Razavi, T., and Coulibaly, P. (2013) .Streamflow Prediction in Ungauged Basins: Review of Regionalization Methods. Journal of Hydrologic Engineering, 18(8), 958–975.

The research presented in this work is an extensive literature review on the regionalization of streamflow. We have mainly focused on the research works in the period of 1990-2011. The main topics which are discussed in the paper include:

- Discussion of developments in continuous streamflow regionalization
- Model parameter optimization methods
- The application of uncertainty analysis in regionalization
- Limitations and challenges
- Further research directions

In this paper streamflow regionalization studies are categorized into two main categories of: Hydrologic model-dependent and hydrologic model-independent methods. The results of this study indicate that:

- Streamflow regionalization has been done mostly through hydrologic models
- Conceptual hydrologic models , HBV and IHACRES , have been the most frequently used tools for streamflow regionalization
- In arid to warm temperate climate (e.g., Australia) physical similarity and spatial proximity approach, in warm temperates (most European countries), regression-based methods, in cold and snowy climates (e.g., Canada), spatial proximity and physical similarity approaches seem to outperform other hydrologic model–dependent methods.

2.1.Abstract

The paper presents a comprehensive review of a fundamental and challenging issue in hydrology: the regionalization of streamflow and its advances over the last two decades, specifically 1990-2011. This includes a discussion of developments in continuous streamflow regionalization, model parameter optimization methods, the application of uncertainty analysis in regionalization procedures, limitations and challenges, and future research directions. Here, regionalization refers to a process of transferring hydrological information from gauged to ungauged or poorly gauged basins to estimate the streamflow. Huge efforts have been devoted to regionalization of flood peaks, low flow and flow duration curves (FDCs) in the literature, while continuous streamflow regionalization is helpful in deriving each of these variables. Continuous streamflow regionalization can be conducted through rainfall-runoff models or hydrologic model-independent methods. In the former case, model parameters are used as instruments to transfer hydrological information from gauged to ungauged basins; while the latter case transfers streamflow directly through data-driven methods.

According to the reviewed regionalization studies, streamflow regionalization has been done mostly through hydrologic models, while the focus of these studies is on identifying the best methods to transfer the model parameters. Conceptual rainfall-runoff models such as HBV (Hydrologiska Byråns Vattenbalansavdelning) and IHACRES (Identification of unit Hydrographs And Component flows from Rainfall, Evaporation and Streamflow data) have emerged as the most frequently used models in this category. Physiographic attributes (e.g. catchment area, elevation, slope of basins or channels) and meteorological information (e.g. daily time series of rainfall and temperature) are the most commonly used in the regionalization studies. Diversity in catchment physical attributes and climatic variability produces different performances for each regionalization method's application in various regions. However, overall, spatial proximity and physical similarity have shown satisfactory performance in arid to warm temperate climate (e.g. Australia) and regression-based methods have been preferred in warm temperate regions (e.g. most European countries). Similarly, in cold and snowy regions (e.g. Canada) spatial proximity and physical similarity approaches seemed to be good options among the hydrologic model-dependent methods. Hydrologic model-independent methods have been applied only in few cases and the results have indicated that in warm temperate regions linear and nonlinear regression methods perform well.

Author keywords: Continuous streamflow, Regionalization, Ungauged basins, Rainfall-runoff models, Uncertainty analysis, Parameter optimization

2.2.Introduction

Continuous streamflow estimation is an important issue in surface hydrology, especially in ungauged watersheds. According to Sivapalan et al. (2003), ungauged basins are ones with inadequate records (in terms of both data quantity and quality) of hydrological observations. A catchment is ungauged or poorly gauged with respect to a variable of interest. The International Association of Hydrological Science (IAHS) initiated the decade 2003-2012 with the Prediction in Ungauged Basins (PUB), defined as the prediction or forecasting of the hydrological responses of ungauged or poorly gauged basins and its associated uncertainty (Sivapalan et al. 2003). Most of the studies in this context were conducted after 2003. An example of the earlier studies is Burn and Boorman's (1993) work that investigated hydrologic model parameters estimation based on the classification of catchments according to hydrologic similarity, rather than traditionally used methods such as regression equations. Uncertainty analysis in PUB has also gone relatively less addressed.

The majority of rivers and stream reaches and tributaries in the world are ungauged or poorly gauged (Sivapalan et al. 2003; Young 2006; Mishra and Coulibaly 2009). Such ungauged streams are often located upstream (e.g. mountain areas in Niadas 2005), in maritime and mountainous Apenninic regions (e.g. Castellarin et al. 2007), in 'unregulated' basins (e.g. Stainton and Metcalfe 2007; Mishra and Coulibaly 2009), or in rural and remote areas (e.g. Makungo et al. 2010). Although ungauged basins are often located upstream due to inaccessibility or lack of developer intentions; this state also occurs in many potential sites downstream (Goswami et al. 2007).

Reliable continuous streamflow forecasting is an important factor in watershed planning and sustainable water resource management, as it is instrumental in obtaining a deeper sense of flow variability in ungauged basins. Furthermore, the estimation of flood peaks, low flow characteristics, and FDCs can be derived once the synthetic continuous flow time series is generated. Streamflow data is also used in the design of critical engineering structures such as highways, drainage systems, reservoirs, etc.

Streamflow in gauged and/or ungauged basins is currently forecasted using distributed physically-based models (e.g. BTOPMC [Block wise use of TOPMODEL with Muskingum-Cunge flow routing method], Mike 11 NAM, MIKE-SHE , etc.), conceptual and semi-distributed models (e.g. HBV, SimHyd, IHACRES), and data-driven models (e.g. MLR [Multiple Linear Regression], ARMA [Auto Regressive Moving Average], ANNs [Artificial NeuralNetworks]).

When predictions of streamflow response are required, less complex conceptual lumped models have been shown to be equally reliable and are often preferred (Yadav et al. 2007). The application of physically-based models in which model parameters are derived from physical catchment attributes to ungauged catchments is associated with high levels of uncertainty, reflecting uncertainty in the prior distribution of parameter values (Bulygina et al. 2011).This sometimes causes over-parameterization and model structural errors (Goswami et al. 2007; Yadav et al. 2007). Such models require considerable data and human effort compared to conceptual or semi-distributed models, such as the HBV model (Bergström 1976) and SAC-SMA (Sacramento Soil Moisture Accounting, Burnash et al. 1973). Therefore, usually non-distributed models are preferred. One example of applying physically-based models for streamflow simulation in ungauged basins is Stoll and Weiler's approach (2010), which estimates parameters of a distributed hydrological model (Hill-Vi) in ungauged basins by the explicit simulation of a stream network, and compares the simulated networks to mapped stream networks .They achieved some promising results but also encountered some limitations, such as the problems caused by simplification and modification of the model to achieve fast and robust runs. More recently, data-driven methods (e.g. ANNs, MLR, etc.) which are potentially applicable for streamflow prediction, have been investigated as alternative models to estimate streamflow in ungauged catchments.

In data-driven and conceptual/semi-distributed hydrological models, the model parameters have to be estimated through calibration against observed streamflow in the process of parameter adjustment (automatic or manual), until catchment and model behavior show a sufficient agreement. Since in ungauged basins an observed streamflow time series is not available, the transposition of either gauged streamflow or model parameters from a similar and/or nearby gauged basin, called regionalization, is well recognized as a low-cost and popular solution to provide time series of streamflow at ungauged basins (Young 2006; Samuel et al. 2011).

The term “regionalization” has been used in the literature with almost identical concepts but some minor differences among writers. In Germany since 1993, the priority program “Regionalization in Hydrology" funded by the German Science Foundation (DFG) was concluded in 1998. The conference on Regionalization in Hydrology held in 1997 aimed to explore new mathematical and computational tools to describe and analyze the behaviour of hydrological systems at all relevant scales, from the point to the global, for whole systems and subsystems. The priority program has identified spatial scaling as the main problem of transferring hydrological information between spatial objects and emphasized the need for the acquisition, management, analysis and cartographic presentation of large hydrological data sets for regionalization of hydrologic information, also application of the GIS technology is recognized as an essential prerequisite (Streit and Kleeberg 1996; Diekkruger et al. 1999). Relevant research works occurred after 1998 have been affected by this program. For example, Hennrich et al. (1999) looked for regionalization techniques to transfer parameters from one scale to another while some other studies (e.g. Chiang et al. 2002; Mwale et al. 2011) used the term regionalization or “hydrologic regionalization” only for classifying the watersheds in terms of hydrologic characteristics, and later on used that classification for transferring hydrological information. Also, Mwale et al. (2011) regionalized runoff variability and accounted for runoff heterogeneity across Alberta, Canada using statistical methods and their further plan is to model the streamflow of clusters with several classes of hydrologic models.

According to Blöschl and Sivapalan (1995), regionalization refers to the process of transferring the information (i.e., "hydrological information") from one catchment (location) to another, and it may be satisfactory if the catchments are similar (in some sense), but error-prone if they are not. Hydrological information can be either the model parameters or the general structure of models which estimate hydrological responses, e.g. streamflows. According to this definition, the ungauged catchments should be located in a region homogeneous with the gauged basins. The assumption behind the homogeneous region of runoff responses is that similar climate, geology, topography, vegetation, and soils in the homogeneous region would generally produce similar runoff responses, but not necessarily in geographically neighboring basins (Smakhtin 2001). In this paper, regionalization is considered as the process of transferring hydrological information from gauged to ungauged basins.

Regionalization can be used to transfer hydrological information between spatial objects, spatial dimensions (which classify the objects according to their number of independent directions in space), and scale (a general idea of looking at objects in a more or less generalized manner) (Streit and Kleeberg 1996). It can be done by using predictive approaches such as an extrapolation of hydrologic information from gauged to ungauged basins, observation by remote sensing and hydrologic model simulation, and integrated meteorological and hydrological modeling (Goswami et al. 2007).

Regionalization is widely regarded as a challenging task in hydrological science (Sivapalan et al. 2003; Oudin et al. 2008; Stoll and Weiler 2010; Samuel et al. 2011), firstly, because of the lack of runoff data which is normally used to calibrate parameters of hydrological models, limits the success of simulation (Sivapalan et al. 2003). Secondly the studies on regionalization methods usually produce different results, as they have been examined on different sites and also the available catchment characteristics vary from one case to another (Oudin et al. 2008). As a result there is no universal method for regionalization.

Considering the rapid pace of regionalization-method development in the literature and the importance of continuous streamflow estimation in ungauged basins, we intend to present a comprehensive review of continuous streamflow regionalization approaches and their developments. Our overall motivations are to review regionalization approaches which have been developed and applied in estimating streamflow or runoff (streamflow per unit area of catchment) in ungauged basins; show the key steps in regionalization procedures, catchment attributes used in these studies, related uncertainty analysis and hydrologic model optimization; and finally present recent developments in the streamflow regionalization. He et al. (2011) have recently reviewed continuous streamflow regionalization methods, but they have only reviewed hydrologic model-dependent approaches. This paper provides a more comprehensive review including model-dependent and model-independent methods, and discusses the developments and emergent directions in continuous streamflow regionalization.

2.3. Main steps in the regionalization approach

In general, a regional model can be stated in a simplified form as follows Eq.2-1 (Wagener and Wheater 2006):

$$\hat{\theta}_L = H_R(\theta_R|\Phi) + \upsilon_R \quad \text{Eq. 2-1}$$

where $\hat{\theta}_L$ is the estimated hydrological variable of interest at the ungauged site (it can be an estimated model parameter, probability or cumulative distribution function parameter or hydrological response such as streamflow or flow events), $H_R(.)$ is a functional relation for $\hat{\theta}_L$ using a set of catchment attributes (physiographic and/or meteorological attributes - Φ), θ_R is a set of regional hydrological variables of interests (e.g. model parameters); and υ_R is an error term. Clearly, regionalization requires information of catchment attributes (physiographic and meteorological attributes) and a function (linear/nonlinear) for relating predictors to the predictand.

There are at least five main important steps in a regionalization strategy. The first step is to collect and manage catchment attributes, which includes meteorological attributes (such as mean annual rainfall, temperature, etc.) and physiographic information (such as the location of stream gauges or centroid of the drainage basins, area covered by grass, trees, etc., and soil types, permeability of soils, etc.). Unfortunately, the required information on catchment attributes is sometimes difficult to obtain. This raises the question on what minimum number and types of catchment attributes should be collected for a proper regionalization procedure, and also which regionalization methods are proper when all of the required catchment attributes are not available. In the next section different catchment attributes which are applied in streamflow regionalization studies are discussed.

The second step in a regionalization procedure is to determine and clarify hydrological variables of interests. In the case of continuous streamflow regionalization, the collected streamflow data of nearby and/or similar gauged basins will be used to generate hydrological model parameters or relationships with catchment attributes. The Third step is to develop a relationship between streamflow or runoff indices or hydrological model parameters and catchment attributes. This relationship is the regionalization method which will be discussed in detail in the next section. The fourth step is to evaluate model performance using pseudo-ungauged basins before the model is applied to the real ungauged basins. Once a relationship between catchment attributes and hydrological variables is established, it is necessary to validate the model before it can be applied in ungauged basins. The leave-one-out cross-validation procedure is normally used to assess the validity of regionalization approach (e.g. Samuel et al. 2011; Parajka et al. 2005; Merz and Blöschl 2004).Other cross-validation techniques such as split-half and bootstrapped are not usually applicable to regionalization studies because they can only be applied to poorly gauged basins and for the periods in which the observed flow data is available. In leave-one out approach, each catchment is in turn considered as being ungauged for obtaining a flow simulation in that catchment, the actual discharges are afterwards used to evaluate the performance of the flow estimation procedures for the catchment. Statistical tests are then used to evaluate the performance of the flow estimation in the “pseudo” ungauged basins. Table 2-1 presents some error metrics commonly used. Among them are the Nash-Sutcliffe efficiency, Root Mean Square Error (RMSE), relative RMSE, mean bias (BIAS), relative BIAS, Volume Error (VE), and Correlation coefficient. The fifth and final step is to include uncertainty analysis. A major recent improvement in regionalization procedures is to include uncertainty analysis, which is necessary due to uncertainties in selecting catchment properties and regionalization procedures, and identifying gauged and regional model structures and their parameters (Wagener and Wheater 2006). A discussions and outline of the general uncertainty analysis procedure will be presented later on.

The main steps presented above provide an overview of the general procedure of the regionalization of any hydrological variable. Step 3 is where the regionalization model can be changed for different hydrological variables (e.g. select a different hydrologic model). Regionalization can be adjusted for specific purposes, such as linking to ecological implications (Stainton and Metcalfe 2007) or combining the approach with integrated data processing tools such as Geographical Information Systems (GIS, e.g. Streit and Kleeberg, 1996; Cheng et al. 2006).

2.4. Catchment attributes

Catchment attributes are different across various studies, and it seems that an initial hypothetical judgment is required to identify which potential catchment attributes would have an impact on the runoff responses of interests. Merz and Blöshl (2004) and Parajka et al. (2005), for example, use the help of expert judgments to take into account the interaction between the runoff regime, climate, and physiographic attributes. Kokkonen et al. (2003) point out that catchment attributes used for regionalization purposes should characterize the factors that drive the hydrological response of a catchment and should also be derivable from existing and readily available data sources, such as topographical maps. Some researchers select catchment properties with the objective that the sample of catchments is representative of the statistical population of catchments in the region, both in geographical and in parameter space (Mwakalila 2003). Some might use step-wise regression analysis to identify landscape-climate descriptors that are good predictors of percentile flows (e.g. Mohamoud 2008) while some of the relationships identified by step-wise regression, even though statistically significant, might be an accident of the data (Sefton and Howarth 1998).

Table 2-1 Validation test (error metrics) which are normally used for regionalization studies

Validation test	Equation	Note of variables in the equation
Nash-Sutcliffe efficiency	$NSE = 1 - \left(\frac{\sum_{i=1}^{N} (y_i - y_i^{'})^2}{\sum_{i=1}^{N} (y_i - y_{mean})^2} \right)$	yi= observed streamflow at time-step i
Volume Error	$VE = \frac{\sum_{i=1}^{N} y_i^{'} - \sum_{i=1}^{N} y_i}{\sum_{i=1}^{N} y_i}$	$y_i^{'}$ =modeled streamflow at time-step i ymean = the mean of the observed values
Mean Bias	$BIAS = \sum_{i=1}^{N} (y_i^{'} - y_i)$	N = number of time-steps (data points)
Mean Relative Bias	$BIASr = \sum_{i=1}^{N} \frac{(y_i^{'} - y_i)}{y_i}$	

Table 2-2 presents the catchment attributes which have been used in reviewed papers. Types of catchment attributes collected to perform regionalization vary among studies. By simply comparing the types of data attributes used in a regionalization process it can be summarized that physiographic information (e.g. catchment area, elevation, slope of basins or channels) and meteorological attribute (e.g. mean annual or mean daily rainfall and temperature) are most often incorporated in regionalization studies (either in regionalization or hydrologic model calibration). Other catchment attributes which are also occasionally incorporated in some studies are: (1) the percentage of area that is covered by water (e.g. lakes, swamp, wetland, and groundwater) or by land use (e.g. forest, grass, woodland, urban/non-urban area); (2) location of stream gauges or centroid of catchments; and (3) other meteorological attributes such as mean annual evaporation and snowfall. According to Mwakalila (2003), methods which are used to quantify the catchment attributes usually include topographical indices, geology and soil index, climate indices, and vegetation cover indices. Croke et al. (2004) collected catchment attributes on soil covers and physiographic characteristics, since their study focused on predicting hydrologic responses to land cover changes due to agricultural intensification in gauged and ungauged basins.

In general, the most widely used attributes by researchers in continuous streamflow regionalization are catchment area, elevation, slope of basins or channels, and mean annual or daily rainfall and temperature.

Table 2-2 Catchment attributes used in streamflow regionalization studies

References	Catchment attributes	References	Catchment attributes
Vandewiele and Elias1995	Location of basins	Merz and Blöschl 2004	Area, elevation, slope, porous aquifers, land covers, geologic units, soil types, river network density, lake index, mean annual precipitation, maximum annual daily precipitation
Sefton and Howarth 1998	Morphometric (elevation, area, channel slope, etc); Soils (% groundwater, %shallow groundwater, % peaty soil, etc); Land use (%grass heath, mixed woodland), rainfall and temperature	Lee et al. 2006	Daily precipitation, streamflow and potential evaporation, 17 physical catchment characteristics e.g. catchment drainage area, altitude, slope
Post and Jakeman 1999	Area, elongation, slope of lid, gradient and drainage density	McIntyre et al. 2005	Daily precipitation, streamflow and potential evaporation, drainage area , standard- period average annual rainfall , mean catchment altitude (m above sea level),index of fractional urban extent
Siebert 1999	Area, % forest, % field of meadow, and % lake	Parajka et al. 2005	Similar as Merz and Blöschl (2004)
Peel et al. 2000	Climate, terrain (90th percentile minus 10th percentile elevation in catchment), soil depth, and plant water holding capacity	Boughton and Chiew 2006	Rainfall, runoff , median elevation ,elevation range , leaf area index; percent of woody vegetation on catchment; plant water holding capacity, transmissivity
Chiang et al. 2002	Watershed area, forest area, percentage of contributing drainage area, area of storage, elevation, above mean sea level, stream length per unit area, main channel slope, the mean annual precipitation	Cheng et al. 2006	Land covers: vegetated area (agriculture & natural forest), bare field, vegetation and urban area
Kokkonen et al. 2003	Mean overland flow distance to a stream , mean flow distance in a stream , mean solar radiation index , mean topographic wetness index , catchment area ,elevation at the weir , mean catchment slope	Heuvelmans et al. 2006	Area, slope, height (masl), dominant land use, dominant soil texture
Mwakalila 2003	Catchment area and slope , drainage density and land use types, indexing topography, geology, and land use, mean annual rainfall (RAIN) and potential evapotranspiration	Wagener and Wheater 2006	Basefow index derived using the HOST classification, soil moisture deficit, catchment size and drainage path configuration, catchment steepness, dominant aspect of catchment slopes, average annual rainfall, median annual maximum 2-day rainfall
Croke et al. 2004	Forest cover area, catchment area, soil and topography classes	Young 2006	Catchment area, Mean catchment altitude, The mean aspect of direction of all slopes, The longest drainage path, etc.
Cutore et al. 2007	Area, average altitude (masl) , permeable area (%) , stream length , record size	Post 2009	Daily rainfall ,mean average wet season rainfall, total length of streams, percent cropping and percent forest in the catchment , minor till (>1 m deep) ,thin till, rock ridges peat pond bedrock outcrops
Goswami et al. 2007	Area, length of longest stream, altitude at outlet and the highest point, mean latitude and hydrological variables	Reichl et al. 2009	Geomorphic characteristics e.g. min / max/ mean elevation, Climate e.g. mean winter & summer precipitation, Soils e.g. mean soil depth mean plant available water holding capacity etc.
Götzinger and Bárdossy 2007	Flow time, land use, soil properties, area and geology	Seibert and Beven 2009	The monthly long-term mean potential evaporation, the areal, corrected precipitation, Temperature
Yadav et al. 2007	Dynamic response characteristics in seven categories , magnitude of high flows, low , average flows, duration of flows, frequency, rate of change in flows, and timing of flow events & and 13 physical watershed characteristics e.g. climate, watershed topography and subsurface geology and soils	Zhang et al. 2008	Maximum & minimum temperature, incoming solar radiation, actual vapor pressure and precipitation, potential ET, area, aridity index, mean elevation, mean slope in degree, stream length, mean Solum thick, water holding capacity, Mean woody vegetation fraction

References	Catchment attributes	References	Catchment attributes
Bastola et al. 2008	Rainfall, Potential Evapotranspiration (PET) and runoff data	Besaw et al. 2010	precipitation and temperature , streamflow time series
Hundecha et al. 2008	Percentages of the different land use and soil classes, size and mean slope of the subwatershed, a shape factor defined as the ratio between area of a subwatershed and the square of the distance from the outlet of the watershed to the farthest point in the watershed.	Bocchiola et al. 2010	Glaciers meteorological data including temperature, precipitation and snow and ice ablation.
Kim and Kaluarachchi 2008	Drainage area , soil depth , percent of cultivated area , percent of forest area, mean Channel density , slope of main channel , ratio of main stream length to basin length , ratio of basin width to basin length , saturated hydraulic conductivity of the upper zone , precipitation of the wet season, dry precipitation of the non-wet season, mean annual potential evapotranspiration , total channel length	Castiglioni et al. 2010	Drainage area; percentage of permeable area; maximum, mean and minimum elevations, concentration time; mean annual precipitation; mean annual temperature
Mohamoud 2008	Land use and land cover%, Geomorphology e.g. minimum elevation, basin relief, average slope, etc. Soil e.g. total soil depth, geology: e.g. dominant lithology	Lima and Lall 2010	Drainage area, flood and streamflow time series
Oudin et al. 2008	Catchment area, mean slope, median altitude, river network density, fraction of forest cover, aridity index (E/P)	Makungo et al. 2010	Rainfall, evaporation, uncontrolled spills, downstream flow releases, dam water levels , domestic abstractions, area under irrigation, crop factors, types of crops grown and the irrigation schedule.
Buttle and Eimers's 2009	Physiographic characteristics e.g. area (ha), mean slope (%), drainage density (m) , fraction of basin area	Parada & Liang 2010	Historical streamflow records for gauged basins in the proximity of the ungauged watershed and streamflow prediction for ungauged basins, mean annual precipitation, area, location of outlet, elevation
Li et al. 2009	Hydro_climatic characteristics e.g. mean annual precipitation , mean annual potential evapotranspiration , mean annual runoff , Runoff coefficient ,ratio of potential evapotranspiration to precipitation, catchment slope, plant available water capacity of soil, fraction of total woody vegetation	Samaniego et al. 2010	Area, mean & median slope , drainage density, shape factor , percentage of north and south facing slopes (%) , mean elevation (m) , saturated areas (%), mean available soil water capacity (mm) , fraction karstic formations (%) ,mean percentage of forest covered areas (%) , mean percentage of impervious areas mean percentage of permeable areas (%), mean annual precipitation (mm) , mean & maximum temperature
Jin et al. 2009	Area and position of basins	Samuel et al. 2011	The location of the centroid of the catchments (i.e., latitude and longitude), the morphology of the catchments (i.e., mean elevation, mean catchment slope and area), the percentage of area covered by water , the land use , water drainage, rooting depth and the surface geology , precipitation and temperature
		Bulygina et al. 2011	Hourly records of precipitation, incoming solar and net radiation, wet and dry bulb temperature, and wind speed and direction, area, mean channel slope, forest%, soil (HOST)%

2.5. Developments in continuous streamflow regionalization from 1990-2011

Regionalization approaches can be classified into hydrologic model-dependent and hydrologic model-independent groups (Figure 2-1). The methods employed by the first group transfer rainfall-runoff model parameters between basins. Those model parameters are then used to generate continuous streamflow in the target basin. The second group does not estimate streamflow time series through rainfall-runoff models (in ungauged basins), and therefore instead of hydrologic model parameters, the equation structure and its parameters are transferred. These models usually develop and employ an equation representing input-output relationships, such as rainfall and temperature as input and streamflow as output. Hydrologic models require more catchment attributes to be parameterized and more knowledge and expertise while the structure of data-driven models is simpler and can be defined with less data compared to the former. An interesting study has been the comparison of the two approaches. Goswami et al. (2007) have used both categories; conceptual hydrologic models and ANN models to simulate daily flow in 12 French catchments considered as ungauged. The result of their study indicated that ANN model had better performance. Although such comparative study requires more resources, it appears a good approach in identifying the optimum regionalization method for a case of interest.It is noteworthy that the good potential of data-driven methods (e.g. ANN) for streamflow regionalization can be particularly useful for cases where data is not available for applying hydrologic model.

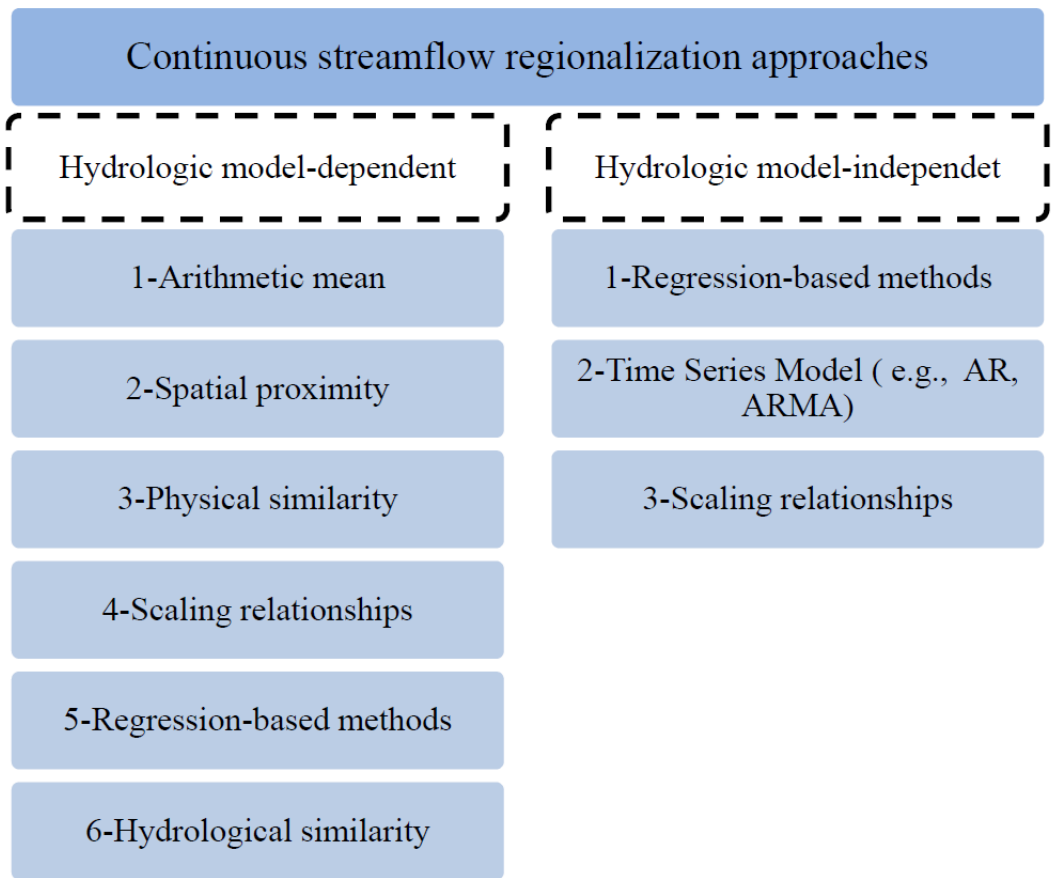

Figure 2-1 Schematic of two classes and subdivisions of continuous streamflow regionalization methods

There are about 70 published studies involving streamflow regionalization within the last two decades (which are cited in the paper). The summary of 43 representive studies is tabulated in Table 2-3 and Table 2-4. Most of these regionalization studies estimate streamflow through hydrologic models and investigate the methods which transfer model parameters from gauged to ungauged basins while a lesser number use data-driven methods to infer streamflow directly in ungauged basins. Table 2-3 presents the former category and contains references (authors' names and publication year), study area, climate classification of the study area, temporal scale and key objectives, name of the hydrologic model, regionalization methods which extrapolate the model parameters, and finally the major findings of the papers. Table 2-4 shows the latter category and indicates the hydrologic model-independent methods which regionalize streamflow from gauged to ungauged basins (see column "regionalization methods").

Table 2-3 and Table 2-4 indicate that regionalization approaches have been widely used in many parts of the world such as North America, Asia, Australia, Africa, and Europe. The approaches have been applied to estimate streamflow from small basins (e.g. 0.04 km^2) to large basins (e.g. 823000 km^2) (see column "Study Area" in both tables). These approaches have also been applied to various landscapes, climatic regions, and different topographies. Parajka et al. (2005) and Merz and Blöschl (2004), for example applied the regionalization approaches in the catchments located in different topographies in Austria .Some examples of the streamflow regionalization approaches in both groups will be further described and discussed in the following sections.

Table 2-3 Studies on hydrologic model-dependent streamflow regionalization approaches (1990-2011)

References	Study area	Climate*	Temporal scale and key objectives	Hydrological model	Regionalization methods	Class**	Major findings
Vandewiele and Elias1995	75 Belgian basins (19-1597 Km^2)	Warm temperate	To obtain the monthly water balance of ungauged catchments	A monthly water balance model obtained by geographical regionalization	Spatial Proximity (kriging and the use of few neighbouring basins)	2	Kriging is acceptable (RMSE<7%) in 72% of the basins, whereas the second is acceptable in 44%.
Sefton and Howarth 1998	60 catchments in England and Wales (8.7-893.6 Km^2)	Warm temperate	To estimate daily flows in ungauged basins	IHACRES with GIS databases	Multiple regression	5	The relationships are limited in terms of statistical accuracy but robust enough to reproduce daily flows, NSE = 0.56 - 0.72
Post and Jakeman 1999	17 small catchments (4 to 65 (ha)) Victoria, Australia	Warm temperate	To estimate daily continuous flow in ungauged basins	IHACRES	Multiple regression (linear & nonlinear)	5	NSE around 0.72 ,errors in the representation of hydrologic response by the model and the limited availability of appropriate landscape attributes caused some poor results
Siebert 1999	11 catchments in flat regions (7 to 950 km^2) Central Sweden	Snowy	To develop a model to obtain optimized hydrological parameters and daily hydrograph simulation	HBV (plus Monte Carlo simulation to obtained optimized parameters)	Regression equations (linear, exponential, power and log)	5	Observed and simulated hydrograph : R_{eff} values:0.70-0.88- fuzzy measure=0.85 , About half of the parameters were significantly correlated to catchment characteristics
Peel et al. 2000	331 catchments (50 to 2000 km^2) in Eastern & southwestern Australia	Warm temperate	To determine the relationships between hydrological model parameters and catchment attributes and estimate daily streamflow in ungauged basins	SIMHYD	Linear regression between model parameters and catchment attributes	5	The correlations between the model parameters and the climate index are more statistically significant compared to other attributes (NSE : 0.12-0.24))
Schreideret al.2002	Gauged and ungauged subcatchments of Thailand (68- 2157 km^2)	Equatorial	Prediction of monthly discharge in ungauged basins	IHACRES	Disaggregation procedure using measured streamflow data from a larger gauged catchment in which the ungauged sub catchments may be nested	4	Relative error for the monthly time step: 13–17%
Kokkonen et al. 2003	13 catchments in North Carolina, USA (1626 ha)	Warm temperate	Investigation of regionalization approaches for daily streamflow prediction	IHACRES	Arithmetic mean, regression, similar hydrological behavior	1,5,6	Arithmetic mean more often gives poor results in comparison with other methods; Elevation was the most powerful explanatory variable in the regressions
Croke et al. 2004	3 subcatchments in northern mountainous regions of Thailand (68-2157 Km^2)	Equatorial	Prediction of hydrologic response to land use changes by simulating daily flow in ungauged catchments	IHACRES combined with CATCHCROP (conceptual crop model)	Scaling of parameters according to the ratio of the area of the gauged to ungauged catchments	4	The procedure was able to predict the relative pattern of annual and seasonal flows-Bias= 0.4-0.18 % , NSE<=0.85
Merz and Blöschl 2004	308 catchments in Austria (3 to 5000 km^2)	Arid and warm temperate	Estimation of continuous daily flow in ungauged basins	HBV	Multiple regression	5	All model parameters are associated with some uncertainty-NSE=0.63-0.67

*Climate classification according to Köppen-Geiger climate classification , source: http://koeppen-geiger.vu-wien.ac.at/present.htm ** Class is according to the predefined classes of approaches in Figure 1-2 . , NSE: Nash and Sutcliffe efficiency

References	Study area	Climate	Temporal scale and key objectives	Hydrological model	Regionalization methods	Class	Major findings
Lee et al. 2006	131 catchments in UK (1-1700Km^2)	Warm temperate	Prediction of daily runoff in ungauged catchments	Aversion of PDM of Moore & a routing module	A step-wise multiple regression	5	Loss in NSE less than 0.04 in 90% of catchments (regressed model parameter values and locally optimized set)
McIntyre et al. 2005	127 catchments in UK (1- 1700 km^2)	Warm temperate	Predictions of daily runoff in ungauged catchments	Probability distribution model (PDM) of Moore	Regression; ensemble modeling and similarity weighted averaging (SWA) method	5,3	Ensemble modeling & SWA method provides the best results and performs significantly
Parajka et al. 2005	320 catchments in Austria (10-9770 km^2)	Arid and warm temperate	Regionalization of catchment model parameters to produce daily runoff	HBV (lumped model but allowing different model states in different elevation)	Arithmetic mean (global and local mean), spatial proximity, regression and physical similarity	1,2,3, 5	Spatial proximity (Kriging) and physical similarity perform best; NSE = 0.62 and 0.66
Boughton and Chiew 2006	213 catchments in Australia (50-2000 km^2)	Arid and warm temperate	Estimation of average annual runoff	Australian Water Balance Model (AWBM)	Multiple linear regressions	5	Two-thirds of the estimates of average annual runoff were within 25% of the actual value. NSE=0.3 to 0.97
Cheng et al. 2006	18 drainage basin, Great Toronto Area (6000Km^2)	Snowy	Predicting daily runoff for ungauged basins using gauged basins and precipitation data	SCS curve number (CN) and model and IHACRES	Multiple regression	5	The SCS curve model is more parsimonious than the IHACRES
Heuvelmans et al. 2006	25 catchments in Belgium (2.24-209 Km^2)	Warm temperate	Daily stream flow simulation in ungauged basins	SWAT (Soil and Water Assessment Tool)	ANN-based and linear regression	5	ANNs delivered more accurate parameter estimates than linear regression
Wagener and Wheater 2006	10 catchments, Southeast of England (28.5-1261 Km^2)	Warm temperate	Investigation of uncertainty of rainfall-runoff model parameters and structure in streamflow regionalization	Rainfall-Runoff Modeling Toolbox (RRMT)	Linear and multivariate regression analysis	5	The uncertainty in the locally estimated model parameters is a function of their importance in representing the response of a given catchment
Young 2006	260 catchments within the UK (median area=110.25Km^2)	Warm temperate	Estimation of daily streamflow in ungauged catchment	IHACRES	A regression-based approach ; nearest neighbour based approach	2,5	The regression-based approach yields the best predictive results
Cutore et al. 2007	9 sub-basins in Italy (47-1832Km)	Warm temperate	Monthly runoff prediction in ungauged basins	Simple rainfall-runoff models	Regression-based approaches :one-step and two step, ANN	5	The "one-step" approach appear to be robust and adequate for estimating the streamflow in ungauged basins
Götzinger and Bárdossy 2007	The Nectar catchment in Germany (14,000 km^2)	Warm temperate	Estimation of continuous flow in ungauged basins	Distributed HBV model (the use of square grid cells as primary hydrological units)	Transfer function (linear of log relationships between model and transfer function parameters), Modified Lipschitz, monotony condition and combination of modified Lipschitz and Monotony condition	5	Best NSE for Lipschitz condition =0.5 and for 3 other methods 0.47

References	Study area	Climate	Temporal scale and key objectives	Hydrological model	Regionalization methods	Class	Major findings
Bocchiola et al. 2010	Pantano basin in the Italian Alps (11 km^2)	Warm temperate	Evaluation of the daily flow discharges	A developed model contains snow and ice melt calculation and semi distributed flow routing	Regression	5	Nash–Sutcliffe efficiency=0.67-0.75, results show a somewhat good capability of the model to evaluate the average flow discharge within the stream
Castiglioni et al. 2010	52 catchments located in northern central Italy (14-3082 Km^2)	Warm temperate	Parameter estimation for rainfall-runoff models and daily streamflow estimation	HYMOD	Regional calibration using a maximum likelihood function based on regression relationship	5	Approximate likelihood cannot take into account the low frequency behaviors (long term autocorrelation) ,Nash–Sutcliffe efficiency=0.22-0.67,the results are inferior to classical calibration but it is encouraging
Masih et al. 2010	Karkheh river basin , Western part of Iran (50,764 km^2)	Arid	Simulation of daily streamflow for poorly gauged catchments based on hydrological similarity	HBV	hydrologic similarity based on FDC, similarity of drainage area and spatial proximity	2,3,6	FDC similarity produces better runoff simulation compared to the other three methods
Makungo et al. 2010	A quaternary catchment in Nzhelele River Catchment in South Africa (92Km^2)	Arid	Generating natural streamflow in ungauged catchment	Mike 11 NAM and AWBM (Australian Water Balance Model)	Modified nearest neighbour regionalization approach	2	The approach can be applied in near-real time modeling. NSE of verification period Mike 11 NAM : 0.74, AWBM :077 .
Samaniego et al. 2010	38 German basins (70 to 4000 km^2)	Warm temperate	Using copula-based dissimilarity measures for daily streamflow simulation in ungauged basins	A conceptualized hydrologic model	Dissimilarity measures that are estimated from pair wise empirical copula densities of runoff	3	The achieved reasonable results NSE=0.76-0.86
Samuel et al. 2011	The main watersheds across the Province of Ontario, (85-100000 km^2)	Snowy	Estimation of daily flows in ungauged basins	MAC-HBV (McMaster-HBV)	Spatial proximity (i.e., kriging, inverse distance weighted (IDW) , spatial averaging), physical similarity, and regression-based approaches	2,3,5	An approach coupling the spatial proximity (IDW) method and the physical similarity produce better model performances than the remaining three
Bulygina et al. 2011	2subcatchments in Wales (10.55km^2 and 8.7 $km^{2)}$	Warm temperate	Using a formal Bayesian approach to estimate daily runoff	PDM model (Moore, 2007)	A probabilistic method (based on base flow index (BFI) and CN)	5	Nash–Sutcliffe efficiency ranging from 0.70 to 0.81-both CN and HOST are potentially valuable sources of information for hydrological modeling of ungauged catchments within a stochastic modeling framework

References	Study area	Climate	Temporal scale and key objectives	Hydrological model	Regionalization methods	Class	Major findings
Hundecha et al. 2008	101 sub watersheds of Rhine basin, ,German (400 - 2100 km^2)	Warm temperate	Estimation of model parameters from watershed attributes to estimate daily streamflow	Swedish Meteorological and Hydrological Institute(SMHI) and the HBV model	Kriging based on identifying the spatial structures of the parameters within a space defined using watershed physiographic and climatic attributes	2,3	NSE : 0.86 , slight improvement of performance compared to linear relationship between the model parameters and the watershed descriptors
Kim and Kaluarachchi 2008	Upper Blue Nile River Basin of Ethiopia (176,000 km^2)	Warm temperate and arid	Parameter estimation and monthly runoff regionalization in ungauged basins	A two-layer monthly water balance model with six parameters	Global mean, , multiple regression (regular , regional calibration aggregated calibration, and volume fraction calibration)	1,5	Regional calibration performed better in simulating the runoff of lumped basins than multiple regression (Nash–Sutcliffe efficiency=0.61 &.81)
Oudin et al. 2008	913 catchments; French catchments (10-9390 Km^2)	Warm temperate	Estimation of daily continuous flow in ungauged basins	GR4J and TOPMO(inspired by TOPMODEL)	Spatial proximity, physical similarity and multiple regression	2,3,5	Spatial proximity provides the best regionalization results- NSE=0.7-0.8
Jin et al. 2009	13 sub-basins in south-china (100-1000 km^2)	Warm temperate	Simulation of daily stream flow in ungauged basins	HBV	Proximity approach and global mean	1,2	NSE for global mean method is 0.74 and for second method is 0.72
Li et al. 2009	210 catchments in south-east Australia (area is not mentioned)	Arid to warm temperate	Prediction of daily runoff in ungauged catchments	Three versions of Xinanjiang rainfall–runoff model	The spatial proximity method and the physical similarity method	2,3	In terms of Nash–Sutcliffe Efficiency two method for the 3 versions give almost similar result (0.20-0.70)
Post 2009	24 catchments in the dry tropics of Australia (68–130.146km^2).	Arid	Estimation of daily streamflow in ungauged basins	IHACRES	Linear Regression	5	The predicted values of mean annual streamflow are within 20% of the observations (NSE around 0.7)
Reichl et al. 2009	184 Australian catchments (Area Kurtosis=3.214)	Arid to Warm temperate	Optimization of a similarity measure to produce the best monthly streamflow predictions	SIMHYD	Ensemble Techniques and Model Averaging model based on catchments similarities	3	The method is inferior to local calibration but it is superior to regression and spatial proximity (NSE=0.7-0.8)
Zhang and Chiew 2009	210 catchments in southeast Australia (51-2000Km^2)	Warm temperate	Daily runoff prediction in ungauged catchments	Xinanjiang and SIMHYD	Spatial proximity ,physical similarity, integrated similarity approach(combines the spatial proximity and physical similarity)	2,3	The spatial proximity approach performs slightly better than the physical similarity and the integrated similarity approach performs only very marginally better than the spatial proximity approach.

Table 2-4 Studies on hydrologic model-independent streamflow regionalization methods (1990-2011)

References	Study area	Climate	Temporal Scale and key objectives	Regionalization methods	Class	Major findings
Chiang et al. 2002	94 candidate stations in Alabama, USA (~37 to 30,810 mi^2)	Warm temperate	Using watershed characteristics to synthesize monthly streamflow hydrographs	Integrated Time series model and Multiple regression analysis (MRA) to estimate TSM parameters using catchment attributes	1,2	Integrated Time series model outperform simple regression analysis method
Goswami et al. 2007	12 basins in France (32.1 - 371 km^2)	Warm temperate	Estimation of daily continuous flow in ungauged basins	Parametric and non-parametric simple linear model, perturbation model, linearly varying gain factor , ANN	1	The non-linear ANN is best in nine out of the 12 catchments in calibration
Yadav et al. 2007	30 small to medium sized watersheds in the UK (50–1100 km^2)	Warm temperate	Ensemble predictions of daily flow in ungauged basins in an uncertainty framework	Stepwise linear regression between 39 dynamic response characteristics & 13 physical watershed characteristics	1	This approach is not impacted by problems of parameter calibration or model structural uncertainty and could guide an improved approach to watershed classification
Buttle and Eimers 2009	22 small basins (3.4–190.5 ha) on the Precambrian Shield in south-central Ontario, Canada	Snowy	Explain inter-basin variations in streamflow metrics in terms of basin scale and physiographic and predict annual maximum and mean daily stream flow	Scaling relationships based on basin size and physiographic properties	3	Annual maximum and mean daily stream flow can be well-predicted using simple scaling relationships, (NSE=0.21-0.63)
Isik and Singh (2008)	26 river basins in Turkey (~700000km2 in total)	Warm temperate and Snowy parts	Regionalization of monthly streamflow in Watersheds of Turkey	FDCs model after basin classification using k-means partitioning method	1	Monthly discharge data with correlation coefficients between 95 and 100% for 85.7% of the gauging stations
Mohamoud 2008	29 catchments n Mid-Atlantic Region, US (23-4250 Km^2)	Warm temperate	Prediction of daily flow duration curves (FDCs) and streamflow for ungauged catchments	Regional FDC & drainage area ratio methods and Step-wise multiple regression analysis using catchment descriptors to find the parameters	1	FDC-based method shows great promise for predicting streamflow in ungauged basins.NSE=0.60-0.97
Besaw et al. 2010	The Winooski River basin, northwestern Vermont, USA (2700 km^2)	Snowy	Streamflow forecast (hourly and daily) in ungauged basins	GRNN and CPN with recurrent feedback loops , linear regression and time series autoregressive moving average	1,2	Both ANNs better captured the climate-flow relationships when trained on hourly data reflecting the basin-scale characteristics-CPN, GRNN and MLR provide the most accurate and unbiased estimates of stream flow
Lima and Lall 2010	40 hydropower sites in Brazil (2588 to 823,555 km^2)	Equatorial	Modeling of non-stationary monthly streamflow series and annual maximum flood series	Hierarchical Bayesian models : the Bayesian estimation of the scaling relationship with drainage area for annual maximum flows and monthly streamflow accounting for nonstationary and seasonal variability	3	Statistics of the streamflow time series in particular moments scale with physical properties of the drainage basin (The correlation between simulated and observed flow=0.63-0.97)
Parada & Liang 2010	North Fork Cache Creek watershed (510 km^2) and Bluestone River watershed (1023 km^2) , USA	Warm temperate	Inference of daily streamflow for ungauged basins combining concepts from both kernel methods and data assimilation	Kernel-based inference method	1	The inference method can estimate streamflow for ungauged basins with unknown and nonlinear dynamics. RMSE=0.37 & 0.21-Bias=0.23 & 0.02

Hydrologic model-dependent methods

The regionalization methods which use hydrologic models to estimate streamflow in ungauged basins are essentially methods which transfer the model parameters from gauged basins to ungauged ones. In recent studies, Peel and Blöschl (2011) and He et al. (2011) have reviewed the methods which are used to estimate model parameters of ungauged catchments. According to the classification of Peel and Blöschl (2011), these approaches are split into groups which estimate model parameters *a priori* (without calibration using relationships between model parameters and catchment characteristics), regionalize calibrated model parameters from gauged to ungauged basins (e.g. regression relationships, spatial proximity, and physical similarity), use multi-objective and regional calibration to assess predictive uncertainty, model (output) averaging, and hydrological signatures (indices) modeling. The described classification is a very general one, regardless of simulated hydrologic variables and includes the studies which aim to estimate uncertainty. The classification scheme employed by He et al. (2011) includes distance-based (using geographical and hydrological similarities) and regression-based methods. This classification and the described examples, cover only the hydrologic-model dependent methods presented in the next paragraph.

In a more specific classification, we classify techniques which have been used to extrapolate hydrologic model parameters to estimate streamflow at ungauged basins into the following groups: (a) arithmetic mean method (e.g. Merz and Blöschl 2004; Oudin et al. 2008; Jin et al. 2009); (b) spatial proximity (spatial distance) approach (e.g. Merz and Blöschl 2004; Parajka et al. 2005; Oudin et al. 2008; Li et al. 2009); (c) physical similarity approach (Oudin et al. 2008; Samaniego et al. (2010) ; Samuel et al. 2011); (d) scaling relationships (e.g. Croke et al. 2004; Schreider et al. 2001); (e) regression-based methods (linear and nonlinear), such as ANNs, MLR (e.g. Sefton and Howarth 1998; Post and Jakeman 1999; Merz and Blöschl 2004 ; Parajka et al. 2005; Cheng et al. 2006; Young 2006; Heuvelmans et al. 2006; Götzinger and Bárdossy 2007; Oudin et al. 2008; Mohamoud 2008) (f) hydrological similarity approach (e.g. Masih et al. 2010) .

With techniques such as arithmetic mean and spatial proximity, in which catchment attributes are not directly involved, one assumes that all catchments within the particular radius are similar and differences in the parameter values arise only from random factors (as in studies performed by Merz and Blöschl 2004; Parajka et al. 2005). All techniques which transfer model parameters from one basin to another are based on the assumption that two basins are similar and will respond identically to the same input (Stoll and Weiler 2010). In the arithmetic mean approach, the rainfall-runoff model parameters of surrounding basins (local) or all basins (global) are averaged. Parajka et al. (2005), for example, used the arithmetic mean of parameters of a region within a radius of 50 kilometers from the catchment of interest for the local technique and all basins for the global technique. Arithmetic mean might also be used as a computation technique after basin classification using other regionalization methods. Spatial proximity approaches transfer the model parameter sets based upon a spatial distance technique, i.e., an interpolation technique which is a function of the geographic location. The most popular interpolation technique in this context is kriging. Vandewiele and Elias (1995), applied a monthly water balance model to 75 Belgian basins which were considered as ungauged in turn and used two spatial proxy techniques (kriging and the use of parameter values of a few neighboring basins) to compute their parameter values. In their experience, kriging gave satisfactory results (root mean squared error less than 7% or relative error less than 20%) in 72% of the basins, whereas the second technique gave satisfactory results in only 44% of basins. Jin et al. (2009) used both of the described regionalization methods. They applied the HBV model using proxy-basin and global mean to regionalize model parameters in 13 sub-basins in southern China to simulate daily streamflow. With the global mean method, they constructed three different sets of regional mean parameters: an arithmetic mean regardless of the size and position of basins, area-weighted mean values of parameters, and a proxy-basin method. The parameter set of simple arithmetic mean values produced the best results compared to other applied methods.

The third method is a physical similarity approach. The concept of this approach is to transfer hydrological model parameters from gauged to ungauged basins according to the similarity of their physical attributes. An example of such an approach is presented by Oudin et al. (2008) and Samuel et al. (2011). In this method, catchments are first grouped according to their physical or non-hydrological similarities. Multivariate statistics analysis is normally used to group the catchments. It is recommended that one use a ranked proximity technique if catchment attributes have different units and ranges. Then, rainfall-runoff model parameters of gauged basins are computed and model parameters located in the same group are arranged, for example by using an arithmetic mean, to obtain a regional rainfall-runoff model parameter set. That parameter set is then used to generate streamflow in the target basin having physical similarity. Some might use physical catchment attributes to find dissimilarity measures. For example, Samaniego et al. (2010) proposed a procedure to find a metric on the basis of dissimilarity measures that are estimated from pair wise empirical copula densities of runoff. They defined a metric in a transformed space of basin descriptors consisting of 22 physical characteristics of the basins, such as area, slope, elevation, permeability, imperviousness, and estimated streamflow in an ungauged basin by transferring parameters from gauged basins on the basis of the selected metric. Simulated daily discharge using their proposed methods has NSE=0.76-0.86, which is considered as a reasonable result. Reichl et al. (2009) selected an ensemble of hydrological models to optimize similarity measures among 27 geometric, climatic, soil and vegetative attributes of catchments to transfer SIMHYD model parameters to 184 Australian catchments and predict monthly streamflow. Their results indicate that flow prediction using an optimized model averaging method (based on physical similarities) is superior to regression and spatial proximity approaches.

The fourth method is scaling relationships based on area or other catchment attributes. For instance, Croke et al. (2004) computed model parameters in ungauged basins by scaling the area, deep drainage, and surface runoff of gauged basins according to area and estimates of surface runoff and deep drainage of ungauged basins obtained from other models e.g. an agricultural model. This method can be used for simulation of subcatchments' streamflow in ungauged subcatchments, assuming that the streamflow contribution from each subcatchment to the total catchment yield is proportional to a ratio of the catchment area or other attributes (Schreider et al. 2002).

Another type of approach is the use of regression-based methods, which include nonlinear regression methods such as ANNs and linear regression methods. Within this group, a linear or nonlinear relationship is developed between model parameters and catchment attributes. Kokkonen et al. (2003) applied a regression scheme to the six-parameter IHACRES model and physical catchment descriptors (Table 2-3) on thirteen Australian catchments to produce daily flow time series which provided to be more accurate than those produced by arithmetic mean method. Sefton and Howarth (1998) conducted a multiple regression analysis to find the relationship between IHACRES model parameters and the selected catchment attributes in 60 basins in the UK. They selected the important catchment attributes in defining hydrologic response by correlation matrix, step wise regression and principal component analysis. Some studies, such as those by Götzinger and Bárdossy (2007) and Cheng et al. (2006) used the multiple regression approach in their regionalization studies, albeit with some modifications due to the use of distributed hydrological model parameters in their model which results in large number of model parameters. Götzinger and Bárdossy (2007) used the transfer function approach to ensure consistent parameter estimation, whereas Cheng et al. (2006) used the multiple regression approach to govern the relationship between the areas of different land cover types occupying the drainage basins. Cutore et al. (2007) tested particular regionalization procedures to transfer the parameters of simple rainfall-runoff models, based on a “two-step” approach in which the first step is a simple regression-based between rainfall and streamflow and the second step is regression equations between model parameters and the geomorphological characteristics, such as average altitude, soil permeability, stream length, etc. The "one-step" approach is only based on regional rainfall–streamflow model calibration for gauged basins. According to their experience models based on the "one-step" approach appeared to be robust and adequate for estimating the streamflow in ungauged basin.

The last method in this category considers hydrological similarities between basins to transfer the model parameters. A simple method based on hydrological similarity assumes that all catchments within the region are similar in their hydrological behavior. In this case, a mean of available or an entire set of calibrated parameter values is typically used to estimate the value in the ungauged catchment instead of deriving quantitative relationships between catchment descriptors and model parameters (Kokkonen et al. 2003; Mohamoud 2008). Flow duration curves (FDCs) similarity is also considered as a hydrological similarity which is used by Masih et al. (2010). They found that the HBV model parameters transferred from similar gauged basins based on FDCs' similarity to a data-limited gauged catchment is a better basis for streamflow time series generation than similarity approaches based on drainage area and spatial proximity. This may be due to the fact that FDCs account for climatic factors.

Some studies resort to a combination of the aforementioned methods to transfer hydrologic model parameters. For example, after basin classification according to physical or hydrological similarities or spatial proximity criteria, regression-based or averaging techniques can be used to transfer the model parameters. More examples and details about reviewed studies in these categories are presented in Table 2-3.

The wide spectrum of regionalization studies uses hydrologic models and involves methods which transfer or estimate the hydrologic model parameters of ungauged basins using the gauged ones. Different approaches can produce different results in various regions. Using a cross-validation procedure and basing its results on model validation statistics, each study claims that one method is more suitable than the others. But, in general, the best performing method is site-specific which seems driven by climate and physiographic conditions that play an important role in the differences of method performance from one region to another. Therefore a major challenge may lay ahead with climate change suggesting that an optimal regionalization method for a given basin may not be the appropriate one in the future. Further research is needed on that topic.

Hydrologic model-independent methods

As displayed in Figure 2-1, hydrologic model-independent (mainly data-driven methods) can be classified into three groups. The first group is regression-based analysis which includes linear regression (e.g. MLR, parametric simple linear model used by Goswami et al. 2007), and nonlinear regression (e.g. ANNs) between streamflow and catchment attributes. For instance, nonlinear regression methods are used in Besaw et al. (2010) and Parada & Liang (2010). The former trained the recurrent ANNs on climate-flow data from one basin and used them to forecast streamflow in a nearby basin with different (more representative) climate inputs, and found that ANNs that always converge and avoid stochastic training (e.g. General Regression Neural Network (GRNN) and Counter Propagation Neural Network (CPNN)) are straightforward to execute and widely applicable to small ungauged basins. The latter presented a Kernel-based methodology, which is applicable to those ungauged basins whose hydrological and system properties/behavior are non-linear and non-Gaussian and inferred streamflows for two basins in the US treated as ungauged. The next category is time series models, e.g. AutoRegressive (AR) models. Chiang et al. (2002a) used Multiple Regression Analysis (MRA) to construct relationships between the parameters of streamflow time series (dependent variables) and watershed characteristics (independent variables). The predicted streamflow parameters from the MRA equations were then used to synthesize hydrographs under the time series model. The regression equations might be developed between streamflow percentile and catchment attributes. For example, Mohamoud (2008) developed a linear regression between the parameters of a FDC model and landscape-climate descriptors identified through a step-wise regression method for gauged basins, transferred these equations to ungauged basins, and converted the simulated FDCs to a streamflow time series. Isik and Singh (2008) also used FDC models to compute streamflow discharge at ungauged sites in 26 river basins in Turkey after defining homogeneous regions with a hierarchical clustering algorithm. They found that FDCs constructed for each homogeneous region estimated monthly discharge data with correlation coefficients of 95-100% for most of the gauging stations. The last category of these approaches is scaling methods. Buttle and Eimers'(2009) study on the Precambrian Shield in south-central Ontario indicates that annual maximum and mean daily streamflow can be well-predicted using simple scaling relationships. These scaling relationships between streamflow metrics and basin size are potentially capable of the extrapolation of data from gauged basins to ungauged sites (Yue and Wang 2004). A similar study on the Mackenzie River Basin in northern Canada estimated streamflow for ungauged basins using streamflow-area relationships of gauged basins (Woo and Thorne 2003). In addition to streamflow time series, the statistics of these time series are also potentially applicable in scaling analysis. Lima and Lall (2010) remarked that statistics of the streamflow time series also scale with physical properties of the drainage basin such as catchment area. More examples of the second category of regionalization methods are presented in Table 2-4.

The accuracy of predictions can be impacted by time scale, i.e., the time step of prediction based on catchment area. In Besaw et al. (2010) study which examines the case of streamflow prediction at two small sub basins of about 2,700 km^2, predictions using hourly data were slightly more accurate than those using daily data (Root Mean Square Error of 5.5 versus 5.2) . However such minor difference in model performance may not allow drawing conclusion on the time scale effect on model performance. More studies are needed to clarify that issue.

In conclusion, among the hydrologic model-independent methods for streamflow regionalization described above, regression equations (including linear and nonlinear) developed between the desired hydrologic responses, (e.g. streamflow) and catchment attributes are the most commonly used ones. One of the advantages of hydrologic model-independent methods is the lower data requirement of these approaches and the simplicity of their structure which does not require special knowledge and expertise of hydrological modeling. However, the identification of an appropriate model structure (e.g. ANN architecture) requires some expertise. Data-driven methods do not simulate the actual rainfall-runoff process and therefore they are not impacted by uncertainty due to the physical process being modeled; however, they are still affected by other sources of uncertainty, e.g. the estimation method and its parameterization.

2.6. Hydrologic models in streamflow estimation in ungauged basins

Compared to conceptual and semi-distributed models (e.g. SAC-SMA), fewer studies have used fully distributed physically-based models (e.g. MIKE SHE) to estimate streamflow time series in ungauged basins. Using fully distributed physically-based models for streamflow estimation in ungauged basins is not usually involved with regionalization process due to *a priori* parameter calibration. However, Gotzinger and Bardossy (2007) used a grid-based modification of the HBV model concept for simulation of catchment runoff in ungauged basins using regionalization approaches. While majority of studies calibrate them *a priori* . For example, Ibrahim and Cordery (1995) developed a model which represents hydrological processes in a physically realistic manner to estimate runoff volumes from generally available geophysical data of ungauged basins. The inputs to the model were monthly rainfall, monthly climate data, and reference soil characteristics. The model was able to provide good estimates of volumes of flow on ungauged catchments in New South Wales. Nyabeze (2005) estimated runoff using a distributed parameter value estimation approach for various poorly gauged catchment sizes in Zimbabwe, and simulated runoff of different segments independently, in which each segment represents an area of different rainfall, soil condition, vegetation cover, and land use, which all influence runoff. Ao et al. (2006) proposed a mixed model structure BTOPMC (Block wise use of TOPMODEL with Muskingum-Cunge flow routing method), which is a physically-based model that has the advantages of both lumped and distributed models to avoid large data requirements , uncertainty and high cost, which often limit the distributed model's applicability. Their experience finally resulted in a reasonable agreement between the simulated and recorded runoff .The application of more detailed physically-based hydrologic models along with regionalization methods appear to yield some improvement but at a quite high cost. This approach is data intensive, and may not be appropriate in data poor regions.

In hydrologic model-dependent regionalization methods (Table 2-3), a rainfall-runoff model is first selected (see column "Hydrologic Model"). The rainfall-runoff models selected in regionalization studies are usually conceptual and semi-distributed models such as HBV (e.g. Jin et al. (2009) , IHACRES (e.g. Young2006), HYMOD (e.g. Castiglioni et al. 2010) , RRMT (e.g. Wagener and Wheater 2006), SIMHYD (e.g. Peel et al. 2000), PDM (McIntyre et al. 2005), AWBM (e.g. Boughton and Chiew 2006), Xinanjiang (e.g. Li et al. 2009), GR4J and TOPMO (e.g. Oudin et al. 2008) , SMHI (Hundechha et al. 2008) , SWAT (e.g. Heuvelmans et al. 2006) and TOPMODEL (e.g. Bastola et al. 2008) and rarely physically-based models such as Mike 11 NAM (Makungo et al. 2010) . The full names of these models can be found in Table 2-3.

In selecting an appropriate model, there is a consideration of data-availability and that the model should be simple (parsimonious with less model parameters), able to capture more hydrological variability and behaviors required in the study catchments (such as snowfall, lakes, etc.), and has been effectively applied in similar regions. In the regionalization approach, a parsimonious hydrologic model structure is usually selected and calibrated to observable watershed responses for a large number of gauged watersheds (Yadav et al 2007). Next step is the selection of regionalization model to govern the relationships between catchment attributes and model parameters in gauged basins and transfer them to ungauged basins.

The most widely used hydrologic models in streamflow regionalization studies are HBV and IHACRES. This may be due to the fact that those models represent well the key components of rainfall-runoff process without unnecessary details. To identify the best model for streamflow estimation in ungauged basins in a certain region, both physically-based and conceptual hydrologic models are suggested to be examined. Makungo et al. (2010) applied both Mike 11 NAM (a physically-based model) and AWBM (a conceptual model) for estimation of daily discharge in ungauged basins of a catchment in South Africa using regionalization method of spatial proximity and found that AWBM slightly outperforms the other model. But, in practice, usually both categories of models available for streamflow estimation in ungauged basins are not examined for various reasons. In future studies, the benefit of using methods from each category should be further emphasized.

2.7. Model parameter calibration (optimization process)

In conceptual and semi-distributed rainfall-runoff models, most parameters are not measurable and have to be estimated by calibration using observed runoff data.

Optimized model parameters are required in model parameter regionalization, since the most common approach in this context is to look for relationships between optimized parameter values and catchment characteristics in gauged basins. Parameter sets can then be compiled for ungauged catchments from measurable variables (Seibert 1999). The range of parameter values is usually selected based on authors' knowledge of the study area and the experience of other studies (Seibert 1999) as well as initial model runs for the study area. Recent advances in optimizing rainfall-runoff model calibration have focused mainly on incorporating multiple objective measures of model performance and improving optimization algorithms (Li et al. 2010). Some examples of model parameter optimization efforts in the reviewed studies are presented in this section.

Oudin et al. (2008) used local gradient search procedure as an optimization algorithm for GR4J and TOPMODEL, with four and six parameters respectively on gauged catchments. Li et al. (2010) combined multi-objective optimization with averaging across multiple calibration sites and estimated model parameters by multi-objective optimization at each calibration site, and then finalized it by weighted averaging of the parameter values across sites. The weight for each site was calculated from the prediction error at that site. Mwakalila (2003) calibrated the Data-Based Mechanic (DBM) model using the Generalized Likelihood Uncertainty Estimation framework whereby, using the Monte Carlo simulation technique, the model was run 5,000 times with different randomly chosen parameter sets. The feasible range of parameters to be sampled was based on the initial estimated parameter values. The optimum values of parameter sets for each catchment were selected through an evaluation of the likelihood measure. Kim et al.

(2008) used the large scale trust-region method to solve nonlinear large scale optimization problems. Li et al. (2009) used the Particle Swarm Optimization (PSO) to optimize the model parameters. PSO is a relatively new addition to the evolutionary computation methodology and is expected to provide the global or near-global optimum. Samuel et al. (2011) used Brent's parabolic interpolation method to optimize the MAC-HBV model parameters.

In most of the mentioned optimization algorithms, multiple objective measures of model performance are used to improve the optimization algorithm and pick the least uncertain set of model parameters.

2.8. Developments in continuous streamflow regionalization with uncertainty estimation

In 2003, PUB focused on the estimation and subsequent reduction of predictive uncertainty as its central theme (Sivapalan et al. 2003). In regionalization studies, the inclusion of uncertainty analysis is necessary, firstly because model uncertainty is inherent and unavoidable (Yadav et al. 2007) and secondly because there are uncertainties in selecting catchment properties and regionalization procedures, and identifying gauged and regional model structures and their parameters (Wagener and Wheater 2006). In addition, calibration procedure to obtain regional model parameters increases the uncertainties (Wagener and Wheater 2006; Yadav et al. 2007; Zhang et al. 2008; Samaniego et al. 2010). Clearly, uncertainty analysis needs to be incorporated within the regionalization procedure to provide better predictions of streamflow in ungauged basins.

However, this has been a challenging task over the last decade because of the various sources of uncertainties involved.

Some examples of studies applying uncertainty analysis in regionalization include: Wagener and Wheater (2006); Yadav et al. (2007); Zhang et al. (2008); Samaniego et al. (2010); and Masih et al. (2010). Briefly, the methodology of uncertainty analysis is performed by calculating prediction limits, determining upper and lower bounds for each parameter, simulating Monte Carlo or any other multi objective function tools to obtain behavioral or non-behavioral parameter sets, and then using a behavioral simulation to create ensemble predictions in the ungauged basins. Wagener and Wheater (2006) detected the uncertainties that resulted from difficulties in identifying model parameters, finding an appropriate calibration strategy and model structure errors by investigating the role of each model parameter and model structure behaviors' effects on streamflows in ungauged basins. Yadav et al. (2007) used a Monte Carlo simulation, whereas Zhang et al. (2008) applied the ε-NSGAII algorithm. Zhang et al. (2008) claimed that the use of the ε-NSGAII is more efficient and robust in finding behavioral parameter sets, and it can reduce uncertainty bounds of streamflows in ungauged basins. McIntyre (2005) regionalized conceptual rainfall-runoff models on the basis of ensemble modeling and model averaging. They remarked that the ensemble of candidate models provides an indication of uncertainty in ungauged catchment predictions, although this is not a robust estimate of possible flow ranges, and frequently fails to encompass flow peaks. Samaniego et al. (2010) accounted for uncertainty of parameterization by running the hydrologic model in an ungauged basin with sets of global parameters obtained from the k nearest neighboring donor basins using various metrics. With 22 basin descriptors, a Monte Carlo experiment was carried out to assess the explanatory power of possible combinations of these predictors. Masih et al. (2010) assessed the impact of parameter uncertainty on the regionalization results using the best parameter set of a study catchment in the regionalization procedure among 50 different parameter sets of a catchment that yielded in the highest Nash Sutcliffe Efficiency (NSE) values during the automatic Genetic Algorithm (GA)-based optimization procedure while Heuvelmans et al. (2006) assessed the uncertainty of the regionalization procedures with a non-parametric bootstrap method. Samuel et al. (2011) calculated a measure of the goodness of fit between the observed streamflow and model predictions (NSE) for each parameter combination in each basin. If the goodness-of-fit value for any parameter combination was inside the accepted range, the parameter set was accepted to provide flow-prediction confidence limits.

An effective approach to reduce the impacts of parameter uncertainties on model simulations might be an appropriate reduction of the number of model parameters as is found by Huang and Liang (2006).They introduced a subsurface flow parameterization based on the concepts of kinematic wave and hydrologic similarity, with one parameter for calibration into VIC-3L model to reduce the impacts of model parameter uncertainties on model simulations by reducing the number of model parameters that need to be estimated through a calibration process. More recently, Samuel et al. (2011) resorted to a Monte Carlo simulation technique to capture flow variability in ungauged basins in Ontario. Significant developments in streamflow regionalization with uncertainty estimates have been achieved in the last decade. However, there is still no general method that could be applied to streamflow regionalization. This is in part due to the variety of the regionalization methods, and the different level of details of hydrologic models and data involved. This remains an interesting research avenue specially in a context of changing climate and land use/cover.

2.9. Discussion and Conclusion

This paper provides a comprehensive review of regionalization methods for estimating continuous streamflow or runoff in ungauged basins. Continuous streamflow regionalization can be carried out through a hydrologic model in which its model parameters are used as instruments to transfer hydrological information from gauged to ungauged basins. An alternative method is the use of hydrologic model-independent approaches which are usually based on data-driven methods. The use of rainfall-runoff models causes some sources of uncertainties due to errors in computing local and regional model parameters and the relationship between local parameters and catchment attributes, and due to the uniqueness of the catchments (Wagener and Wheater 2006) and the structure of the rainfall-runoff model. Conversely, hydrologic model-independent methods such as data-driven models avoid the impact of hydrologic model structure and parameter uncertainty, but still contain uncertainties due to the estimation method which is derived from the gauged basin and uncertainty due to the data-driven model's calibration. Data-driven methods usually require less data and expertise which might be useful to deal with constraints of data-availability. There is no clear indication from the literature on which regionalization approach should be preferred for a given case. Comparative study using methods from each category (model-independent and model-dependent) appears the best approach to identify appropriate regionalization method for a given site or region.

Since the regionalization process is inherently involved with using catchment attributes, it is not possible to establish a universal approach as the best method for all of the catchments. Therefore a specific study needs to be done on any region of interest to identify the best approach among hydrologic model dependent or independent methods. For example most reviewed studies on hydrologic model-dependent methods in arid to warm temperate climate (e.g. Australia) indicate that physical similarity and spatial proximity appears to be the best approach, while in warm temperate (most European countries) regression-based methods have been preferred. Similarly, in cold and snowy climate (e.g. Canada) spatial proximity and physical similarity approaches seem to outperform other hydrologic model-dependent methods. It has been found that the HBV and IHACRES are the most frequently used hydrologic models. Among the hydrologic model-independent methods, linear and nonlinear regression methods have performed well in warm temperate regions (e.g. European countries) while in cold and snowy climate (e.g. Canada) and warm humid climate (e.g. Brazil) scaling relationships have shown good performance. This highlights the site-specific nature of the regionalization methods and the need for comparative study before selecting a regionalization method for a given site or region. Existing studies summarized in this review can provide some guidance and reduce the number of methods to be investigated.

Wagener and Wheater (2006), and later followed by other researchers such as Yadav et al. (2007), Zhang et al. (2008), Besaw et al. (2010), and Samaniego et al. (2010) suggested and then applied uncertainty analysis in their regionalization studies. The use and development of the regionalization approach, including uncertainty estimate, is in line with the central theme of the PUB initiative promoted by the International Association of Hydrological Sciences (IAHS, see Sivapalan et al. 2003). Although significant developments have been achieved on that topic, in general, there is still no standard method for estimating uncertainty in streamflow estimation at ungauged basins using regionalization techniques. This issue remains a challenging research topic in a context of climate change along with changes in land use and cover. Thus it is raising the emerging issue of nonstationarity that is generally overlooked by most regionalization methods that assume stationarity. Future research should focus on those key issues to advance the regionalization techniques for streamflow estimation in ungauged basins.

There has been some preliminary work in studding the nonstationary effects on streamflow prediction in ungauged basins. For instance, Lima and Lall (2010) developed and applied hierarchical Bayesian models, to assess regional and at-site trends in time in a spatial scaling framework and to reduce parameter and model uncertainties. They used a log–log scaling law of annual maximum series and catchment area to estimate varying scaling parameters.

This review provides a comprehensive overview of various methodologies used in continuous streamflow regionalization over the last two decades. Clearly, after 1990 hydrologic variables regionalization approaches have remarkably progressed. Recent improvements in this area include for example the use of data-driven methods in both hydrologic model's parameters extrapolation and hydrologic response inference such as the ANN approach proposed by Heuvelmans et al (2006), Goswami et al. (2007), Besaw et al. (2010); and the statistical inference methods for watersheds with non-linear behavior (Parada and Liang 2010); the transfer function approach (Götzinger and Bárdossy 2007); the use of uncertainty analysis with an optimum multi-objective function (Zhang et al. 2008); nonstationarity analysis (Lima and Lall 2010), and the incorporation of multi-objective measures of model performance and improved optimization algorithms for watershed models calibration (Li et al. 2010).

The rapid development of streamflow regionalization, in terms of its methodologies after 1990 and applications as shown in this paper brings greater confidence that accurate streamflow estimation at ungauged basins can be achieved. However, there are still many particular aspects that require more research to improve regionalization analysis and results. For example the problem of data-availability raises questions about which approaches of streamflow estimation in ungauged basins should be taken. When a rainfall-runoff model is to be selected, which model is most efficient and applicable and also parameter calibration or optimization approach needs to be addressed. Uncertainty analysis is always required and strongly recommended in regionalization efforts; however a well-established method for uncertainty estimation in the context of streamflow regionalization is still to be developed. The emerging issue of nonstationarity in hydrological time series (e.g. streamflow time series) due to climate change and changes in land use and cover, raises question as to the validity of most of the regionalization methods used with the assumption of stationary. Significant work still lies ahead to properly address both the issue of "nonstationarity" and "uncertainty estimate" in the context of streamflow regionalization.

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Chapter 3 : Classification of Ontario Watersheds Based on Physical Attributes and Streamflow Series

Summary of Paper II : Razavi, T., and Coulibaly, P. (2013) . Streamflow Prediction in Ungauged Basins: Review of Regionalization Methods. journal of Hydrologic Engineering, 18(8), 958–975.

Summary:

In this research work two novel techniques for watershed classification i.e. Non-Linear and Compact Non-Linear Principal Component Analysis are proposed, and SOM as another technique for watershed classification technique using catchment attributes and streamflow series is investigated. The watershed classifications of two benchmarks: the standard Principal Component Analysis (PCA) and K-means classification based on recently proposed runoff signatures are used for comparison.

The results of this research work imply that:

- SOM, NLPCA and CNLPCA can be robust tools for the classification of ungauged watersheds using watershed attributes prior to regionalization.
- The classifications are sound from the hydrological point of view since further analysis of the classification results using SOM, NLPCA and CNLPCA based on watershed attributes indicated distinct patterns of FDC slope, timing of event flows (annual hydrograph) shape, and dominant physical attributes in each cluster.

3.1. Abstract

Nonlinear cluster analysis techniques including Self Organizing Maps (SOMs), standard Non-Linear Principal Component Analysis (NLPCA) and Compact Non-Linear Principal Component Analysis (Compact-NLPCA) are investigated for the identification of hydrologically homogeneous clusters of watersheds across Ontario, Canada. The results of classification based on catchment attributes and streamflow series of Ontario watersheds are compared to those of two benchmarks: the standard Principal Component Analysis (PCA) and K-means classification based on recently proposed runoff signatures. The latter classified the 90 watersheds into four homogeneous groups used as a reference classification to evaluate the performance of the nonlinear clustering techniques. The similarity index between the first largest group of the reference classification and the one from the NLPCA based on streamflow, is about 0.58. For the Compact-NLPCA the similarity is about 0.56 and for the SOM it is about 0.52. Furthermore, those results remain slightly the same when the watersheds are classified based on watershed attributes – suggesting that the nonlinear classification methods can be robust tools for the classification of ungauged watersheds prior to regionalization. Distinct patterns of flow regime characteristics and specific dominant hydrological attributes are identified in the clusters obtained from the nonlinear classification techniques -- indicating that the classifications are sound from the hydrological point of view.

Keywords: Nonlinear Principal Component Analysis (NLPCA), Self Organizing Maps (SOMs), Principal Component Analysis (PCA), Cluster analysis, Watersheds classification, Ungauged watershed.

3.2. Introduction

Classification of watersheds in hydrology is needed for different purposes. It has been used in the prediction or extension of shorter records of flow characteristics such as floods or low flows in ungauged watersheds (e.g. Cavadias et al., 2001; Natahan and McMahon 1990), regional flood frequency analysis (e.g. Rao and Srinivas, 2006; Castellarin et al., 2008), generalization of hydrologic system understanding (Sawicz et al. 2011), and to generate streamflow hydrographs in ungauged watersheds (e.g. Chiang et al., 2001a, 2001b; Kahya et al., 2008). According to Blöschl and Sivapalan (1995), regionalization, the process of transferring hydrological information from gauged watersheds to ungauged ones, may be satisfactory if the watersheds are similar (in some sense), but error-prone if they are not . Therefore, the main advantage of watersheds' classification is its application in regionalization. In fact, regionalization is expected to be more accurate if it is applied on similar watersheds i.e., considering the similarities in the selection of donor watersheds. Streamflow records are affected by hydro-climatic variability at local or regional scale (Coulibaly and Burn, 2005) and the estimation of streamflow in different regions is affected by hydrological or physiographic characteristics. Therefore, the classification of watersheds can make a significant difference in regionalization studies.

Watersheds' classification is generally based on watershed physiographic characteristics or its hydrologic behavior e.g. streamflow metrics. The first one is appropriate for ungauged watersheds while the later one is not applicable to ungauged watersheds since streamflow time series are not adequately available in those. Some examples of watershed classification studies are presented in Table 3-1.

Most of these studies apply linear classification techniques such as principal component analysis and k-means clustering.

For example Burn and Boorman (1993) applied k-means clustering on the flow response variables of watersheds and classified the watersheds according to the hydrological similarity. They assigned ungauged watersheds into groups based on physical characteristics of the watersheds and finally transferred hydrological parameters e.g. the unit hydrograph time to peak and standard percentage runoff from gauged to ungauged watersheds. Chiang et al., (2002a) used 16 streamflow parameters estimated by a time series model to classify 94 watersheds into 6 regions and using principal component analysis (PCA), they identified the regional membership in the classification by the watershed variables of elevation, forest, area, and channel slope. The limitation of linear classification techniques is that they may not capture the nonlinear patterns in data, hence, it should not be considered as the only option in watershed classification. The authors agree with Wagener et al., (2007) that hydrology has not yet recognized a generally agreed upon watershed classification system. However, a discussion on outstanding components that should be included in such classification framework constitutes a step in that direction.

One can assume that when the goal of watershed classification is to estimate hydrological responses (e.g. streamflow) streamflow metrics used in first-order analysis are the most reliable variables as the basis of classification. Sawicz et al., (2011) introduced six signatures defined as hydrologic response characteristics and possible universal metrics to identify homogeneous groups of hydrologically similar watersheds.

The signatures include: runoff ratio, baseflow index, snow day ratio, slope of flow duration curve, streamflow elasticity and rising limb density. Ssgane et al., (2012) used three of these indices to identify reference watersheds classified as homogeneous and compared them with classification performance of four watershed variable groups using a similarity index. Earlier, Di Prinzio et al., (2011) compared a reference watersheds' classification identified using available indices of streamflow regime e.g. mean annual runoff and sample L-moments of the annual maximum floods with four alternative classifications using watershed descriptors.

In Canada some efforts have been devoted to classify the watersheds or/and identify the streamflow variability in various regions of the country. For example Mwale et al., (2011) applied wavelet analysis, independent component analysis (ICA) and empirical orthogonal function (EOF) to regionalize runoff variability and account for runoff heterogeneity across Alberta (western Canada) and identified three hydrologic clusters from 59 stations of watershed runoff data using ICA and EOF.

Table 3-1 Summary of watershed classification and runoff variability studies

Author	Purpose of classification	Classification techniques	Study area	Major findings
Ssegane et al. (2012)	Flow predictions in ungauged watersheds	K-means clustering using: geographic proximity; watershed hypsometry; causal selection algorithms; PCA and stepwise regression	Three Mid-Atlantic ecoregions within USA	Classification performance was highest using causal algorithms
Di Prinzio et al. (2011)	Predicting streamflow indices i.e. mean annual runoff, mean annual flood, and flood quantiles in ungauged watersheds	SOM on the available catchment descriptors and derived variables obtained by applying PCA and Canonical Correlation Analysis (CCA)	~300 Italian catchments scattered nationwide	PCA and CCA on the available catchment descriptors before applying SOM improve the effectiveness of classifications.
He et al. (2011)	Set up and test a non-parametric catchment classification scheme	Multidimensional scaling (MDS) and local variance reduction (LVR) using hydrologic model performance as a measure of similarities	27 catchments in Germany	The scheme is potentially useful for prediction in ungauged watersheds and provides an alternative to conventional regression-based regional approaches.
Mwale et al. (2011)	Regionalize runoff variability and establish baseline predisturbance hydrologic regimes	Wavelet, independent component analysis (ICA), and empirical orthogonal function (EOF) analysis	59 stations of catchment runoff data in Alberta, Canada	ICA identified hydrologic clusters that agree better with the five ecoregions of Alberta.
Sawicz et al. (2011)	Understanding hydrologic similarity in a 6-dimensional signature space	A Bayesian clustering applied on 6 hydrological signatures including: runoff ratio, baseflow index, snow day ratio, slope of the flow duration curve, streamflow elasticity, and rising limb density	280 catchments located in the Eastern US	Identification of nine clusters with a relatively clear separation which suggests that spatial proximity is a good indicator of similarity.
Kahya et al. (2008)	Delineating the geographical zones having similar monthly streamflow variations	Hierarchical clustering applied to streamflow data	80 watersheds in Turkey	The zones having similar streamflow pattern were not overlapped well with the conventional climate zones of Turkey.
Stainton and Metcalfe (2007)	To identify reference watersheds in Ontario for understanding the ecological significance of hydrological variability	Classify the full range of flow variability using five components of the natural flow regime: the timing, magnitude, duration, frequency and rate-of-change	135 watersheds in the province of Ontario, Canada	Cluster analysis using mean monthly hydrographs identified a total of 8 hydroclimatic groups and FDC identified 13 groups.
Rao and Srinivas (2006)	Estimation of flood Quantiles in ungauged watersheds	Fuzzy clustering algorithm (FCA) on attributes and flow records	245 gauging stations in Indiana, USA	FCA derives homogeneous regions, effective for flood frequency analysis.
Chiang et al. (2002)	Streamflow estimation in ungauged watersheds	Discriminant Analysis and PCA using 16 parameters of streamflow time series	94 watersheds in Alabama, Georgia, and Mississippi (USA)	The 6 regions seem to be separated by physiographical boundaries and regional membership is mainly identified by some of the watershed variables

Author	Purpose of classification	Classification techniques	Study area	Major findings
Cavadias et al. (2001)	Estimation of flood characteristics of ungauged watersheds	Canonical correlation	20 watersheds in Ontario , Canada	The homogeneous regions determined in the canonical space of the flood variables are based on relationship between the watershed and flood variable.
Burn and Boorman (1993)	Estimation of rainfall-runoff model parameters in ungauged watersheds	K-means clustering on flow response variables and determination of group membership based on catchment attributes	99 Catchments , UK	Methods are effective in estimating the unit hydrograph time to peak and standard percentage runoff.
Natahan and McMahon (1990)	Prediction of low flow characteristics which can be used in ungauged watersheds	Cluster analysis, multiple regression, principal component analysis	184 catchments in southeastern Australia	Use of watershed characteristics makes the grouping very sensitive to the initial choice of predictor variables.
Acreman and Sinclair (1986)	Flood frequency analysis	Multivariate clustering algorithm applied on 11 watershed variables	168 watersheds in Scotland	Four of the five identified regions yield homogenous distributions of flood frequency.

Using mean monthly hydrographs they identified a total of 8 hydro-climatic groups, and the classification based on flow duration curve (FDC) identified 13 separate FDC groups, irrespective of their hydro-climatic group. Their study classifies the flow variability of watersheds using only flow characteristics; consequently, it is only applicable to gauged watersheds.

In the current study the performance of the selected nonlinear classification techniques (SOMs, NLPCA, Compcat-NLPCA) is evaluated on both watershed attributes and daily streamflows which is essential to assess their applicability for both gauged and ungauged watersheds. So far, to our best knowledge, NLPCA and Compact-NLPCA models have not been investigated as watershed classification techniques.

3.3. Study Area and Data

Study area covers 90 natural watersheds across the Province of Ontario, Canada. The climatology and landscape vary from the northern to the southern region. The annual mean precipitation is 400–600 mm in the northern region and 800–1,200 mm in the southern part. In the northern regions, with more severe air temperatures, the average air temperature ranges approximately between -20°C (in January) and 17°C (in July); and in the southern regions, it ranges between -10°C (in January) and 19°C (in July). The relief varies between 300 m and 500 m above mean sea level (msl) in the southern region, and down to 100 m–200 m above msl in the northern region. Most of the natural watersheds in the northern region are covered with coniferous forest, with gaps of swamp, muskeg, and small lakes, whereas the southern region is dominated by mixed forests (Atlas of Canada, available at http://atlas.nrcan.gc.ca).

Meteorological data, i.e., daily precipitation and air temperature, were obtained from the Canadian Daily Climate Data (CDCD, provided by the Environment Canada).Only precipitation/temperature stations which have less than 20% missing data (for the period of 1960–1995) are selected for this study. The daily flow data were obtained from the HYDAT database (Environment Canada, 2004). The number of natural watersheds with active flow station that has more than 20 years continuous flow records of sufficient quality, and approximately more than 100 km^2 of drainage watershed area resulted from the initial screening were 135 watersheds (used by Stainton and Metcalfe, 2007), 90 watersheds out of 135 watersheds are selected for this study due to the availability of data for the selected time period (1976–1994). The areas of the watersheds range from approximately 100 to 100,000 km^2, representing different types and sizes of watersheds.

Table 3-2 Catchment attributes

Classification		**Catchment attribute**	**Unit**	**Notes**
Location of watersheds (centroid)		Latitude	deg	
		Longitude	deg	
Morphology of watersheds		Area	km^2	
		Mean slope	%	
		Mean elevation	m	
Percentage of area covered	Water	Lakes	%	Percentage of area covered by lakes.
	Land use	Forests	%	sum of percentage of area covered by coniferous, deciduous and mixed forest
	Drainage class	Rapid	%	sum of percentage of area covered by rapid, well and moderately well drainage class
	Rooting depth (RD)	RD deeper than 150 cm	%	percentage of area covered by RD deeper than 150 cm
	Surficial geology	Glaciofluvials	%	sum of percentage of area covered by glaciofluvial plain and complex
		Glaciodeposits	%	sum of percentage of area covered by till blanket and till veneer
		Rocks	%	Percentage of area covered by undivided

3.4. Methodology

Nonlinear classification techniques including: Self-Organizing Maps (SOMs), Non-linear Principal Component Analysis (NLPCA) and Compact-NLPCA are applied to watershed attributes and daily streamflows of 90 watersheds across Ontario, Canada, to classify the watersheds into four clusters and the results of classification using benchmark methods i.e. principal component analysis (PCA) and K-means clustering based on streamflow signatures are compared with those of investigated techniques to identify the method with highest performance. Figure 3-1 illustrates the flowchart of the methodology used in the study.

Benchmark Methods

Principal Component Analysis (PCA) and K-means Clustering

Principal Component Analysis (PCA) finds combinations of the original variables (known as latent variables or principal components—PCs) which describe the dominant patterns and the main trends in the data (Jackson, 2003). In datasets with multiple variables, usually more than one variable determine the same driving principle which controls the behavior of the system. In this case, replacing a group of variables with a smaller set of new variables can make the analysis simpler.

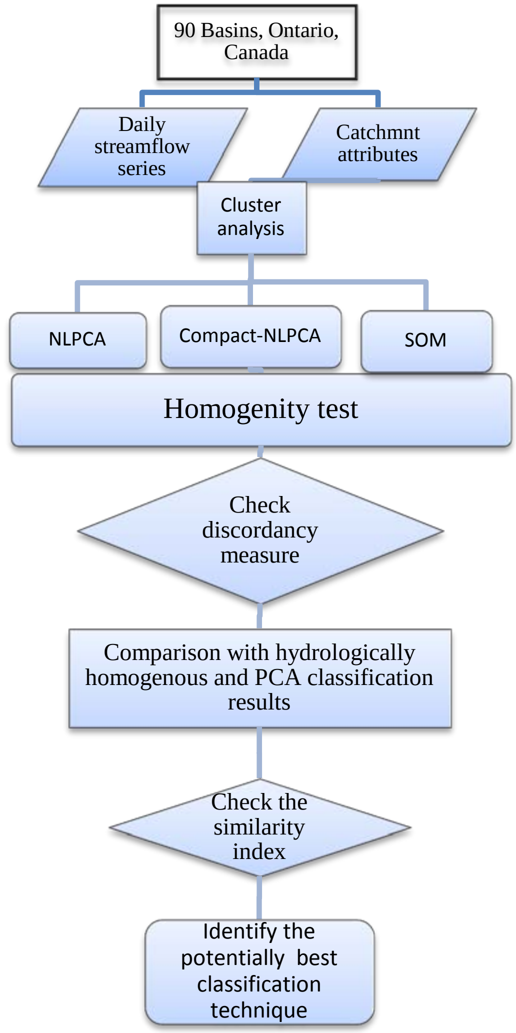


Figure 3-1 Flow chart of methodology

This new set of variables, are principal components. Each principal component is a linear combination of the original variables. PCA is done through an eigenvector decomposition of the covariance matrix of the original variables. The extracted latent variables are sorted according to their eigenvalue. With PCA the high dimensional space described by matrix X is modeled as (Aguado et al., 2008):

$$X = TP^T + E \qquad \text{Eq. 3-1}$$

Where T is the score matrix (composed by the PCs), P the loadings (composed by the eigenvectors of the covariance matrix) and E the residual matrix (variance that was not captured by the model). Principal Component Analysis (PCA) maximizes the rate of decrease of variances (Haykin, 1999). Usually the sum of the variances of the first few principal components exceeds 70% of the total variance of the original data . In the current study PCA is carried out on physiographic and land cover attributes (Table 3-2) and daily streamflows of 90 watersheds across Ontario. MATLAB 7 (2011b) is used to make PCA calculations and graphs.

K-means algorithm is used to distinguish the boundaries of PCA scores. The k-means method developed by MacQueen (1967), assigns each data point to the cluster where the distance between the data points to the cluster centroid is smallest. This non-hierarchical clustering first chooses some initial clusters of data then alters the cluster memberships in order to obtain new clusters that minimize the variance within each cluster.

The Davies–Bouldin (DB) index introduced by Davies and Bouldin (1979) is a metric for evaluating clustering algorithms. This DB index is defined as:

$$DB = \frac{1}{n}\sum_{i=1, i\neq j}^{n} \max\left(\frac{Si+Sj}{d(Ci,Cj)}\right) \qquad \text{Eq. 3-2}$$

Where n is the number of clusters, Si and Sj are the average distances of all points in clusters i and j to their cluster centers (within cluster scatter) and $d(Ci, Cj)$ is the distance between cluster centers (Ci and Cj). Small values of this index correspond to clusters that are compact, and whose centers are far away from each other (Aguado et al., 2008). This index is calculated for classifying PCA scores using K-means algorithm. Therefore, the number of clusters that minimizes Davis-Bouldin index is taken as the optimal number of clusters

Streamflow Indices and K-means Clustering (namely Reference Classification)

Streamflow signatures which measure characteristics of hydrologic response are used in first order analysis to classify watersheds or runoff variability. In this study we apply K-means clustering on five streamflow indices of 90 watersheds across Ontario including runoff ratio, slope of flow duration curve (FDC), base flow index (BFI), streamflow elasticity and snow day ratio, a subset of six signatures recently introduced by Sawicz et al., (2011). The resulting clusters from this analysis are made homogenous in terms of discordancy measure (D) which is defined as (Hosking and Wallis, 1997):

$$D_i = \frac{1}{3} N(u_i - \bar{u})^T A^{-1} (u_i - \bar{u}) \qquad \text{Eq. 3-3}$$

Where N is number of sites (watersheds) in a cluster, u_i is the vector of sample L-moments including L-CA, L-skewness and L-kurtosis and A is the matrix of sums of squares and cross-products defined as:

$$A = \sum_{i=1}^{N} (u_i - \bar{u})(u_i - \bar{u})^T \qquad \text{Eq. 3-4}$$

D indicates site i to be discordant if D_i is large i.e. more than 3 for 15 or higher number of sites in the group. Using this measure the discordant watersheds are moved to other groups until hydrologic homogeneous clusters are identified. Watershed classification using this method is considered as reference classification and it is compared with the results of other methods in section 4. A brief definition of each of the indices is provided hereafter following Sawicz et al., (2011):

- *Runoff ratio*

Runoff ratio (R) is defined as the ratio of long-term average streamflow (Q) to the long-term average precipitation (P).

$$R = \frac{Q}{P} \qquad \text{Eq. 3-5}$$

A high runoff ratio indicates that large amount of precipitation turned into streamflow while lower values of R shows that larger amount of precipitation converted to evapotranspiration.

- *Slope of FDC*

Flow duration curves represent the percentage of time or probabilities of streamflow equaled or exceeded. FDCs can be developed using hourly, daily or monthly streamflow. The normalized daily streamflows by drainage area are used to develop FDCs for the watersheds. The slope of the curves (S) between probabilities of exceedance of 33 % and 66% is used as the slope of FDC:

$$S = \frac{\ln(Q_{33\%}) - \ln(Q_{66\%})}{(0.66 - 0.33)} \qquad \text{Eq. 3-6}$$

The shape of the flow duration curve can also be used as an indication of physiographic characteristics of watersheds including slopes and drainage distribution and plant cover (Peters and Driscoll, 1987).

- *Base Flow Index (BFI)*

BFI is defined as the ratio of long-term base flow to total streamflow (Sawicz et al., 2011). The digital filter method has been widely used in base flow separation. This method provides a good match between filtered base flow and measured base flow values (Arnold and Allen 1999; Lim et al. 2005). $q_t = \alpha \times q_{t-1} + \frac{1+\alpha}{2} \times \ (Q_t - Q_{t-1})$ Eq. 3-7 shows the digital filter method used for baseflow separation:

$$q_t = \alpha \times q_{t-1} + \frac{1+\alpha}{2} \times \ (Q_t - Q_{t-1}) \qquad \text{Eq. 3-7}$$

Where q_t and q_{t-1} are filtered direct runoff at time step t and t-1, α is the filter parameter and Q_t and Q_{t-1} are the total values of streamflow at the time step t and t-1.

However, Champan (1991) pointed out that this method provides constant streamflow and baseflow when the direct runoff has ceased. The algorithm proposed by Champan (1991) and simplified equation proposed by Champan and Maxwell (1996) is used in this paper to calculate base flow values using daily streamflows :

$$b_t = \frac{\alpha}{2-\alpha} \times b_{t-1} + \frac{1-\alpha}{2-\alpha} \times \ Q_t \qquad \text{Eq. 3-8}$$

Where b_t and b_{t-1} are the filtered base flows at time step t and t-1 and α is the filter parameter. α is set at a value of 0.925 (based on Eckhardt (2008)).The Based flow index (I) can be then calculated as the summation of all ratios of daily baseflow (Q_B) to daily total streamflow (Q) as follows:

$$I = \sum \frac{Q_B}{Q} \qquad \text{Eq. 3-9}$$

- *Streamflow elasticity*

Streamflow elasticity (E) indicates the rate of changes in streamflow with respect to changes in precipitation. It is calculated as the median of the values of inter-annual difference between annual streamflow (dQ) divided by the inter-annual difference between annual precipitation (dP), normalized by ratio of mean annual precipitation ($\bar{P}$) to mean annual streamflow ($\bar{Q}$) (Sawicz et al., 2011) :

$$E = median(\frac{dQ}{dP}\frac{\bar{P}}{\bar{Q}})$$ Eq. 3-10

Snow day ratio

Snow day ratio(R) uses the time series of temperature, precipitation; therefore it represents both the climatic and hydrologic characteristics of watersheds. It is defined as the ratio of the number of wet days (days with precipitation, N_S) when the average daily air temperature is below 2 ºC to the total number of days with precipitation (N_P) (Sawicz et al., 2011):

$$R = \frac{N_S}{N_P}$$ Eq. 3-11

Nonlinear Techniques

Self-Organizing Maps (SOMs)

Kohonen maps (or Self Organizing Maps, SOMs) are one type of neural networks which are capable to solve unsupervised rather than supervised problems. Self-organizing maps learn to recognize groups of similar input vectors. (Kohonen, 1995; Aguado et al., 2008). The SOMs can be used as data compression technique by mapping high-dimensional data into a lower-dimensional grid or to identify groups of observations with similar characteristics. SOMs have shown a good potential for watershed classification in Italy (Di Prinzio et al., 2011) and is therefore selected here for further analysis and comparison with NLPCA and Compact-NLPCA for watersheds classification based on streamflows and watershed attributes respectively.

Two layers compose a typical SOM: the input layer and the output layer (also known as competitive layer). A schematic 3 × 3 two dimensional SOM is displayed in Figure 3-2. The input layer contains neurons representing variables (i.e. watershed attributes) fully connected to neurons of output layer by applying weight vectors. The number of neurons in output layer is predetermined by modeler and here it is considered as the number of desired clusters. Each neuron from the output layer represents its position in the grid and its weight vector. In the network training process the weights are gradually changed in order to span the weight vectors across the input data set and the dimension of the weight vector equals the dimension of the input data vectors. At the end of the network training, samples are placed in the most similar neurons of the Kohonen map. The training is both competitive and cooperative because the weights of the neuron which resembles most to that input data are updated (competitive) and also the weights of both the winning neuron and neighboring neurons are updated (cooperative). The trained neural network is to achieve a topology preserving characteristics of the data, for example if two input data vectors are similar (close in the input space), the corresponding winning neurons should be close (Aguado et al., 2008). Some toolboxes for calculating supervised and unsupervised SOMs are proposed in the literature e.g. SOM toolbox developed at Helsinki University of Technology (Aguado et al., 2008) and Kohonen and CP_ANN toolbox developed at University of Milano Bicocca (Ballabio et al., 2009) which are used in this study.

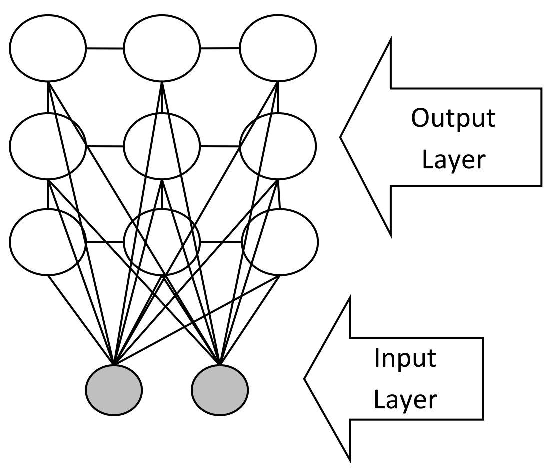


Figure 3-2 Schematic of a two-dimensional Self Organizing Map (SOM)

Non-Linear Principal Component Analysis (NLPCA)

Standard PCA is a suitable option to identify the classification pattern in the data if the structure of the data is inherently linear otherwise if the data contain nonlinear structure it will not be detected by PCA (Monahan, 1999). In 1991, Kramer introduced a neural network–based generalization of PCA for the nonlinear feature extraction problem which is referred to as Nonlinear Principal Component Analysis (NLPCA). In NLPCA the mapping into feature space is defined as (Kramer 1991):

$$T_i = G_i(Y) \qquad \text{Eq. 3-12}$$

Where G_i is the i_{th} nonlinear factor of Y (input) and T_i (output) represents the i_{th} element of T. The inverse transformation is implemented by a second nonlinear vector function H:

$$Y_j^{'} = H_j(T) \qquad \text{Eq. 3-13}$$

The functions G and H are mapping and de-mapping functions and are selected to minimize the loss function L:

$$L=\left\|(Y - Y^{'})\right\| \qquad \text{Eq. 3-14}$$

A basis function approach which is used by Kramer (1991) to generate G and H is based on the following nonlinear functions suggested by Cybenko (1989) which fits any nonlinear function $v = f(u)$ to an arbitrary degree of precision:

$$v_k = \sum_{j=1}^{N_2} w_{jk2}\ {}_{\sigma(\sum_{i=1}^{N1} w_{ij1}\, ui+\theta_{j1})} \qquad \text{Eq. 3-15}$$

$\sigma_{(x)}$ is any continuous and monotonically increasing function such as a sigmoid function:

$$\sigma_{(x)} = \frac{1}{1+e^{-x}} \qquad \text{Eq. 3-16}$$

Equations 15 and 16 describe a feedforward artificial neural network with $N1$ inputs, a hidden layer comprised of N_2 nodes with sigmoidal transfer functions and a linear output node for each k . W_{ijL} in Eq. 3-15 represents the weight on the connection from node i in layer L to node j in layer L+1. The θ are nodal biases, treated as adjustable parameters like the weights.

Neural networks are able to fit arbitrary nonlinear functions owing to the hidden layers and nonlinear transfer functions between the nodes. G and H in $T_i = G_i(Y)$

Eq. 3-12 and $Y_j^{'} = H_j(T)$

Eq. 3-13 can be represented by two single hidden layer neural networks. The network for G operates on Y as input vector with m nodes and its hidden layer is called *mapping* (or encoding) layer with sigmoidal transfer function and its output is T with n nodes. The network representing the inverse function H takes T as input and its hidden layer is called *de-mapping* (or decoding) layer and its output is reconstructed data, Y. Figure 3-3 (a) displays the architecture of the described neural networks for modeling G and H. Since T is unknown and it is the output of G and input of H, the two networks are combined so that G feeds directly into H and a network is obtained whose inputs and desired outputs are known. The second hidden layer is referred to as *bottleneck* layer because it has the smallest number of nodes. Therefore, standard NLPCA model consists of an auto-associative feedforward neural network (having same input and output), with five layers of neurons including: input, three hidden layers (encoding, bottleneck, decoding) and output layer. The neural network is called auto-associative because the output neurons are in pairs with input neurons.

In the current study, watershed attributes and daily streamflows of 90 watersheds are used as input to the three-hidden-layer feedforward neural network. The number of encoding and decoding neurons are adjusted for an optimal fit of output to the target and is set to be the same (following Kramer, 1991 and Lu and Panadolfo , 2011). The number of neurons in the middle hidden layer or bottleneck layer should be less than neurons in the encoding and decoding layers and dimension reduction is achieved in bottleneck layer. The outputs of this layer, representing the network output are considered as nonlinear principal components. In this study a single neuron bottleneck layer gives the nonlinear principal component vector (of 90 watersheds).

To overcome the common problem of overfitting , methods such as "early-stop during the training phase" and "weight penalty" can be applied (Hsieh, 2001; 2004; 2007). MATLAB codes for nonlinear principal component analysis developed by Hsieh (2007) at the University of British Columbia are used. The NLPCA training algorithm used avoids overfitting by determining the best weight penalty. For further details on the NLPCA model as used herein, the readers are referred to Hsieh 2007.

Compact-NLPCA

Lu and Pandolfo (2011) modified the structure of the three hidden layer neural network introduced for NLPCA because they found that the three-hidden-layer neural network can cause the non-uniqueness of solutions and data-over-fitting due to the linear transfer function which convert encoding signals to bottlenecks (output layer in the neural network representing function G in Figure 3-3 (a)). The encoding layer and also output bias terms are removed in this new model structure. Therefore, the bottle neck neurons make up the first hidden layer and encoding layer is the second hidden layer and both having nonlinear transfer functions. This model is called compact-NLPCA because it has two hidden layer and four layers in total rather than the five layers of standard NLPCA model (see Figure 3-3 a,b). This simplified neural network is expected to obtain more stable nonlinear components. The bottleneck signal in this model is the output of nonlinear function e.g. sigmoid operated on input vector. It can be expressed as:

$$T = \sigma(\sum_{i=1}^{m} W_i \, y_i + \theta) \qquad \text{Eq. 3-17}$$

Where W_i is the weight of the bottleneck neuron to signal from the i_{th} input neuron, y_i , and θ is the bias term. The architecture of this two-hidden layer neural network is displayed in Figure 3-3 (b).

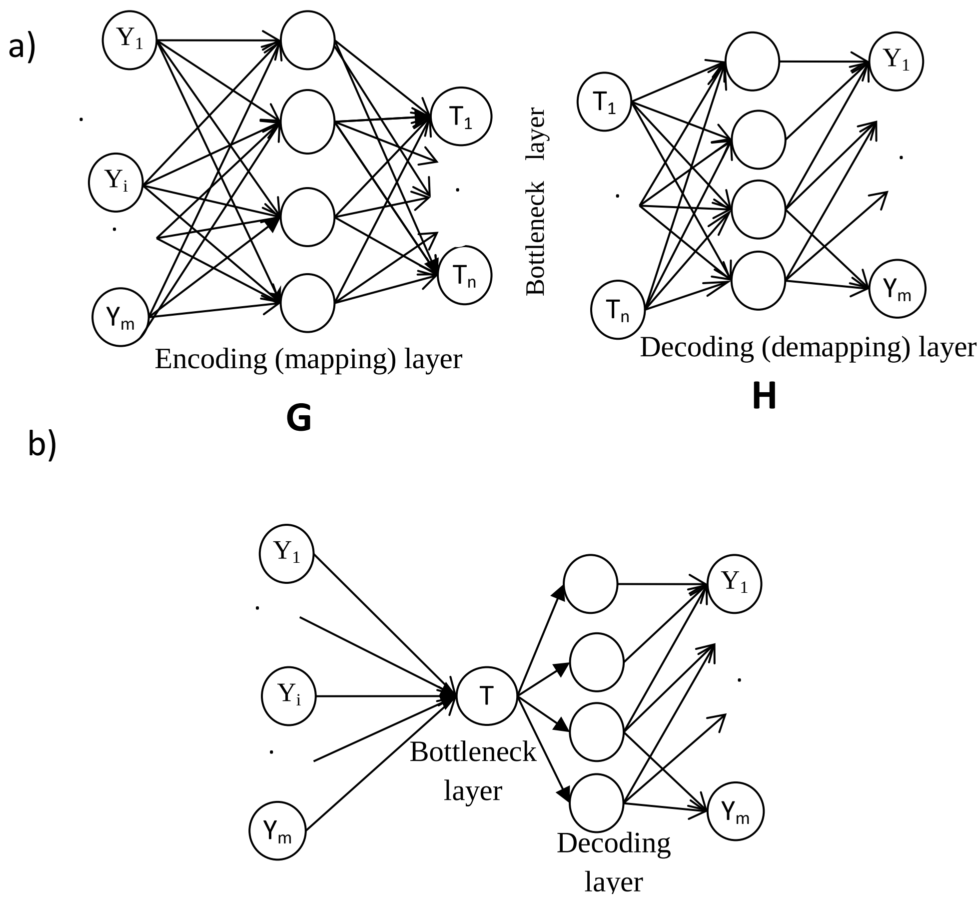


Figure 3-3 Schematic architecture of feed forward neural network used for NLPCA model

a) Standard NLPCA with three hidden, one input and one output layers following Kramer, 1991

b) Compact-NLPCA with two hidden, one input and one output layers; the first hidden layer is called bottleneck layer consists of a single neuron and the second hidden layer is called decoding layer introduced by Lu and Pandolfo (2011)

3.5. Results

K-mean clustering on PCs and streamflow signatures

PCA is first applied on watershed attributes, considered as variables of 90 watersheds (observations). Prior to classification the raw data (attributes) are mean-centered and scaled to unit variance to handle the different measurement units of attributes and giving equal importance to each attribute. After the standardization all attributes have zero mean and unit variance. Figure 3-4 shows a plot of the percentage of variability explained by each principal component of watershed attributes. The graphical plot shows that the first three principal components explain almost 90 percent of the total variability in the standardized data, so that is considered as a reasonable way to reduce the dimension in order to visualize the principal components (PCs).

To visualize the analysis results, both the principal component coefficients (loadings) for each attribute and the principal component scores for each observation (watershed) are presented in a single plot in Figure 3-5. Each of the 12 variables (watershed attributes) is represented in this plot by a vector, and the direction and length of the vector indicates how each variable contributes to the two principal components. For example, the first principal component has positive coefficients for 7 out of 12 watershed attributes and negative coefficients for the remaining five attributes. That corresponds to the seven vectors directed into the right half of the plot. Each of the 90 observations is represented by a point in the plots, and their locations indicate the score of each observation for the principal components. For example, in the first plot points near the left edge of the plots have the lowest scores for the first principal component. In the plot of loading vectors, variables (watershed attributes) which are positively correlated are grouped together (in the same quadrant) and if they are inversely correlated they are located in opposite sides of the plot origin. From the first graph, it can be seen that slope and elevation are correlated since they have same direction and almost same magnitude. Also the two graphs show that the two first principal components are more affected by latitude, area, elevation/slope and forest, therefore classification is expected to be more affected by these attributes.

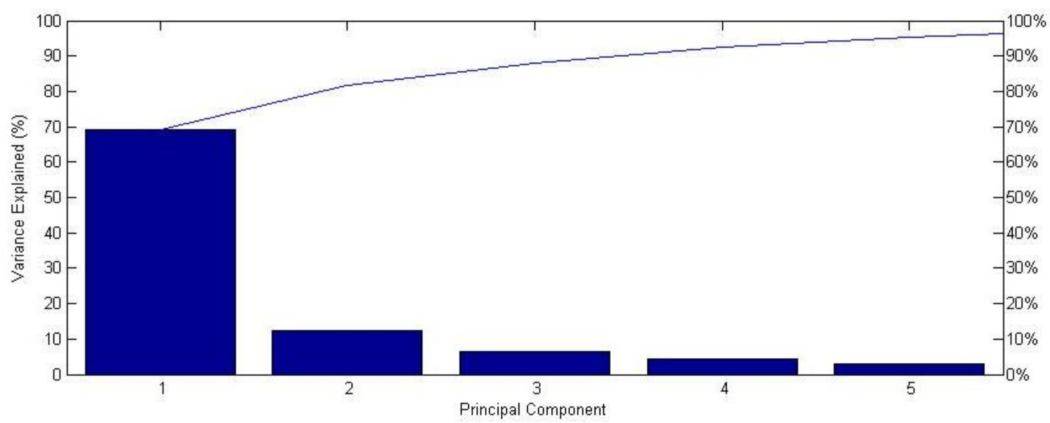


Figure 3-4 Percentage of total variability explained by each principal component of catchment attributes

K-means algorithm with Davies-Bouldin index is applied to the scores of the first three principal components to discover groups of observations (watersheds) with similar characteristics. K-means partitions the points into K clusters.

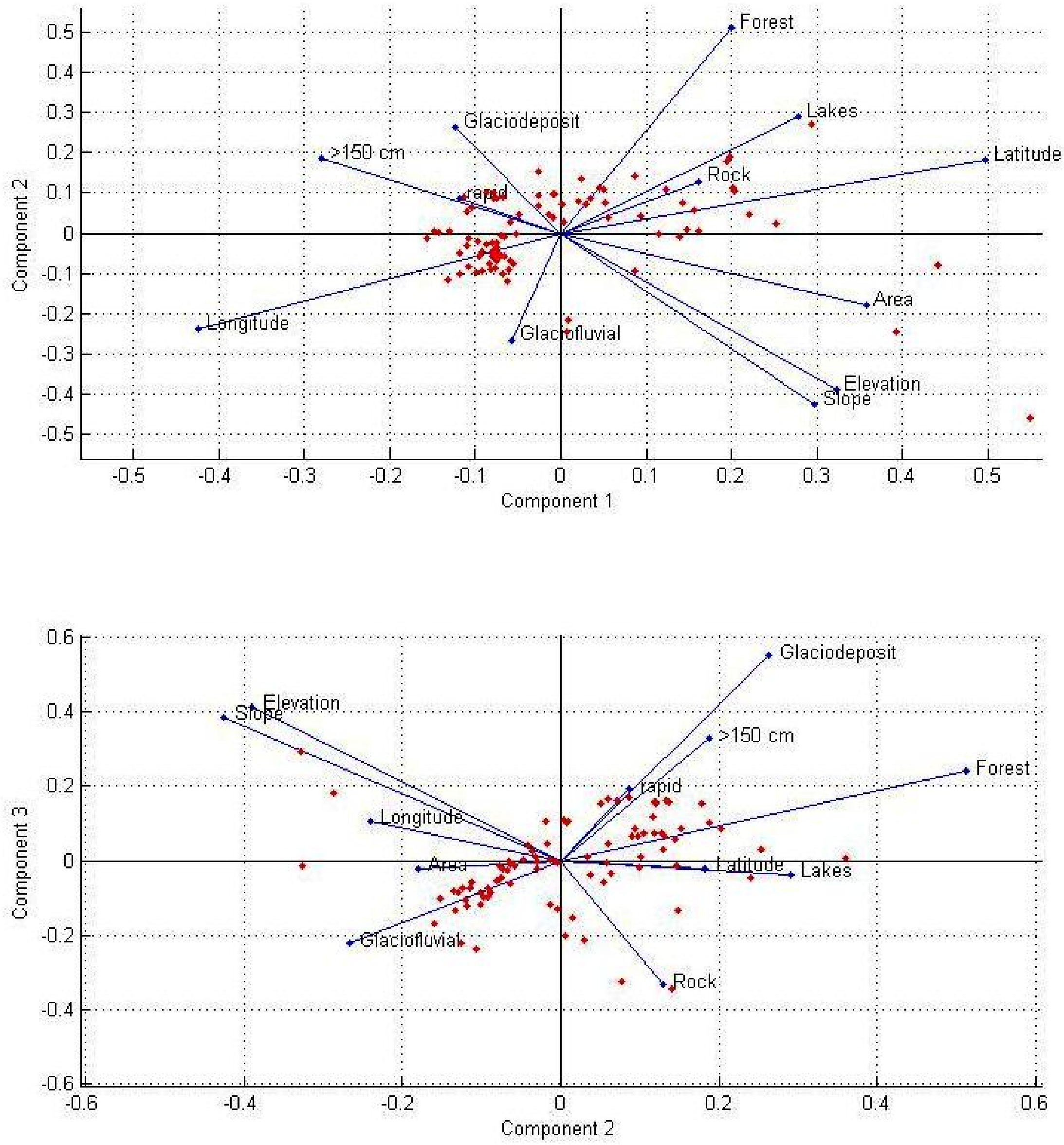


Figure 3-5 PCA loading plots for (a) the two first principal components and (b) the second and third principal components of catchment attributes (Table 3-2)

The optimal number of clusters is obtained by minimizing the Davies-Bouldin index. The value of this index for different number of clusters is averaged after 10 runs and it is shown in Figure 3-6. The results indicate a lower value of Davies-Bouldin index for four and nine clusters, four is taken as an appropriate number of clusters for the simplicity of analysis. K-means algorithm is applied on the first three principal components (scores) of watersheds attributes and classified them into four clusters.

PCA is also applied on the watershed daily streamflows. The continuous daily streamflows for the 90 watersheds are used for this analysis. Streamflow time series for each watershed are normalized by the watershed area. Similarly to watershed attributes, the graphical plot of watershed daily streamflow indicated that the first three components account for most of the variance in the flow (more than 70 percent) and K-means algorithm is applied on the scores of the first three principal components of daily streamflows to classify the watershed into four clusters.

Runoff ratio, slope of FDC, streamflow elasticity, baseflow index and snow day ratio are calculated for 90 watersheds. The summary of statistics of the calculated indices is presented in Table 3-3. Precipitation and temperature time series are obtained from the closest meteorological station to the center point of each watershed with less than 20 percent missing data. Since meteorological stations are not homogeneously distributed throughout the province and may not be coincident with the streamflow gauges calculated indices are involved with some source of uncertainty which can also affect the classification results. The correlation between baseflow index and slope of FDC was highest among the remaining signatures which is 0.53. Since the correlation between the signatures is negligible all the five indices are used for the classification using K-means algorithm into four clusters. Discordancy measure (D) is calculated for the four identified clusters (each cluster consists of more than 15 watersheds). Two of the clusters are homogeneous according to this measure and for the two largest clusters only one watershed in each was discordant and was moved to another cluster, and D was recalculated until the watersheds in all groups became homogenous. The clusters resulted from this method are used as reference classification.

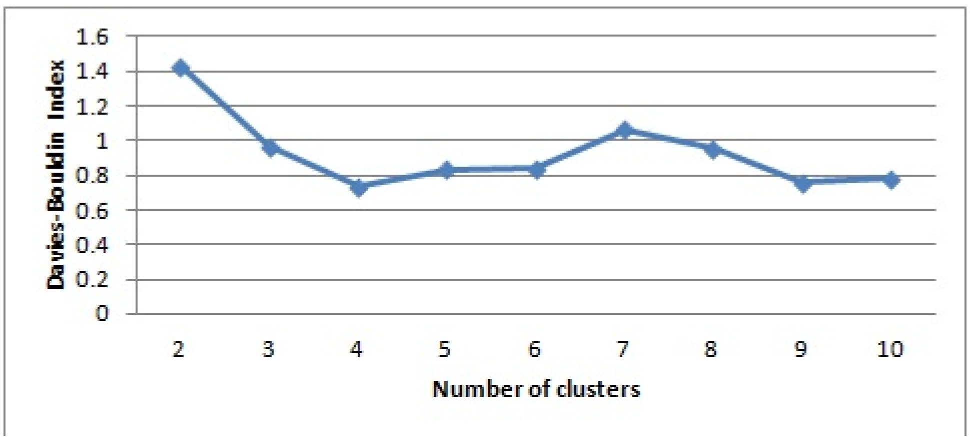


Figure 3-6 Davies-Bouldin index for the K-means clustering algorithm applied to the PCs of catchment attributes (average of 10 runs)

SOM

Component planes allow the visualization of correlation patterns among the process variables. In order to visualize the relationships among the variables, the component plane of a given variable shows the estimated value of that variable in all neurons of the map. Each component plane is composed by many hexagons (neurons), and the color of each hexagon informs on the value of the component in that neuron.

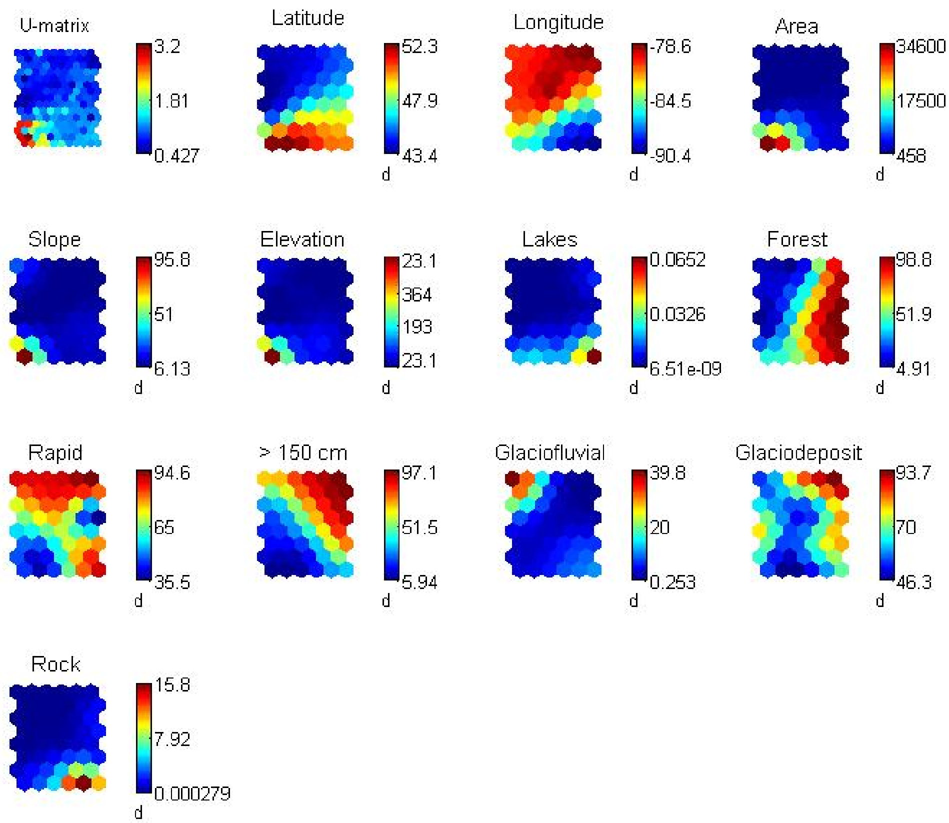


Figure 3-7 U-matrix and component planes of the trained SOM (Attributes have same units as in Table 3-2)

Figure 3-7 displays the component planes of 12 watershed attributes used as input variables to SOM. Comparing the color gradient of the component planes some correlation patterns among the variables can be discovered. Similar dark and light areas on different component planes indicate positive correlation. Therefore, area, slope and elevation exhibit positive correlation. Also, the component planes of the percentage of area covered by root depth deeper than 150 cm and rapid drainage class are almost similar reflecting that the larger area covered by root depth deeper than 150 cm in a watershed is related to larger area of rapid drainage class and the similarities between latitude and lakes indicate the watersheds with higher latitudes are covered with more percentage of lakes.

Table 3-3 Summary of statistics of runoff signatures for 90 watersheds across Ontario

	Runoff ratio	**FDC slope**	**streamflow elasticity**	**Snow day ratio**	**Baseflow index**
Min:	0.252	1.278	-0.288	0.228	0.502
1st Qu.:	0.377	2.499	0.808	0.294	0.541
Mean:	0.413	3.034	1.277	0.340	0.569
Median:	0.410	2.98	1.29	0.342	0.563
3rd Qu.:	0.447	3.67	1.63	0.398	0.601
Max:	0.610	5.30	3.84	0.500	0.668
Std Dev.:	0.071	0.907	0.6878	0.0637	0.0425

The analysis of the component planes reveals the watersheds with similar characteristics. The U-matrix plan in Figure 3-7 shows the distances between neighbouring neurons on the whole map: high values (dark colour) correspond to large distances between neighboring neurons and indicates cluster borders. This plane reveals that 3 to 4 distinct clusters that are visible in the whole data set. The number of four clusters is in line with the results of K-means algorithm on watershed attributes along with Davis-Bouldin index.

Table 3-4 Discordant sites for the two largest groups from each classification technique

	PCA,att			PCA,St		
	n[1]	DB[2]	Percent%	n	DB	Percent%
C_1	40	0	0	31	2	6.45
C_2	31	1	3.23	24	1	4.17
	NLPCA,att			**NLPCA,St**		
	n	DB	Percent%	n	DB	Percent%
C_1	39	0	0	41	0	0.00
C_2	33	0	0	27	1	3.70
	SOM			**CNLPCA,St**		
	n	DB	Percent%	n	DB	Percent%
C_1	43	1	2.33	40	0	0.00
C_2	28	1	3.57	26	1	3.85
	CNLPCA,att					
	n	DB	Percent%			
C_1	41	0	0.00			
C_2	20	1	5.00			

C1: First largest group [1]n is the number of watersheds in the group

C2: Second largest group [2]DB is the number of discordant watersheds

NLPCA and Compact-NLPCA

The architecture of three hidden layer auto associative neural networks used for the standard NLPCA is *I-m-u-m-I* and for the Compact-NLPCA is *I-u-m-I* where *I* is the number of both the input and output neurons (they are the same), *m* is the number of hidden neurons in encoding and decoding layers and *u* is the number of bottleneck neurons. In this study watershed attributes of 90 watersheds and also daily streamflow series are used as inputs, *u* is considered as one, *m* is changing from 2:10 and P (weight penalty) having the values of [0, 0.01, 1] . The most appropriate values of P and m, yielding the smallest MSE (Mean Square Error) and also consistent in assigning NLPCs to nearest neighbors are selected by running the NPCA algorithm multiple times. The nonlinear principal components of selected solution are classified according to their magnitude into four clusters.

Inter-comparison of classification results

The number of discordant sites for the two largest groups (as representatives of each classification) resulting from the different methods are presented in Table 3-4. From Table 3-4 NLPCA based on watershed attributes identifies homogenous clusters (i.e. the two largest clusters have no discordant watersheds) and also PCA based on watershed attributes and NLPCA based on streamflow have equally the next least number of discordant watersheds. Figure 3-8 demonstrates the Ontario watershed classification using runoff signatures (Reference one) in comparison with other alternative classifications. The three ecozones of Ontario including Boreal shield, Hudson plain and Mixed wood plain, characterized by bedrock (defined by Ontario ministry of natural resources) are also shown in the background.

A similarity index (SI) (proposed by Ssegane et al., (2012)) is used to show the similarity between clusters. This index combines three existing measures of similarity included the hamming distance (HD) by Dunne et al., (2007), similarity index (S_s) by Kalousis et al., (2007) and a consistency index (CI) by Kuncheva (2007) . This SI accounts for the cardinality of set intersection of A and B ($|A \cap B|$), the cardinality of set difference and unequal number of features in the two sets A and B which are not considered in any single of the mentioned indices:

$$SI = \frac{1}{2}\left(\frac{1-|A\backslash B|+|B\backslash A|-2|A\cap B|}{|A|+|B|}\right)) \qquad \text{Eq. 3-18}$$

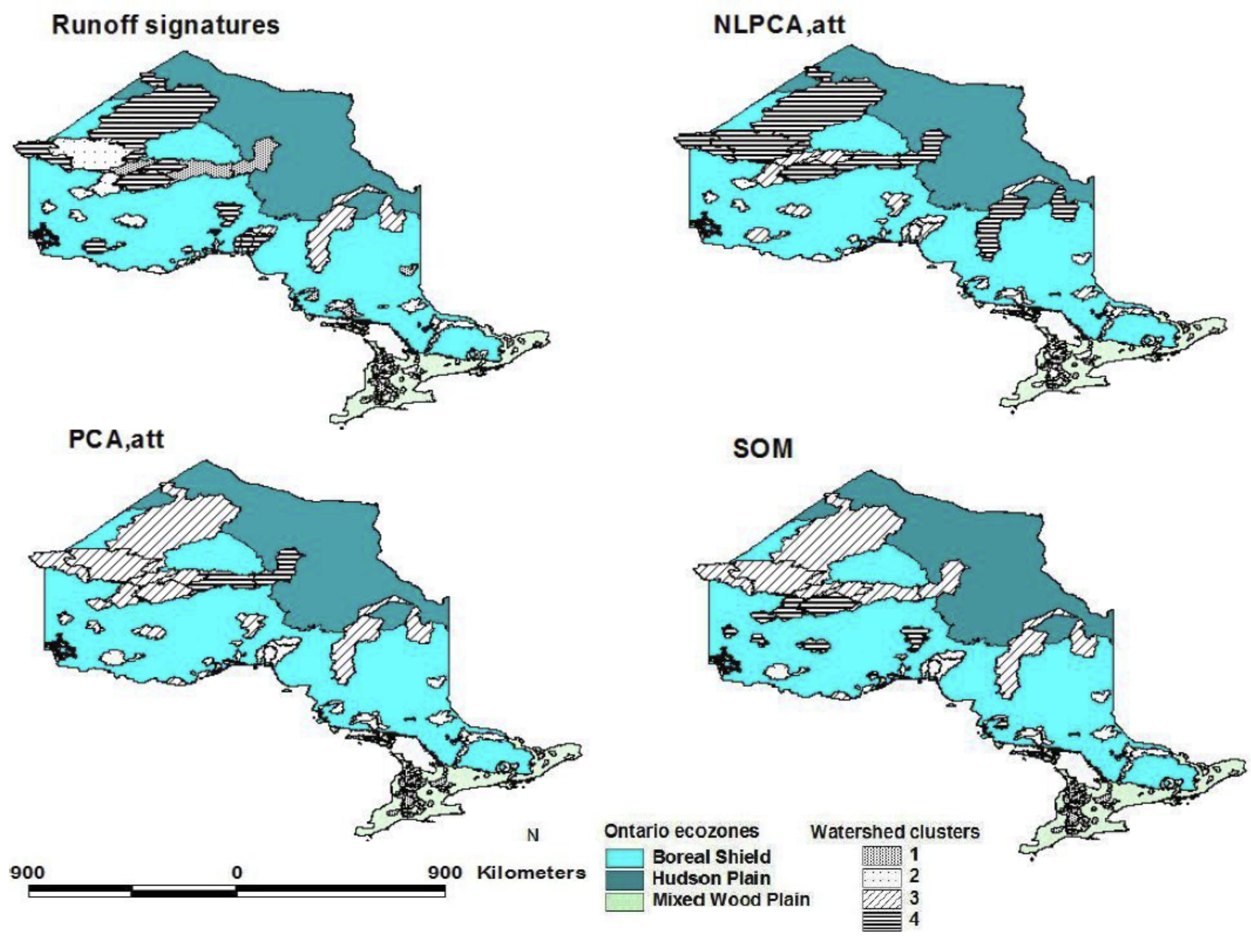
Where $|A|$ is the cardinality of set A and $|B|$ is the cardinality of set B, $|A\backslash B|$ is cardinality of set difference of A from B and $|B\backslash A|$ is cardinality of set difference of B from A. Set A is considered to be one of the homogenous reference clusters (classified using streamflow signature) and set B is one of the clusters classified by alternative techniques. Table 5 presents the SI between the two largest groups (as representatives) of hydrologically homogenous classification and corresponding cluster of other techniques. According to this table the classified groups using NLPCA based on watershed attributes and daily streamflows have the highest similarity in both largest groups (in average) with the corresponding groups of hydrologically homogeneous classification. Also classification results of SOM and Compact-NLPCA (average of both attributes and streamflow) have higher SI compared to standard PCA.

It is also shown that the Compact-NLPCA (an improved version of NLPCA) does not outperform the typical NLPCA model in this experiment. The superior performance of the NLPCA based on watershed attributes suggests that it can be a good alternative for watersheds classification where appropriate streamflow series are unavailable.

Table 3-5 Similarity index between the reference homogenous groups and nonlinear techniques

First largest class							
	PCA-att	PCA-st	SOM	NLPC-att	NLPCA-st	CNLPCA-att	CNLPCA-st
A	38	38	38	38	38	38	38
B	40	31	43	39	41	41	40
A/B	20	19	17	16	15	18	16
B/A	22	12	22	17	18	21	18
A∩B	18	19	21	22	23	20	22
A+B	78	69	81	77	79	79	78
SI	0.46	0.55	0.52	0.57	0.58	0.51	0.56
Second largest group							
A	23	23	23	23	23	23	23
B	31	24	28	33	27	20	26
A/B	18	19	18	12	16	16	17
B/A	26	20	23	22	20	13	20
A∩B	5	4	5	11	7	7	6
A+B	54	47	51	56	50	43	49
SI	0.19	0.17	0.20	0.39	0.28	0.33	0.24

(a)


Runoff signatures
NLPCA,att
PCA,att
SOM
N
900 0 900 Kilometers
Ontario ecozones
Boreal Shield
Hudson Plain
Mixed Wood Plain
Watershed clusters
1
2
3
4

(b)

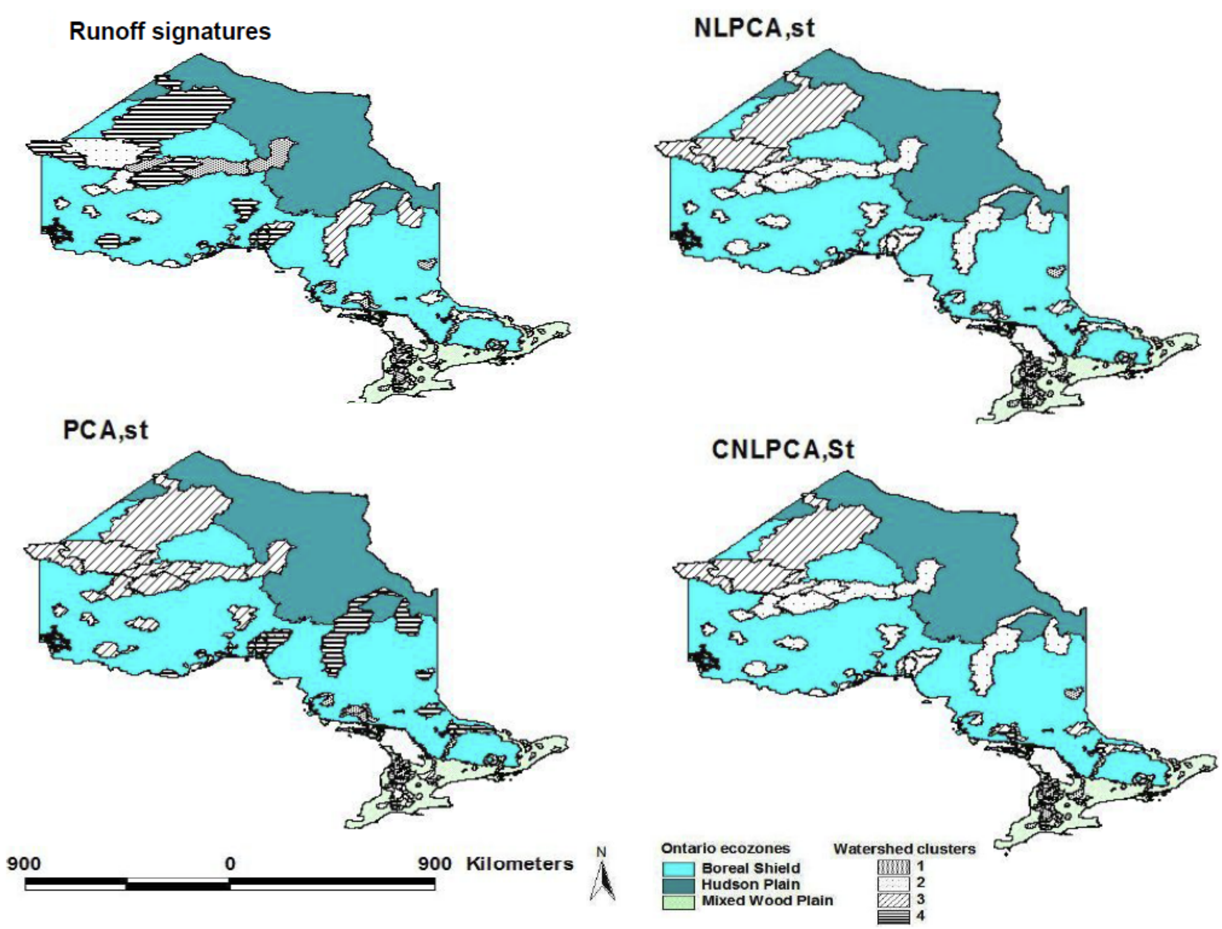


Figure 3-8 Ontario watersheds classified using runoff signatures, PCA and nonlinear techniques (att: catchment attributes, st: daily streamflows)

3.6. Discussion of Hydrologic Implications

The classification results of the nonlinear techniques (SOM, NLPCA,Compact-NLPCA) based on watershed attributes are selected for further investigation of hydrological homogeneity in clusters because of their superior performance and also their applicability for the classification of ungauged watersheds.

Using the PCA the attributes with highest coefficients in each cluster are specified in Table 3-6. Latitude appears the main attribute in the first large cluster (C1) whatever the nonlinear classification method which is consistent with the spatial distribution of the cluster (C1) watersheds shown in Figure 8a,b for the nonlinear methods. The dominant effect of latitude in the largest cluster further confirms (albeit indirectly) the importance of climate-streamflow relationship in the regional hydrology (Coulibaly and Burn, 2005). Elevation, area covered by rooting depth>150cm and forest are the other attributes that differentiate the two largest clusters. The shape of the flow duration curve (FDC) reflects specific attributes of the watershed (Post, 2004) because when flows are ranked according to their frequency of occurrence and plotted on a FDC, the resulting curve shows the integrated effect of all the various factors that affect runoff magnitude and frequency (Searcy, 1959). The slope of FDC (Q5/Q95) which is the ratio of high flow to low flow is selected as a criterion further analysis of the clusters. Table 3-7 presents the number of watersheds in each cluster with high, moderate and low value of FDC slope (Q5/Q95). The majority of watersheds in the first largest cluster (C1) has a high slope whatever the classification method. The majority of the watersheds in the second largest cluster (C2) of SOM and NLPCA-att has a moderate FDC slope while the ones in CNLPCA-att cluster (C2) have a low slope. Since latitude, elevation and area covered by forest are among the principal attributes in the first two largest clusters and also the existence of a dominant pattern in the ratio of Q5/Q95 in the corresponding clusters suggests some physical hydrologic implication of these attributes in the magnitude and frequency of flow. Furthermore, Table 3-8 shows the number of watersheds in each cluster with the same timing of event flows. Timing of low flow, spring snowmelt peak flow, and autumn peak reflect the shape of annual hydrograph. According to previous study (Stainton and Metcalfe 2007), climate and regional physiography influence the timing of event flows in certain areas of the Province of Ontario. In the first largest clusters of all the three classifications, for the majority of watersheds, low flow occurs in July/August, spring snowmelt in March and autumn peak in December. For the second, third and fourth clusters, dominant patterns of the flow timing in majority of watersheds can be observed. There is a consistent pattern in flow timings for the majority of watersheds in each cluster whatever the method. Although, the flow timings for the watersheds in the CNLPA-att clusters (C2, C3, C4) are different for some seasons as compared to those of the SOM and NPCA-att, there is a consistent pattern for each cluster. For example in cluster 1 of CNLPCA-att, majority of watersheds have spring snowmelt in March, in cluster 2 it happens in June/May and for clusters 3 and 4 it happens in April

Stainton and Metcalfe (2007) identified eight hydroclimatic regions in Ontario based on annual flow regime characteristics which are most affected by climate and indicate generally good geographic contiguity (see Figure 3-9). According to their findings, distinct trends in the timing of spring snowmelt and low flow periods with increasing latitude were observed across the Province specially the delayed spring snowmelt with increasing latitude. All the watersheds in the first largest cluster (C1) of SOM and CNLPCA-att and the majority of watersheds in the first largest cluster (C1) of NLPCA-att belong to hydroclimatic regions 1, 2 and 3 which consist of small watersheds in southern Ontario, the most spatially contiguous regions, spanning the mixed wood plains ecozone. Most of these watersheds show a pattern of maximum discharge in the month of March/April, a summer low-flow in July / August, and an autumn peak in December. It appears that the nonlinear classification methods are able to capture the complex patterns in cold region hydrology based only on the watershed attributes. This is particularly important for improved streamflow regionalization for ungauged basins which is the target of future investigation. Further study should evaluate the potential of the nonlinear classification methods for continuous flow regionalization as compared to standard methods.

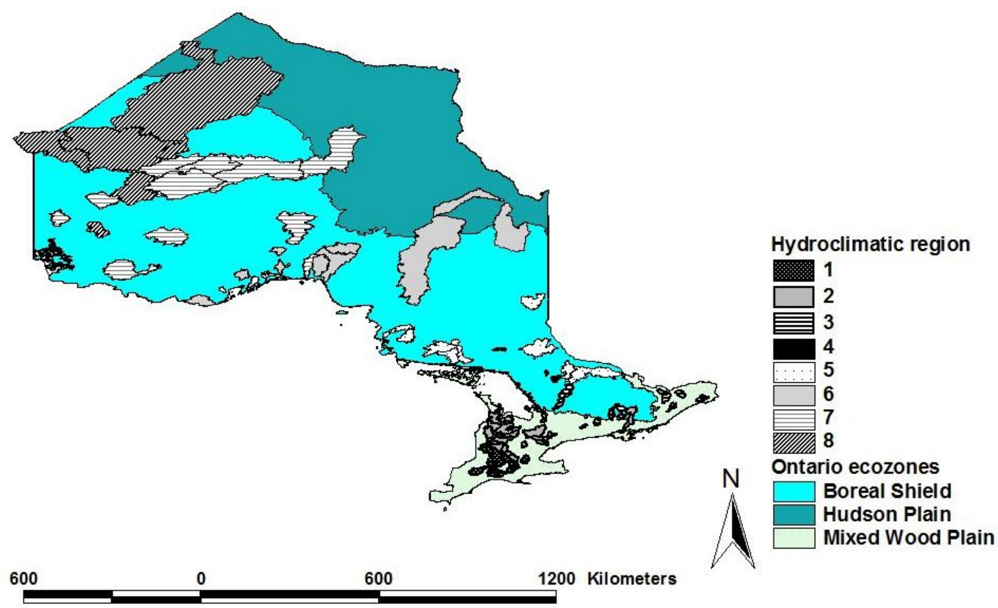


Figure 3-9 Eight hydroclimatic regions of Ontario watersheds identified by Stainton and Metcalfe (2007) .

Table 3-6 Catchment attributes with highest coefficient of principal component in each cluster

Classification Technique	Cluster	Number of watersheds	Principal Attributes
SOM	C1	43	Latitude, Slope, Elevation, >150cm
	C2	28	Latitude, Longitude, >150cm,Glaciodeposit
	C3	10	>150cm,Elevation,Slope,Longitude
	C4	9	Area, Slope,Latitude, Longitude
NLPCA ,att	C1	39	Latitude, Forest, Elevation, Glaciodeposit
	C2	33	Latitude,Longitude, Forest, >150cm
	C3	11	>150cm, Longitude, Glaciofluvial
	C4	7	Slope, Elevation, Glaciofluvial, Area
CNLPCA ,att	C1	41	Latitude, Longitude, Forest, Glaciofluvial
	C2	20	Forest, Rapid, Elevation, Glaciodeposit
	C3	17	Rapid, Forest, Elevation
	C4	12	Forest, Rapid, Lakes

Table 3-7 Number of watersheds with low, moderate and high value of FDC's slope (Q5/Q95) in each cluster

	NLPCA-att				CNLPCA-att				SOM			
	C1	C2	C3	C4	C1	C2	C3	C4	C1	C2	C3	C4
Low	6	11	8	5	9	13	6	2	9	9	5	7
Moderate	12	15	2	1	12	5	8	5	14	12	3	1
High	21	7	1	1	20	2	3	5	20	7	2	1
Number of Watersheds	39	33	11	7	41	20	17	12	43	28	10	9

Table 3-8 Flow timing (time of event flows) in the watersheds of each cluster

Cluster	Event	Time	SOM	NLPCA-att	CNLPCA-att	Cluster	SOM	NLPCA-att	CNLPCA-att
C1	Low flow	July/Aug.	42	37	41	C3	0	2	6
		Feb./March	1	2	0		10	9	11
	Spring Snowmelt	March	32	21	31		0	1	0
		April	10	18	10		0	1	10
		June/May	1	0	0		10	9	7
	Autumn Peak	Oct.	1	1	0		10	8	4
		Nov.	11	14	10		0	1	13
		Dec.	31	24	31		0	2	0
	Number of watersheds		**43**	**39**	**41**		**10**	**11**	**17**
C2	Low flow	July/Aug.	17	20	19	C4	0	0	12
		Feb./March	11	13	1		9	7	0
	Spring Snowmelt	March	2	12	0		0	0	3
		April	18	11	1		2	0	9
		June/May	8	10	19		7	7	0
	Autumn Peak	Oct.	6	8	20		7	7	0
		Nov.	14	12	0		2	0	4
		Dec.	8	13	0		0	0	8
	Number of watersheds		**28**	**33**	**20**		**9**	**7**	**12**

3.7. Conclusion

This study evaluated the ability of nonlinear statistical techniques including SOM, NLPCA, and Compact-NLPCA to classify Ontario watersheds into hydrologically similar clusters. The classification results of two benchmark methods: (1) K-means clustering on PCA scores of watershed attributes/daily streamflow and (2) K-means clustering on streamflow signatures were compared with the results of the proposed nonlinear techniques. Applying K-means clustering to PCA scores of watershed attributes and using Davis-Bouldin index lead to four clusters that appears the best number of clusters of watersheds in Ontario – which was also visible in the SOMs of watershed attributes. The homogeneity of the classified watersheds using each technique was evaluated using discordancy measure and the similarity between the hydrologically homogenous classification and the alternative techniques was evaluated using a similarity index.

Overall, in average, the investigated nonlinear techniques (SOM, NLPCA and Compact-NLPCA) for both watershed attributes and daily streamflow series were consistently superior to PCA in terms of identifying hydrologically homogenous clusters of Ontario watersheds. Surprisingly, despite its more advanced structure, the compact-NLPCA does not outperform the typical NLPCA in the watershed classification experiment. The superior performance of NLPCA based on watershed attributes suggests its potential for the classification of ungauged watersheds. The study results suggest that the nonlinear classification techniques could be reliable alternative methods for the classification of gauged and/or ungauged watersheds.

Further analysis of the classification results using SOM, NLPCA and CNLPCA based on watershed attributes indicated distinct patterns of FDCslope, timing of event flows (annual hydrograph) shape, and dominant physical attributes in each cluster. The identified difference between the clusters can be an indicator of a meaningful watershed classification from the hydrologic point of view. The proposed nonlinear classification methods based on attributes can potentially improve the performance of streamflow regionalization in ungauged watersheds. This needs further study of streamflow regionalization techniques having two scenarios of classified and unclassified watersheds and will be the next stage of our research.

Acknowledgements

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Chapter 4 : Evaluation of Continuous Streamflow Regionalization Using Classified and Unclassified Basins

Summary of Paper III: Razavi, T., and Coulibaly, P. (2014) . Evaluation of Continuous Streamflow Regionalization Using Classified and Unclassified Basins. Submitted to : Journal of Hydrology.

In this research work we used the classified watersheds from the previous study to evaluate the potential of improvement in the performance of continuous streamflow regionalization. We also investigated the combination of watershed classification techniques / regionalization techniques/ rainfall-runoff models. That includes:

1. Four regionalization techniques : IDW , MLP, CPN , SVM
2. Two conceptual hydrologic models : MAC-HBV and SAC-SMA
3. Watershed classification techniques: SOM, NLPCA , CNLPA

The results of this study reveal that:

- MLP model is very competitive with IDW while SVM and CPN have competitive performance in case they are applied on pre-classified watersheds.
- The accuracy of estimated daily mean, low and peak flows is improved when certain combination of regionalization and rainfall-runoff models are used.
- MAC-HBV and SAC-SMA coupled with CPN indicate a clear improvement in daily mean, low and peak flow regionalization after watersheds’ classification using NLPCA.

4.1. Abstract

In this study the potential of watershed classification prior to regionalization in improving the performance of continuous streamflow regionalization as well as the combination of watershed classification and regionalization techniques and rainfall-runoff models is evaluated in Ontario (Canada) watersheds. Four regionalization techniques including a spatial proximity approach (IDW, Inverse Distance Weighted) and three types of neural networks i.e. a Multi-Layer Perceptron (MLP), a Counter Propagation Neural Network (CPN) and a Support Vector Machine (SVM), are applied to transfer the parameters of two conceptual hydrologic models namely MAC-HBV (McMaster University Hydrologiska Byråns Vattenbalansavdelning) and SAC-SMA (Sacramento Soil Moisture Accounting) from gauged to ungauged watersheds in unclassified case as well as homogenous clusters of watersheds obtaining from self-organizing map (SOM), nonlinear principal component analysis (NLPCA) and compact-nonlinear principal component analysis (CNLPA) classification techniques. Overall, it is found that the MLP model is very competitive with IDW which was previously identified as the best regionalization method in the study area, while SVM and CPN have competitive performance in case they are applied on pre-classified watersheds. It is shown that the accuracy of estimated daily mean, low and peak flows is improved when certain combination of regionalization and rainfall-runoff models are used. For example MAC-HBV model coupled with CPN indicates a clear improvement in daily mean, low and peak flow regionalization after watersheds' classification using a nonlinear principal component analysis (NLPCA). Interestingly, a higher improvement is achieved for low flow as well which is usually difficult to estimate in ungauged basins.

Key words: Continuous daily streamflow, Regionalization, Watershed Classification, Neural Networks

4.2. Introduction

Continuous streamflow series are required for water resources' management and for designing various hydraulic infrastructures. Sustainable management decisions can help to maintain the existing water resources for future generations and protect human life from catastrophic flood events. Continuous daily streamflow series are useful for the estimation of daily flow peaks, low flow and flow duration curves. Unfortunately streamflow data are not available in many of the watersheds in the world (Mishra and Coulibaly, 2009). In Ontario (Canada) most of natural basins (more than 60 %) within its one-million-square-km area are still ungauged or poorly gauged (Samuel et al., 2012a). In the United States (US), approximately less than 25000 (10 %) river basins out of 250000 are gauged by US Geological Survey (USGS) (Besaw et al., 2010 ; Geological Survey, 2009). This picture gets worse for many developing countries.

Streamflow series in gauged and/or ungauged watersheds are usually predicted using rainfall- runoff models including fully distributed physically-based and conceptual/semi-distributed models. Other alternative methods recently considered in the literature are hydrologic model-independent or data-driven methods such as regression-based approaches in which streamflow series are not estimated through hydrologic models but based on watershed physiographic and/or meteorological characteristics and data-driven models (detailed discussion on these methods can be found in Razavi and Coulibaly, 2013a).

For prediction of continuous daily streamflow, among rainfall-runoff models, less complex conceptual models are often preferred due to their acceptable and reliable performance. In physically-based models, parameters are usually derived from physical attributes of watersheds which need considerable data and human resources, while parameters of conceptual hydrologic models are calibrated against observed streamflow. Since in ungauged or poorly gauged watersheds, observed streamflow series are not available, the model parameters of gauged watersheds are usually transferred to ungauged ones. This process is called regionalization and it is expected to be more reliable if gauged and ungauged watersheds are similar in some aspects (Blöschl and Sivapalan, 1995). To our best knowledge, watershed classification prior to regionalization has not yet been systematically evaluated in large watersheds such as the Canadian river basins. This study aims to investigate the possibility of improvement in continuous daily streamflow regionalization after systematic watershed classification using nonlinear data-driven approaches such as Artificial Neural Networks (ANNs). Some conventional regionalization techniques are inherently involved with watershed classification. For example in physical similarity or spatial proximity approaches the hydrologic responses are transferred from gauged watersheds to ungauged ones in clusters of similar physical attributes or location. While other types of regionalization approaches such as linear regression or artificial neural networks can be applied on either homogenous groups of watersheds or unclassified ones. Several studies have investigated the potential of improvement in hydrological predictions in ungauged watersheds after classification. They mostly presented a procedure to identify homogenous regions based on watersheds' physical attributes to estimate hydrological responses which can also be used in ungauged watersheds such as low flow characteristics (e.g., Natahan and McMahon, 1990), hydrologic models' parameters (e.g., Burn and Boorman, 1993) , flood characteristics (e.g., Cavadis et al., 2001) and streamflow time series (e.g., Chiang et al., 2002). The focus of these studies has mostly been on the classification's framework and the possibility of its application for ungauged basins or regionalization itself rather than the impacts of classification techniques on the performance of regionalization. A very few studies have investigated the later issue. For example Prinzio et al. (2011) investigated the performance of estimating streamflow indices such as mean annual runoff, flood quartiles and mean annual flood in ungauged watersheds after classification applying a self-organizing map on physical attributes, and they found that watershed classification using SOM could reduce the uncertainty of hydrological predictions in ungauged sites. A more comprehensive analysis is proposed herein; this includes investigating a systematic watershed classification using nonlinear classification techniques prior to regionalization applying two rainfall-runoff models to 90 basins in Ontario.

Nonlinear data-driven methods such as ANNs have been largely used in streamflow prediction (see Abrahart et al. 2012 for a recent review), but very few studies have investigated ANN-based models streamflow prediction in ungauged watersheds. Examples of the later include flood prediction in ungauged watersheds (e.g., Dawson et al. 2006; Wang et al. 2006) and in a few studies daily streamflow prediction in ungauged watersheds either as hydrologic model-independent methods (e.g., Besaw et al., 2010) or to transfer hydrologic model's parameters from gauged to ungauged watersheds (e.g., Heuvelmans et al., 2006). Besaw et al. (2010) used a Generalized Regression Neural Network (GRNN) and a Counter Propagation Neural Network (CPNN) with recurrent feedback loops to connect climate and hydrological data to hourly and daily streamflow in gauged watersheds and used that architecture for ungauged watersheds. They found that the ANNs trained on a climate-discharge record from one watershed are capable of predicting streamflow in a nearby watershed as accurately as the one used for training. Heuvelmans et al., (2006) compared linear regression analysis and a three layer feed forward neural network for estimating the most sensitive parameters of the semi-distributed hydrological model SWAT (Soil and Water Assessment Tool) for ungauged watersheds in Belgium. They found that ANNs can estimate more accurate model parameters than linear regression equations if the physical watershed descriptors of the site under study lie within the range of the descriptor values of the ones used for the construction of the ANNs .

Watersheds' classification can be based on either physiographic characteristics of watersheds or streamflow metrics. Since streamflow series are not available in ungauged watersheds the classification based on watershed physiographic attributes is considered.In this study we will consider three classification scenarios in which watershed clusters are identified as homogeneous regions using nonlinear clustering techniques including Self Organizing Maps (SOMs), standard Non-Linear Principal Component Analysis (NLPCA), and Compact Non-Linear Principal Component Analysis (Compact-NLPCA) on watershed physiographic attributes to classify 90 watersheds into four clusters . The results of these classifications are presented in Table 4-1. It presents the number of watersheds in each cluster, the governing attributes in each cluster along with their ranges and the flow duration curves' slope (Q5/Q95) of majority of watersheds in each cluster. A brief description of the classification techniques is also provided in the appendix. The performance of these nonlinear techniques in watershed classification was compared with principal component analysis and k-means clustering based on runoff signatures (applicable to gauged watersheds) as linear benchmark techniques in a previous study (Razavi and Coulibaly, 2013b). The results suggested that the nonlinear classification techniques on watersheds attributes could be reliable alternative methods for the classification of gauged and/or ungauged watersheds. In this study we apply IDW, MLP, CPN and SVM as regionalization techniques to pre-identified homogenous clusters of watersheds as well as unclassified watersheds to investigate the possible improvement in continuous daily streamflow regionalization. The main objective is to investigate the possible improvement in continuous daily streamflow regionalization by applying nonlinear data-driven approaches to systematically pre-classified watersheds along with different rainfall-runoff models and the combination of them.

Table 4-1 Clusters of homogeneous watersheds identified by SOM, NLPCA and CNLPCA techniques based on watersheds attributes. Ranges of high flow to low flow slope (Q5/Q95) of the majority of watersheds in each cluster are provided (Modified after Razavi and Coulibaly 2013b)

Classification Technique	Cluster	Number of watersheds	Dominant Attributes	Q5/Q95
SOM	C1	43	Latitude , Elevation , Slope	High
	C2	28	Latitude Longitude , >150cm	Moderate
	C3	10	>150cm,Elevation,Longitude	Low
	C4	9	Area ,Slope , Latitude	Low
NLPCA	C1	39	Latitude , Forest, Elevation	High
	C2	33	Latitude Longitude >150cm	Moderate
	C3	11	>150cm, Longitude , Glaciofluvial	Low
	C4	7	Slope , Elevation(28:785 m), Glaciofluvial	Low
CNLPCA	C1	41	Latitude , Longitude , Forest	High
	C2	20	Forest , Rapid , Elevation	Low
	C3	17	Rapid , Forest, Elevation	Moderate
	C4	12	Forest , Rapid , Forest	Moderate

4.3. Study Area and Data

The study area covers 90 natural watersheds across the Province of Ontario, Canada (Figure 4-1), with annual mean precipitation of 400–600 mm in the northern region and 800–1200 mm in the southern part. In the northern regions, the average air temperature ranges approximately between -20°C (in January) and 17°C (in July); and in the southern regions, it ranges between -10°C (in January) and 19°C (in July). Most of the natural watersheds in the northern region are covered with coniferous forest, with gaps of swamp, muskeg, and small lakes, whereas the southern region is dominated by mixed forests (Atlas of Canada, available at http://atlas.nrcan.gc.ca).

Meteorological data, i.e., daily precipitation and air temperature, were obtained from the Canadian Daily Climate Data (CDCD, provided by the Environment Canada). The daily flow data (1976-1994) were obtained from the HYDAT database (Environment Canada, 2004). The climate and streamflow data of 1976-1985 (10 years) are used for models calibration while the data of 1986-1994 (9 years) are used for models validation. The areas of the watersheds range from approximately 100 to 100,000 km^2, representing different types and sizes of watersheds. Watershed attributes used in this study are similar to ones used in Samuel et al, (2011) and Razavi and Coulibaly (2013b). They can be classified as follows: the location of the centroid of the watersheds (i.e., latitude and longitude); the morphology (i.e., mean elevation, mean slope and area); the percentage of area covered by water (the portion of lakes); the land use (the portion of forests); water drainage (i.e., the sum of the percentage of the area covered by rapid and moderate drainage classes); rooting depth (associated to soil depth and available water, i.e., the portion area covered by root depth deeper than 150 cm); and the surface geology (the percentage of region covered by glaciofluvial, glaciodeposit, and rock). Catchment attributes were derived from the digital maps and digital elevation database obtained from the Shuttle Radar Topography Mission (SRTM), available at http://www2.jpl.nasa.gov/srtm/cbanddataproducts.html (Samuel et al. 2011).

Figure 4-1 Location map of selected Ontario watersheds and sample watersheds

4.4. Methodology

An overview of the methodology is provided in a flowchart (see Figure 4-2). The method includes four regionalization approaches: three types of neural networks (i.e. MLP, SVM, CPN), and a spatial proximity method (i.e. IDW) that are applied to the two scenarios of unclassified and classified watersheds using SOM, NLPCA and CNLPCA techniques to transfer the hydrologic model's parameters of gauged watersheds to ungauged ones. The classification techniques are described with details in a previous study (Razavi and Coulibaly, 2013b) and summarized in the appendix. In addition, Table 4-1 presents the final results of the selected classification techniques. The two hydrologic models used to estimate continuous daily streamflow are conceptual rainfall-runoff models described in the next section followed by a brief description of the regionalization techniques and model performance evaluation criteria.

Rainfall-Runoff Models

MAC-HBV

The MAC-HBV (Samuel et al., 2011) is a lumped conceptual rainfall-runoff model, following the structure of the HBV model (Bergström, 1976) which has been widely used in hydrological studies and also in many regionalization studies. The MAC-HBV uses a concept of the HBV model similar to what has been presented earlier by Merz and Blöschl (2004) and modified routing routine following Seibert (1999) with a simplified Thornwaite formula to account for daily potential evapotranspiration (SMHI 2005). The model consists of a snow routine, a soil moisture routine, a response function, and a routing routine. The snow routine represents changes in the snowpack using a simple degree-day concept. The soil moisture routine represents the soil moisture accounting, i.e., changes in soil moisture storage in top soil layer. The response function estimates the amount of runoff from upper zone and lower zone based on the current water storage and the maximum storage. Channel or routing an equilateral triangular weighting function is used to obtain the final streamflow. The parameters of this model are presented in Table 4-2 Detailed description of the MAC-HBV model can be found in Samuel et al. (2011).

SAC-SMA

The SAC-SMA is a conceptual watershed model (Burnash et al., 1973) used by the National Weather Service (NWS) for operational streamflow forecasting and flood warning throughout the United States. This hydrologic model is a conceptual system for modeling the headwater portion of the hydrologic cycle. The first component of the model i.e., rainfall occurring over the basin is considered as falling on two basic areas: the pervious area and impervious area. Pervious area is a permeable portion of the soil mantle and impervious area is a portion of the soil mantle covered by streams, lake surfaces, marshes or other impervious material. This model consists of six state variable reservoirs representing the accumulation of water in two soil zones (upper and lower) in the forms of both “tension” and “free” water. Tension water is considered as water which is closely bound to soil particles and is available for evapotranspiration while free water is the portion of water which is not bound to soil particles and so is free to descend to deeper portions of the soil and move laterally through the soil due to gravitational and pressure forces.

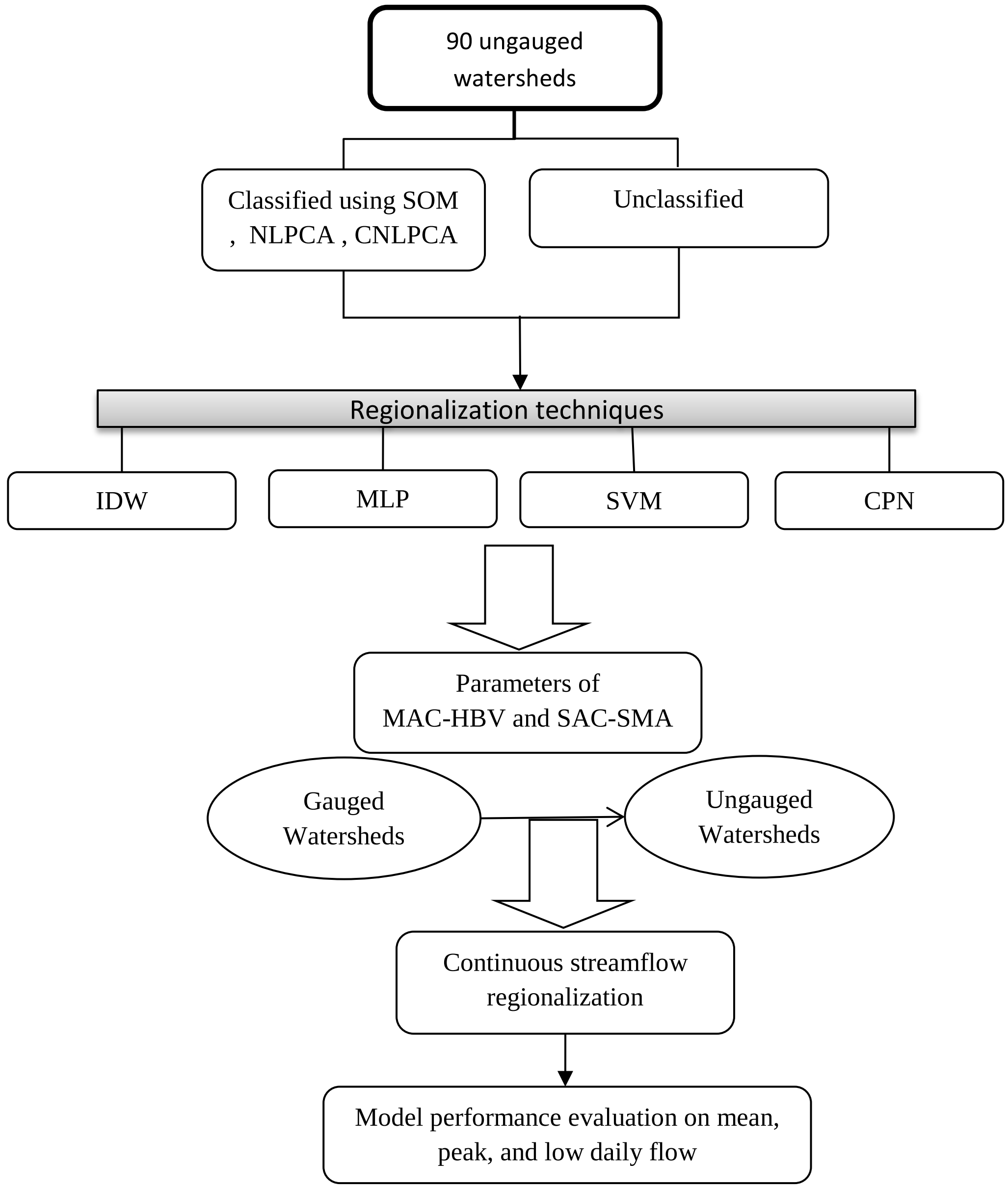

Figure 4-2 Flowchart of methodology showing the four regionalization techniques (IDW, MLP, SVM and CPN) used to transfer the parameters of two hydrologic models (MAC-HBV and SAC-SMA) from gauged to ungauged watersheds considering two scenarios of classified and unclassified watersheds.

Table 4-2 Parameters of MAC-HBV and SAC-SMA models and optimized ranges (using PSO algorithm)

Parameter	Descriptions	Unit	Initial range	Optimized range
MAC-HBV				
tr	Upper threshold temperature, to distinguish between rainfall, snowfall	^{0}C	-1.5 – 2.5	0 – 2.5
scf	Snowfall correction factor	-	0.4-1.6	0.44-1.55
ddf	Degree day factor	mm/(day^{0}C)	0-5	0.5-5
athorn	A constant for Thornthwaite’s equation	-	0.1-0.3	0.1-0.3
fc	Maximum soil box water content	mm	50-800	111-800
lp	Limit for potential evaporation	mm/mm	0.1*fc-0.9*fc	5-717
beta	A non-linear parameter controlling runoff generation	-	0-10	0.25-10
k0	Flow recession coefficient at an upper soil reservoir (for soil moisture exceeds a threshold lsuz value)	days	1_30	1_30
lsuz	A threshold value used to control response routing on an upper soil reservoir	mm	1-100	1_100
k1	Flow recession coefficient at an upper soil reservoir	days	2.5-100	30-100
cperc	A constant percolation rate parameter	mm/day	0.01-6	0.01-6
k2	Flow recession coefficient at an lower soil reservoir	days	20-1000	100-500
maxbas	A triangular weighting function for modeling a channel routing routine	days	1_20	1_17
rcr	Rainfall correction factor	-	0.5-1.5	0.65-1.5
α1	An exponent in relation between outflow and storage representing non-linearity of storage-discharge relationship of lower reservoir	-	0.5-20	0.6-1.5
SAC-SMA				
UZTWM	Upper-zone tension water maximum storage	(mm)	1-150	1-150
UZFWM	Upper-zone free water maximum storage	(mm)	1–150	17–145
LZTWM	Lower-zone tension water maximum storage	(mm)	1-500	1-446
LZFPM	Lower-zone free water primary maximum storage	(mm)	1-1000	1-966
LZFSM	Lower-zone free water supplemental maximum storage	(mm)	1-1000	1-1000
ADIMP	Additional impervious area		0-0.4	0-0.4
UZK	Upper-zone free water lateral depletion rate	(day^{-1})	0.1-0.5	0.1-0.5
LZPK	Lower-zone primary free water lateral depletion rate	(day^{-1})	0.0001-0.025	0.0001-0.025
LZSK	Lower-zone supplemetal free water lateral depletion rate	(day^{-1})	0.01-0.25	0.01-0.25
ZPERC	Maximum percolation rate	-	1-250	1-246
REXP	Exponent of the percolation equation	-	1_5	1_5
PCTIM	Impervious fraction of the watershed area	-	0-1	0-0.1
PFREE	Fraction percolating from upper to lower zone free water storage	-	0-0.6	0-0.6
Rq	Routing coefficient		0-1	0_0.75
ddf	Degree day factor	mm/(day^{0}C)	0-5	0.3-5
scf	Snowfall correction factor	-	0.4-1.6	0.5-1.5
tr	Upper threshold temperature, to distinguish between rainfall, snowfall	0 C	-1.5 – 2.5	0-2.5
athorn	A constant for Thornthwaite’s equation	-	0.1-0.3	0.1-0.3
rcr	Rainfall correction factor	-	0.5-1.5	0.7-1.5
Constant numbers				
RIVA	Riparian vegetation area	-	0	
SIDE	Ratio of the deep recharge to channel base	-	0	
RSERV	Fraction of lower zone free water not transferable to tension water		0.3	

State variables include: Additional Impervious Area Content (ADIMC), Upper-Zone Tension Water storage Content (UZTWC), Upper-Zone Free Water storage Content (UZFWC), Lower-Zone Tension Water storage Content (LZTWC), Lower-Zone Free Primary water storage Content (LZFPC), Lower-Zone Free Secondary water storage Content (LZFSC). The structure of SAC-SMA model used herein is illustrated in Figure 4-3, and the optimized maximum and minimum ranges of each model parameter are presented in Table 4-2. The routing approach used in this model is Nash cascade method and the same snow component and evapotranspiration calculation's method as used in MAC-HBV are added to this model.

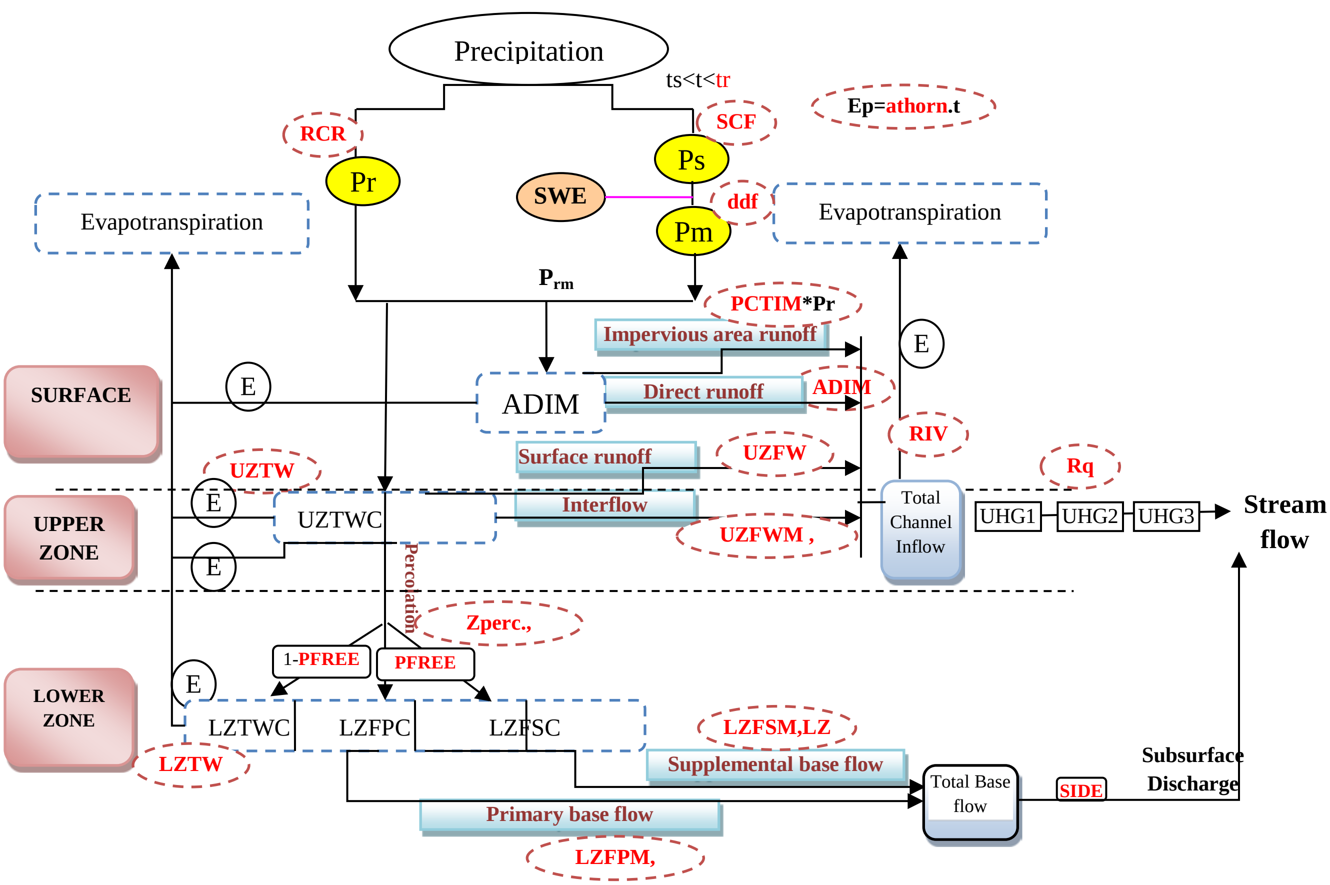

Figure 4-3 Schematic representation of the SAC-SMA model as used in this study showing the model states parameters used. Arrows indicate fluxes between components and the streamflow at the watershed outlet is shown (Adapted after Vrugt et al. 2006)

Model Parameter Optimization

The two rainfall-runoff models are calibrated against observed daily streamflow time series . The time series of 1976-1985 (10 years) are used for models calibration to obtained the optimized parameters while 1986-1994 (9 years) are used for models validation and comparison. The optimization algorithms including Particle Swarm Optimization (PSO) (Eberhar and Kennedy, 1995; Clerc, 2006), Shuffle Complex Efficiency (SCE) (Duan et al. 1994) and Non-Sorted Genetic Algorithm II (NSGA II) (Deb et al. 2001), and a Monte Carlo simulation are used to optimize the parameters of two models. In the Monte Carlo simulation, 100,000 uniformly-distributed random values of the model parameters are selected in their initial ranges and the parameter set which produce the highest model performance is selected as the optimized set of parameters. The criterion of performance evaluation used for all the optimization algorithms is the objective function (NVE) used by Samuel et al. (2011) which addresses mean, low and high flows at the same time:

$$NVE = 0.5NSE - 0.1VE + 0.25NSE_{log} + 0.25NSE_{sqr} \qquad \text{Eq. 4-1}$$

Where

$$NSE = 1 - \left(\frac{\sum_{i=1}^{N} \left(Q_{obs} - Q_{sim}\right)^2}{\sum_{i=1}^{N} \left(Qobs - \overline{Q_{obs}}\right)^2} \right) \qquad \text{Eq. 4-2}$$

$$VE = \frac{\sum_{i=1}^{N} Q_{sim} - \sum_{i=1}^{N} Q_{obs}}{\sum_{i=1}^{N} Q_{obs}} \qquad \text{Eq. 4-3}$$

$$NSE_{sqr} = 1 - \left[\frac{\sum_{i=1}^{N}(Q_{sim}^2 - Q_{obs}^2)^2}{\sum_{i=1}^{N}(Q_{obs}^2 - \overline{Q_{obs}^2})^2}\right] \quad \text{Eq. 4-4}$$

$$NSE_{log} = 1 - \left[\frac{\sum_{i=1}^{N}(\log Q_{sim} - \log Q_{obs})^2}{\sum_{i=1}^{N}(\log Q_{obs} - \overline{\log Q_{obs}})^2}\right] \quad \text{Eq. 4-5}$$

Q_{sim} and Q_{obs} are the simulated and observed streamflow, respectively, and $\overline{Q}_{obs}$ is the average of observed streamflow values and N is the number of data points. The NSE_{log} is better at reflecting the accuracy of low flows; while NSE_{sqr} is better at reflecting the accuracy of high flows. Using this objective function the single-objective algorithms can be useful as a multi-objective one. The model with the highest performance should produce a value close to 1 for NVE and NSE (Nash and Sutcliffe, 1970) and a value close to zero for Volume Error (VE).

Regionalization Techniques

Inverse Distance Weighted (IDW)

IDW is an interpolation technique based on inverse spatial distance of watersheds' centroid. This method is coupled with physical similarity approach as in Samuel et al. (2011), and is recognized as the best regionalization method among the other investigated approaches (i.e. regression-based and physical similarity) for the study area. The spatial distance between watersheds is calculated using latitude and longitude of the watersheds' centroids. The IDW equation (Shepard 1968) used in this study to estimate model parameters in ungauged watersheds is:

$$P_j = \sum_{i=1}^{n} W_i \, p_i \qquad \text{Eq. 4-6}$$

Where n is the number of gauged watersheds; p_i is the model parameter of gauged watersheds; Pj is the model parameter of ungauged watershed; W_i is weight function of each watershed and is calculated as follows:

$$W_i = \frac{({d_i}^{-2})}{\sum_{i=1}^{n}({d_i}^{-2})} \qquad \text{Eq. 4-7}$$

Where d_i is distance from the centroid of the gauged watersheds to the centroid of the ungauged watershed.

First before watershed classification each of the 90 watersheds is assumed to be ungauged in turn and after calculating the weights of other watersheds based on their distance, the model parameters of the ungauged watershed are obtained using the parameters of gauged ones. After classifying the watersheds the weights are calculated within each cluster and model parameters are obtained for each watershed assumed as ungauged based on the distance from other watersheds in the cluster

Multi-Layer Perceptron (MLP)

MLP is a feed forward neural network which maps input data set to output or network target. It is the most widely used data-driven model in hydrologic applications (Maier et al., 2010) and is therefore selected as a benchmark method. The MLP used in this study has one input layer, one hidden layer and one output layer. The neural network toolbox of MATLAB 2012b is used for the MLP model development and computation.

Physiographic watershed attributes (12 attributes) are used as network input's vector and each hydrologic model parameter of MAC-HBV and SAC-SMA , presented in Table 2, as network output in separate networks for 90 samples (watersheds). Data from two third of watersheds are used to train the network and model parameters of the remaining watersheds are obtained from the validation period. To cover all the watersheds, this procedure is repeated three times. For the unclassified watersheds, data from 60 watersheds are used as gauged watersheds to train the network and using the same network architecture, model parameters of remaining 30 watersheds are estimated using their attributes as network's input. This procedure is repeated 3 times so that all the watersheds are considered as ungauged once. For the classified watersheds the same procedure is performed within each cluster separately i.e., two-third of watersheds in each cluster are considered as gauged while the remaining one-third are considered as ungauged watersheds and it is performed three times to encompass all the watersheds in each cluster.

Architecture of the neural network with best performance is achieved by taking the average of Mean Square Error (MSE) of network's output. The network is trained using Bayesian regularization backpropagation training algorithm (MacKay, 1992). Bayesian regularization is a network training process that updates the weight and bias values using Levenberg-Marquard optimization. It minimizes a combination of squared errors and weights, and then determines the correct combination so as to produce a network that generalizes well. A comparison between the networks trained by a regular Levenberg-Marquard and Bayesian regularization algorithms indicated the better performance for the latter. The smallest network MSE was achieved for 3 hidden units for the unclassified watersheds and 2 hidden units for classified ones. Tangent sigmoid ("tansig") function was used as transfer function in both the hidden and output layers. The networks were trained 100 times and the output with highest performance on training data set were selected.

Support Vector Machine (SVM)

Support Vector Machine (SVM) is a neural network based algorithm for solving multidimensional function estimation problems and it was initially developed by Vapnik (1995) for pattern recognition problems and later extended to solve non-linear regression estimation problems by introduction of Vapnik's $\boldsymbol{\epsilon}$-insensitive loss function (Vapnik et al., 1996). Therefore SVMs can be used for classification (Support Vector Classifier – SVC) and regression (Support Vector Regression- SVR). This tool is especially useful for high dimensional input space (in our case 12 catchment attributes) where decision functions are based on nonlinear elements. SVMs apply the structural risk minimization principle which minimizes an upper bound of the generalization error rather than minimizing the training error. Generalization error is bounded by the sum of the training error and a confidence interval term. Therefore, SVMs are expected to result in better generalization performance than other neural network models. Furthermore the solution of SVMs is unique because the training of SVMs is equivalent to solving a linearly constrained quadratic programming, and also it is optimal and absent from local minima, unlike other networks' training which requires non-linear optimization and involves the risk of getting stuck in local minima. The regression function which map a set of data points $\{(xi, di)\}_{i=1}^{n}$ in which xi is the input vector, d_i is the desired target value and n is the total number of data patterns estimated by SVMs and can be approximated by (Tay and Cao, 2001):

$$y = f(x) = w^T \emptyset(x) + b \qquad \text{Eq. 4-8}$$

Where $\emptyset(x)$ maps the input x to a vector in multi feature space. w and b are weight and bias values obtained by minimizing risk function of SVMs (R_{SVMs}) :

$$R_{SVMs\ (C)} = C\frac{1}{n}\sum_{i=1}^{n} L_{\varepsilon}\,(di\ , yi) + \frac{1}{2}\|w\|^2 \qquad \text{Eq. 4-9}$$

Where $L_{\varepsilon}(d, y)$ is ε-insensitive loss function:

$$L_{\varepsilon}(d,y) = \begin{cases} |d-y| - \varepsilon & |d-y| \geq \varepsilon \\ 0 & \text{otherwise} \end{cases} \qquad \text{Eq. 4-10}$$

The MATLAB code of LS-SVMs (Brabanter et al., 2011) is used in this study for support vector regression (SVR) model development. A cross validation procedure is used as a performance measure to determine tuning parameters i.e., regularization and kernel parameters in two steps; first a global optimization technique i.e., Coupled Simulated Annealing (CSA) which determines suitable parameters according to some criterion and parameters which are then given to a second optimization procedure (simplex or grid search) to perform a fine-tuning step. Support vector regression (SVR) has been investigated for hydrological prediction in previous studies but rarely investigated for streamflow prediction in ungauged watersheds. A recent study (Zakaria, 2012) has shown the potential of SVR for streamflow regionalization. Herein the SVM is further investigated as regionalization technique for both classified and unclassified basins, and compared with more advanced techniques such as the counter propagation neural network (CPN).

Counter Propagation Neural Network (CPN)

CPN introduced by Hecht - Nielsen (1987) consists of an input layer, Kohonen layer and output layer called Grossberg outstar. The input layer performs the mapping of the multidimensional input data into lower dimensional array (most often two-dimensional). The mapping is performed by use of competitive learning — often called winner-takes-it-all strategy. The counter propagation algorithm is executed in two phases: a training phase and an operational phase (classification/prediction). The training process of the CPN connects the input vector with N variables (xs=xs,1,…, xs,i,…, xs,N) with the weight vector (wj=wj,1,…, wj,i,…, wj,N) of the neurons in the Kohonen layer. The winning (or central) neuron c is first found among the neurons in the Kohonen layer, then the weights of both Kohonen and output are adjusted according to the pairs of input and target vectors (x, y) using suitably selected learning rate η(t) and neighborhood function $f_{(dj-dc)}$(Kuzmanovski and Novic, 2008) :

$$W_{j,i}^{new} = W_{j,i}^{old} + \eta_t . f_{(dj-dc).}(x_i - W_{j,i}^{old}) \quad \text{Eq. 4-11}$$

$$u_{j,i}^{new} = u_{j,i}^{old} + \eta_t . f_{(dj-dc).}(y_i - u_{j,i}^{old}) \quad \text{Eq. 4-12}$$

Where the difference $(dj - dc)$ is the topological distance between the winning neuron c and the neuron j which weights are adjusted. $W_{j,i}^{old}$ and $W_{j,i}^{new}$are weights of the Kohonen layer before and after its adjustments were performed, while $u_{j,i}^{old}$ and $u_{j,i}^{new}$ are the weights of the output layer before and after the performed adjustments. The CPN MATLAB code developed by Kuzmanovski and Novic (2008) was adapted and used in this study. Similar to MLP, the data set is divided into two parts of training and validation. Attributes and model parameters of two-third of watersheds are used for network's training while the remaining one-third is used for the validation. Performing the same process tree times, all the watersheds are considered as ungauged once. The attributes and parameters were normalized using the maximum and minimum values of attributes and parameters respectively. The best values of parameters of CPN for regression i.e., width and length of network, parameters of rough and fine-tuning training and shape of network were determined by standard trial and error approach.

Model Performance Evaluation

To evaluate the performance of the regionalization models (i.e. combination of regionalization and classification techniques), in addition to mean daily streamflow, the derived daily baseflow time series, peakflow values, streamflow over a threshold value, and monthly flows are estimated. The description of the estimation methods are described as follows.

Baseflow

Baseflow is derived from streamflow series to evaluate models' performance in low flow estimation. Baseflow was separated from total streamflow using a recursive digital filter (Lyne and Hollick, 1979) as follows:

$$f_n = a \times f_{n-1} + 0.5\,(1 + a)(Q_n - Q_{n-1}) \qquad \text{Eq. 4-13}$$

$$Qb_n = Q_n - f_n \qquad \text{Eq. 4-14}$$

Where Qb_n , f_n and Q_n are the baseflow, the filtered quick response and the original streamflow at n_{th} event, respectively, and a is the filter parameter (set to 0.925).

Peak Flow

To evaluate the performance of models for peak flow estimation, usually some threshold values are considered and the error of model in days with flow over that threshold is calculated. Examples of high flow threshold are flow-duration percentile describing the daily mean discharge that is exceeded a given percentage of the time or long term median flow and flows 3, 5,7 or 9 times the long term median flow or 2 times the long term mean flow (Growns and Marsh, 2000). For instance some studies consider (1 to 10 or 15) percent duration flows (U.S. Geological Survey, 2003) as peakflow threshold. We consider 33 percent duration flow as a threshold and the streamflow values above this threshold are considered as high flows. The reason for selecting this threshold is to have almost same number of days with high flow for all watersheds (one-third of data length) and also to obtain a reasonable number of days for error calculation. Volume Error (VE) between the simulated and observed peak flows is calculated for all the simulations. Zero value for VE indicates the best model performance.

4.5. Results

Hydrologic Models' Parameter Optimization

Optimization algorithms including SCE, PSO, NSGA-II and Monte Carlo simulation were applied to calibrate hydrologic models: MAC-HBV and SAC-SMA against observed daily streamflow time series of gauged watersheds for 1976-1985 (10 years) as calibration period and evaluated for 1986-1994 (9 years) as validation period. All variable parameters of MAC-HBV i.e. 15 parameters and all variable parameters (not constant values) of SAC-SMA i.e. 19 parameters presented in Table 4-2 are optimized by changing in their initial ranges while other parameters are kept constant at their average possible value. The initial and optimized ranges of the parameters of the two hydrologic models are presented in Table 4-2.

The box plots of NSE and VE values of the simulated daily streamflow for the validation period using optimized parameters for 90 watersheds for the two hydrologic models are presented in Figure 4-4. Results from PSO and SCE indicate equally superior mean and median of NSE and VE values with less outlier values for PSO compared to other optimization methods. Further analysis on the performance of PSO and SCE was performed by calculating NSE values for daily baseflow and VEs for peak flows. The results indicated almost similar performance but slightly better results for PSO. Therefore, the PSO is selected as hydrologic model optimization method for the regionalization study. Optimized parameters from PSO algorithm for the calibration period (1976-1985) are selected for the regionalization and will be transferred to hypothetical ungauged watersheds.

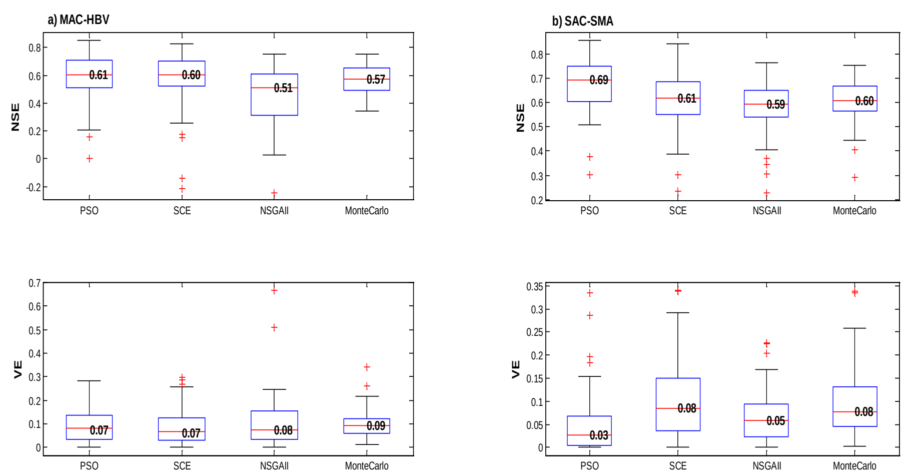

Figure 4-5 Box plots of NSE and VE values of simulated daily streamflow for 90 watersheds across Ontario using calibrated model parameters of a) MAC-HBV, b) SAC-SMA resulted from optimization algorithms: PSO, SCE, NSGAII and Monte-Carlo for validation period (1986-1994).

Continuous Streamflow Regionalization

Daily Streamflow

NSE , RMSE (Root Mean Square Error) and VE values of simulated daily streamflow using the two hydrologic models (SAC-SMA and MAC-HBV) coupled with the four regionalization techniques (IDW, MLP, CPN and SVM) on unclassified and classified homogeneous watersheds using classification techniques (SOM , NLPCA and CNLPCA) for validation period (1986-1994) are calculated. Table 4-3 presents the statistics of NSE values for MAC-HBV and SAC-SMA models coupled with IDW, MLP, CPN and SVR techniques on unclassified and classified watersheds. The mean and median of NSE values for the unclassified watersheds using IDW technique are slightly higher than the corresponding values for the same model coupled with MLP technique and clearly higher than SVM and CPN techniques. These results show that MLP is very competitive with IDW approach. CPN and SVM indicate competitive performance when they are applied on classified watersheds. For both hydrologic models coupled with the four regionalization techniques, the results in average after watershed classification are consistently improved although it might not be the case for some watersheds. For example both MAC-HBV and SAC-SMA models coupled with IDW technique reach their highest performance for classified watersheds using CNLPCA with NSE mean / median of 0.47 / 0.50 and 0.48 / 0.53, respectively. Table 4-5 (a) presents the percent of basins with less than -20% and more than 20% of improvement in RMSE of daily streamflow normalized by long term mean daily streamflow after watersheds' classification. The minus improvements indicate deterioration and imply that watershed classification had negative impact on regionalization performance in some watersheds.

For example the performance of MAC-HBV model coupled with MLP technique indicate <-20% of improvement (deterioration) in normalized RMSE after CNLPCA classification for about 17% of watersheds while this improvement is >20% for 20 percent of watersheds. According to this table, when using CPN as regionalization method, MAC-HBV and SAC-SMA models reach more than 20% improvement in RMSE of daily streamflow for about 39% and 13% of basins after watersheds' classification using NLPCA . In general, results in Table 4-5 (a) indicate that some combinations of hydrologic model, regionalization technique, and basin classification method can yield higher improvement (>20%) in daily streamflow estimation in most of ungauged basins while some other combinations results in deteriorating performance. Two of the combinations (i.e. CPN-NLPCA and CPN-SOM) , which show consistent improvement in daily mean , low and peak flow regionalization using MAC-HBV and SAC-SMA in majority of the watersheds are further analyzed hereafter.

Figure 4-6 (a) and Figure 4-6 (b) demonstrate the spatial distribution of percent of improvement in daily streamflow regionalization using watershed classification techniques, NLPCA and SOM , combined with regionalization technique, CPN with MAC-HBV and SAC-SMA models, respectively. The basins which indicate consistent improvement of ">20%" in daily mean, low and peak flow regionalization are specified with a circle. Furthermore, the hydrographs of observed and simulated daily streamflow using the two hydrologic models coupled with CPN technique on unclassified and classified watersheds for three sample watersheds (specified in Figure 4-1) are presented in Figure 4-7. This figure shows a generally better performance of models after watershed classification.

Daily Baseflow and Peakflow

NSE statistics for daily baseflow are presented in Table 4 4. MLP and CPN become very competitive with the IDW method (in average) when applied to classified basins. In general, the performance of models is superior for daily baseflow compared to daily streamflow. Similar to daily streamflow, the improvements in NSE values of daily baseflow regionalization in average are more significant for CPN and SVR techniques. Table 4 5 (b) presents the percentage of watersheds with less than -20% and more than 20% improvement in VEs of daily baseflow for regionalization models after watersheds' classification. According to this table the baseflow regionalization is improved >20% in high percent of watersheds when using MLP, CPN and SVR techniques after watershed classification. Table 4 5 (c) indicates the percentage of watersheds with less than -20% and more than 20% improvement in VE of daily peak flow. More than 20% improvement in VE of daily peakflow can be achieved in about 61% and 47 % of the watersheds when CPN and SVM are applied respectively to basins classified with NLPCA method while there will be the deterioration of <-20 % in 26 and 19 percent of watersheds , respectively. Figure 4 5 and Figure 4 6 demonstrate the spatial variability of percent of improvement in VE of daily baseflow and peakflow regionalization using watershed classification techniques, NLPCA and SOM, combined with regionalization technique, CPN and MAC-HBV and SAC-SMA models.

Table 4-3 Statistics of NSE values of estimated daily streamflow using MAC-HBV and SAC-SMA models coupled with regionalization techniques: IDW, MLP, CPN and SVM on unclassified watersheds (Unc) and classified watersheds with SOM, NLPCA and CNPLCA for validation perids

Regionalization technique		**IDW**				**MLP**				**CPN**				**SVR**			
Classification technique		Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA
MAC-HBV	Min	-0.75	-0.48	-0.63	-0.14	-2.20	-0.02	-0.25	-0.28	-1.21	-0.47	-0.13	-1.11	-0.82	-0.95	-2.80	-0.89
	Mean	0.44	0.45	0.45	0.47	0.35	0.47	0.43	0.41	0.26	0.41	0.43	0.42	0.29	0.31	0.34	0.33
	Median	0.49	0.48	0.51	0.50	0.43	0.51	0.47	0.45	0.32	0.44	0.46	0.47	0.33	0.36	0.44	0.43
	Max	0.68	0.73	0.69	0.69	0.64	0.68	0.69	0.68	0.72	0.69	0.70	0.70	0.66	0.64	0.68	0.70
SAC-SMA	Min	-1.50	-1.28	-0.41	-0.38	-0.68	-1.07	-0.53	-1.97	-2.52	-1.03	-1.66	-0.70	-3.05	-1.07	-2.85	-0.91
	Mean	0.40	0.45	0.45	0.48	0.40	0.44	0.43	0.45	0.26	0.38	0.39	0.42	0.29	0.34	0.31	0.36
	Median	0.52	0.53	0.53	0.53	0.47	0.52	0.50	0.50	0.40	0.48	0.48	0.49	0.41	0.46	0.46	0.47
	Max	0.70	0.71	0.72	0.71	0.70	0.68	0.70	0.68	0.71	0.69	0.70	0.69	0.68	0.66	0.69	0.67

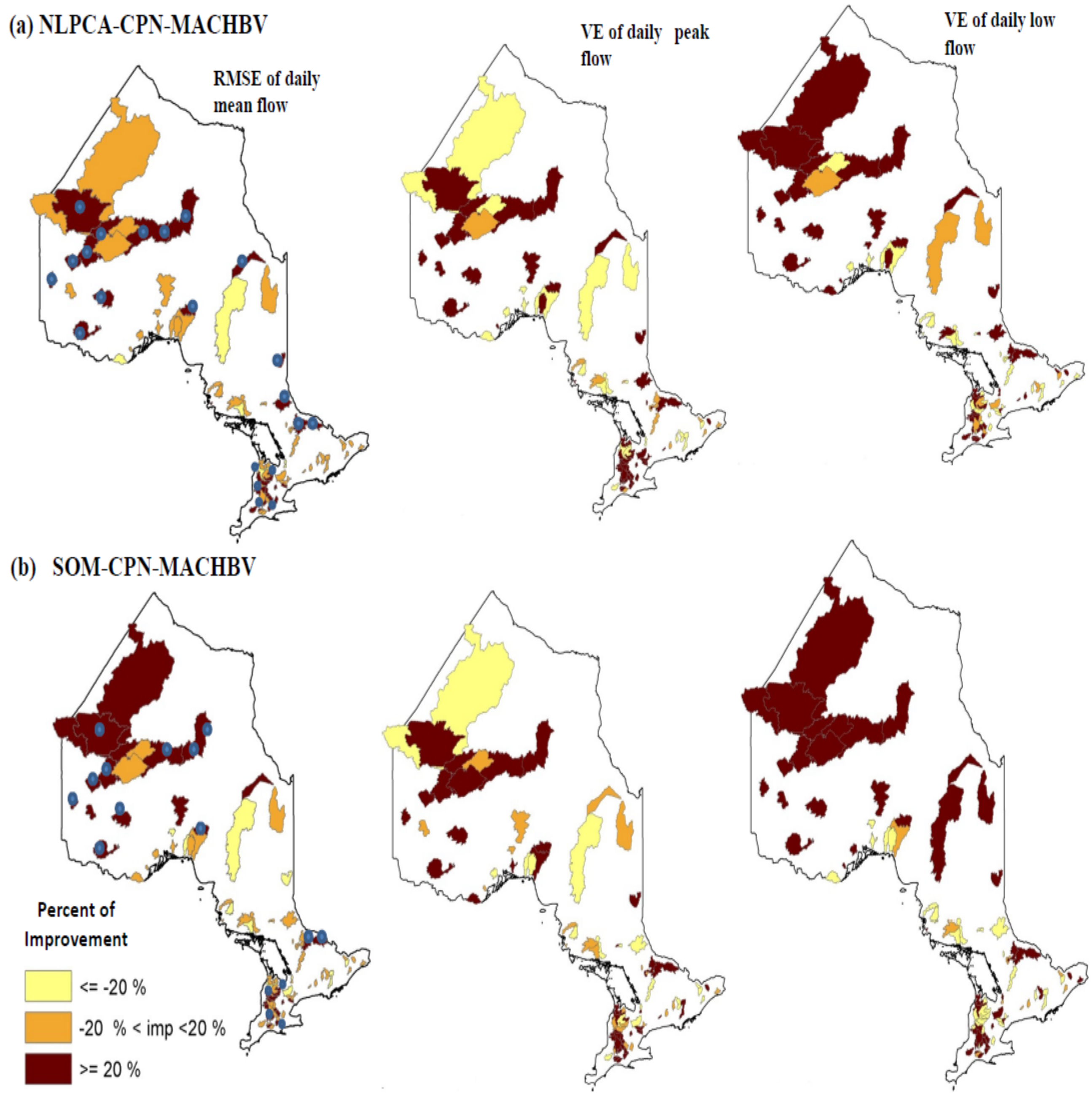

Figure 4-6 Spatial distribution of percent of improvement in daily streamflow , low and peak flow regionalization using (a) NLPCA and (b) SOM classification techniques combined with CPN regionalization technique on MAC-HBV model - small circles specify the basins with consistent improvement of “>20% “in daily mean , low and peak flow regionalization

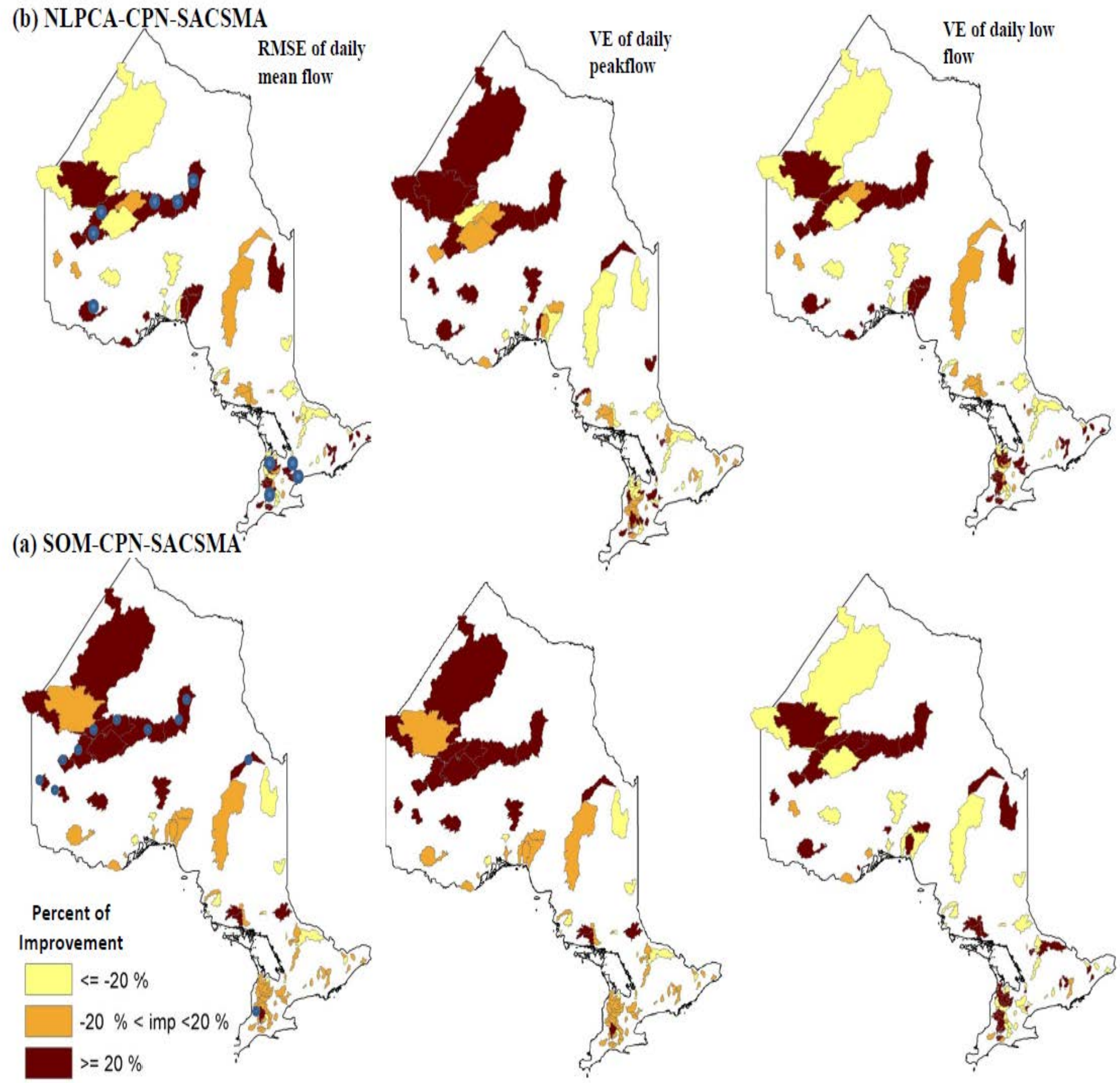

Figure 4-7 Spatial distribution of percent of improvement in daily streamflow , low and peak flow regionalization using (a) NLPCA and (b) SOM classification techniques combined with CPN regionalization technique on SAC-SMA model - small circles specify the basins with consistent improvement of ">20% "in daily mean , low and peak flow regionalization

Table 4-4 NSE statstics of estimated daily baseflow using MAC-HBV and SAC-SMA models coupled with regionalization techniques: IDW, MLP, CPN and SVM on unclassified watersheds (Unc) and classified watersheds with SOM, NLPCA and CNPLCA for validation period (1986-1994

Regionalization technique		IDW				MLP				CPN				SVR			
Classification technique		Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA	Unc	SOM	NLPCA	CNPCA
MAC-HBV	Min	-0.31	-0.43	-0.65	-0.44	-0.73	-0.32	-0.80	-0.29	-1.15	-0.66	-0.40	-0.68	-0.69	-0.55	-1.09	-0.69
	Mean	0.48	0.48	0.48	0.50	0.37	0.50	0.45	0.44	0.27	0.44	0.46	0.47	0.32	0.36	0.38	0.40
	Median	0.51	0.52	0.54	0.54	0.47	0.52	0.51	0.49	0.33	0.47	0.51	0.53	0.36	0.43	0.49	0.49
	Max	0.60	0.73	0.72	0.70	0.66	0.71	0.74	0.70	0.73	0.72	0.72	0.73	0.67	0.67	0.70	0.71
SAC-SMA	Min	-0.91	-0.37	-0.92	-0.36	-1.26	-1.33	-1.41	-1.20	-1.89	-1.32	-0.83	-0.98	-1.37	-0.96	-1.69	-0.80
	Mean	0.46	0.50	0.39	0.52	0.42	0.47	0.45	0.48	0.33	0.42	0.44	0.45	0.34	0.40	0.39	0.41
	Median	0.57	0.58	0.53	0.58	0.52	0.57	0.54	0.52	0.51	0.51	0.53	0.56	0.43	0.50	0.50	0.51
	Max	0.75	0.76	0.78	0.76	0.71	0.72	0.72	0.71	0.73	0.72	0.73	0.72	0.71	0.68	0.70	0.70

Hydrologic implications

According to Figure 4-5 and Figure 4-6 regardless of the hydrologic model used, most of the northern watersheds (except the largest one) reach the improvements of “>20%” after watershed classification consistently for mean, low and high flows, while in small southern watersheds this improvement is less frequent, while in most of the central watersheds and some southern watersheds deterioration is more apparent.

Table 4-5 Percent of basins with percent of improvement in (a) RMSE of daily streamflow (b) VE of daily baseflow (c) VE of daily peakflow less than -20 % or greater than 20 % using classification techniques: NLPCA, CNLPCA and SOM prior to regionalization techniques

(a)

Regionalization	IDW			MLP			CPN			SVM		
Classification	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM
MAC-HBV												
<-20 %	8	3	9	3	17	17	7	43	12	13	14	11
>20 %	4	3	3	16	20	20	39	10	37	16	23	18
SAC-SMA												
<-20 %	12	1	3	7	7	9	8	10	14	11	9	18
>20%	2	11	8	4	10	6	13	17	19	10	9	12

(b)

Regionalization	IDW			MLP			CPN			SVM		
Classification	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SO M
MAC- HBV												
<-20 %	34	16	17	32	38	36	33	44	36	33	34	38
>20 %	41	23	16	53	47	56	56	41	54	51	49	41
SAC-SMA												
<-20 %	51	26	23	34	38	35	33	44	44	31	37	42
>20 %	11	24	23	48	50	41	49	36	48	46	49	46

(c)

Regionalization	IDW			MLP			CPN			SVM		
Classification	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM	NLPCA	CNLPCA	SOM
MAC-HBV												
<-20 %	26	11	12	41	30	22	26	39	20	19	21	29
>20 %	31	19	16	31	43	47	61	36	52	47	47	36
SAC-SMA												
<-20	32	14	17	26	29	18	27	29	44	31	37	42
>20	14	12	11	39	29	42	37	37	48	46	49	46

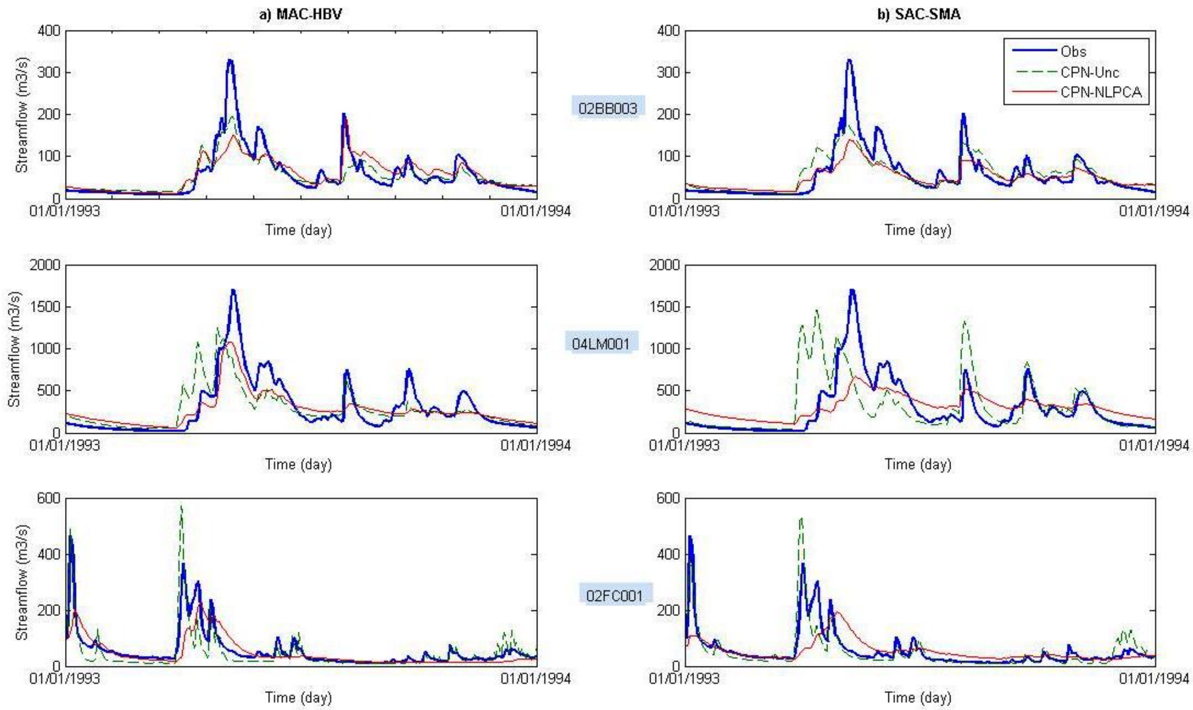

Figure 4-8 Observed and simulated streamflow using hydrologic models: a) MAC-HBV and b) SAC-SMA models coupled with CPN technique on unclassified (CPN-Unc) and classified watersheds using NLPCA (CPN-NLPCA) on three sample watersheds specified on Figure 4-1.

The hydrologic behavior of all basins for the period of 1976-1994 (19 years) is evaluated by determining the timing of monthly low and peakflow and the FDC slope, Q95/Q5 (the proportion of daily low/high daily flow). The shape of FDC's has been shown to be dependent on some watershed attributes such as hydrogeology (Patel, 2006) and drainage for agriculture and urban land use (Smakhtin, 1998). Timing of low and peak flow is governed by climate which acts as a first order control in Ontario (Stainton and Metcalfe 2007), and hydrograph shape is reflected in monthly low and peak flow. The hydrographs of monthly mean flow (Figure 4-9) indicate that in small southern watersheds the minimum monthly flow generally occurs in July/August with early spring snowmelt peakflow in March/April while in northern watersheds minimum monthly flow generally happens in March and spring snowmelt reaches a peakflow in May/June and in central watersheds generally minimum flow happens in February/March and spring snowmelt monthly peakflow occurs in April/May in general.

Figure 4-8 demonstrates the spatial distribution of watersheds' land cover and the amount of FDCs' slope (Q95/Q5). Considering the maps in Figure 5 and 6 , the spatial variability of FDCs' slope (Q95/Q5) (Figure 4-8) indicate that in northern watersheds and part of the southern basins with higher FDC's slope a higher improvement in regionalization can be achieved after watershed classification. The spatial variability of watersheds' land cover (Figure 4-8) indicates that in southern watersheds with lower percent of forest, a higher improvement in streamflow regionalization is achieved compared to the other southern basins. In central watersheds where the most deterioration is apparent, forest cover is relatively high and in watersheds with higher percent of area covered by rapid drainage area and glaciodposits more improvement in regionalization is achieved after watershed classification. Therefore, it can be concluded that among the investigated approaches, nonlinear watershed classification techniques, SOM and NLPCA coupled with CPN as regionalization technique are more likely to improve daily streamflow regionalization in watersheds exhibiting these characteristics: monthly low flow in March, spring snowmelt peak flow in May/June, high FDC's slope (Q95/Q5), less area covered by forest, more area covered by rapid drainage and glaciodeposits.

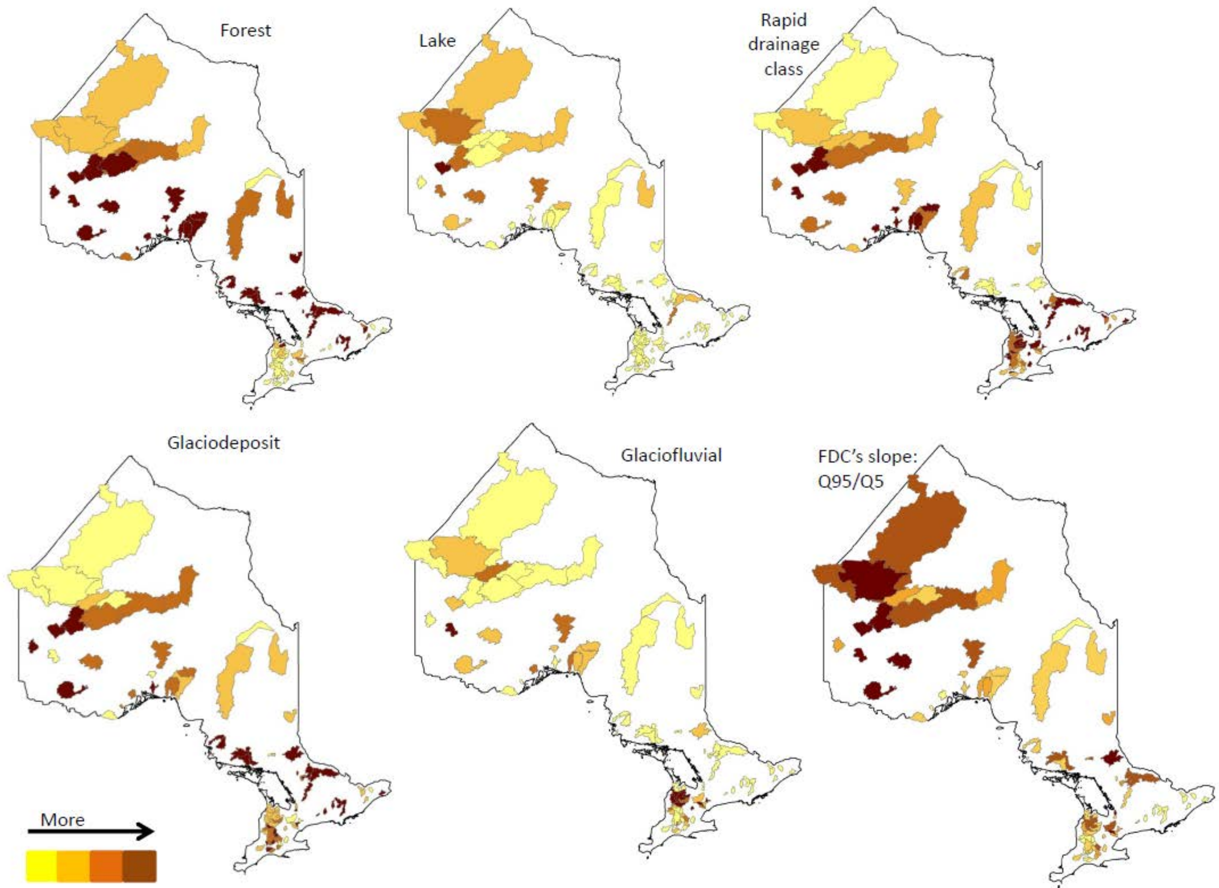

Figure 4-9 Spatial variability of percent of land covered by: Forest, Lake, Rapid drainage, Glaciodeposit, and Glaciofluvial and shape of FDC's slope (Q95/Q5) in selected Ontario watersheds

4.5. Summary and Discussion

In the current study, 90 watersheds across Ontario (Canada) are used to assess the benefit of classified homogenous basins in the regionalization of continuous daily streamflow. Four regionalization techniques (IDW, MLP, CPN, SVM) with two hydrologic models (MAC-HBV, SAC-SMA) are applied to watersheds classified with nonlinear data mining classification techniques (NLPCA, CNLPCA, SOM) and to unclassified watersheds.

The study results show that the MLP model is very competitive with the IDW method which was identified in previous study as the best regionalization method in the study area while the more complicated types of neural networks, CPN and SVR, become competitive when they are applied on classified watersheds. It is shown that the combination of watershed classification and regionalization techniques for a hydrologic model can improve the performance of daily streamflow, baseflow and peakflow regionalization in most of the watersheds while that combination might not be the best one for some of them. For example, each of the hydrologic models coupled with CPN in combination with NLPCA or SOM as a classification technique, reveals a clear improvement in daily streamflow, baseflow and peakflow regionalization. The results of this study reveal that in general these nonlinear data-driven techniques are more likely to improve the performance of daily streamflow regionalization in watersheds with high FDC's slope (Q95/Q5) , less area covered by forest , more area covered by rapid drainage and glaciodeposits, monthly low flow in March and spring snowmelt peak flow in May/June .

Moreover, the improvement of regionalization results for daily baseflow is higher compared to daily streamflow and peak flows. This can have positive implication for environmental flow determination which is based on baseflow. Accurate baseflow estimation in ungauged basins is still a challenging task. This study suggests that appropriate combination of regionalization technique, hydrologic model, and basin classification method, can provide substantially improved streamflow and baseflow estimates at ungauged basins. Furthermore, it appears that neural networks as dynamic nonlinear methods are capable to account for non-stationarity due to urbanisation and climate change in the hydrological modelling for ungauged watersheds. The potential of neural networks for nonstationary hydrological time series modeling has been documented by Coulibaly and Baldwin (2005). Investigation of different types of neural networks in watershed classification and streamflow regionalization as well as their combination with hydrologic models in future studies in regions with different climate pattern and watershed attributes is suggested to further explore the possibility of improvement in hydrologic predictions in ungauged watersheds.

Acknowledgements

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Chapter 5 : Improving Daily Streamflow Regionalization by Multi-Model Combination

Summary of paper IV: Razavi, T., and Coulibaly, P. (2014) . Improving Daily Streamflow Regionalization by Multi-Model Combination. Submitted to Journal of Hydrologic Engineering.

In this research work four regionalization models are developed considering the results of previous papers. That includes:

- IDW-PS : Streamflow values are transferred based on watersheds distance and physical similarity
- MLP-IDW : Streamflow values are transferred using a neural network trained with close and similar watershed attributes ,
- MAC-IDW: Streamflow time series are generated using MAC-HBV model while model parameters are transferred using IDW-PS approach
- SAC-IDW: Streamflow time series are generated using SAC-SMA model while model parameters are transferred using IDW-PS approach

The first two models are data-driven models while the two later ones are hydrologic model- dependent approaches. IDW which is based on the distance between the watersheds and is recognized as the best approach for streamflow regionalization in the area is incorporated to all models. Each model is investigated independently and improved. For example 10 km grid climate data are used to improve each model. The results of the study indicate that:

- IDW-PS perform very well for 90 % of the watersheds while it performs very poor for the rest
- Each model can capture some aspects of the streamflow time series better

Finally a combined model is proposed which combines the output of the four models based on their performance for similar and close gauged watersheds at the same time step. It is shown that this combined model is reliable for all of the watersheds in mean, low and high flow regionalization.

5.1. Abstract

In this study a model combination approach is proposed for improved continuous daily streamflow regionalization. Four regionalization models are developed investigated for continuous daily streamflow. This includes an Inverse Distance Weighted and Physical Similarity (IDW-PS), and a Multilayer Perceptron coupled with IDW-PS (MLP-IDW), and two lumped conceptual hydrologic models namely MAC-HBV (McMaster University Hydrologiska Byråns Vattenbalansavdelning) and SAC-SMA (Sacramento Soil Moisture Accounting) coupled with IDW-PS respectively. In addition to catchment attributes, climate gauged and gridded data are used to improve the regionalization analysis. The comparison of the four models reveals that each of the four models can potentially outperforms other ones for a specific ungauged basin. Although the performance of IDW-PS is superior to other models for most of the watersheds, it does not perform well for all the 90 watersheds selected. The poor performance of IDW-PS for 10 percent of watersheds, which are the large northern and few central ones, can be significantly improved by combining the outputs of the four structurally different regionalization models. Overall, the combined model performs well on all 90 watersheds. The study results also indicate that each model can capture specific characteristics of the flow hydrograph such as low or high flows better than other models. Therefore, the model combination allows taking advantage of the relative strengths of each model. The combination of the four models is more efficient and appears more robust compared to the individual models.

Key Words: Streamflow, Regionalization, model combination

5.2. Introduction

Streamflow time series are required for sustainable water resources management while most of the watersheds over the word are ungauged or poorly gauged. It highlights the need for reliable regionalization models to estimate streamflow time series in ungauged watersheds. In hydrologic studies, regionalization is known as the process of transferring hydrologic information from gauged to ungauged watersheds (Sivaplan et al., 2003). Different approaches have been investigated for continuous streamflow regionalization in the literature (see Razavi and Coulibaly, 2013a for a full review). Continuous daily streamflow regionalization can be conducted through hydrologic models or data-driven approaches. . In the first category the parameters of hydrologic models are transferred from gauged to ungauged watersheds and streamflow time series for ungauged watersheds are estimated/predicted through hydrologic models. In the second category streamflow time series of ungauged watersheds are estimated/predicted through data-driven approaches initially developed for gauged watersheds using catchment attributes or streamflow time series.

In order to reduce the uncertainty of hydrologic predictions in gauged watersheds some studies have investigated multi-model combination approaches. Different studies have shown that using multiple models with different structures can improve the reliability of predictions and reduce the uncertainty of hydrologic predictions (e.g. Li and Sankarasubramanian, 2012; Velazquez et al., 2010; Coulibaly et al., 2005 ; etc.). To combine the outputs of multiple models, different approaches have been studied such as simple or weighted averaging as well as some more complicated approaches such as Artificial Neural networks (Shamseldin et al., 1997) and first-order Takagi-Sugeno method (Xiong et al., 2001) . The most common and popular approach of combining outputs of multiple hydrologic models is a weighted averaging approach due to its understandable basis and high efficiency. However, the optimal selection of weights remains a challenge. Li and Sankarasubramanian (2012) investigated two weighted averaging methods to combine two hydrologic models for improved prediction of monthly flow discharge. In the first one a dynamic-weighting approach determines weights based on the inverse value of models' error at each time step while the second method is based on a static optimized weighting approach that assigns weights to individual models by minimizing the errors over calibration period. They found a superior performance for the second approach. Coulibaly et al. (2005) proposed a static weighting approach that assigns weights based on the variance and correlation of model errors in the whole calibration period to combine outputs of a conceptual hydrologic model, a neural network model, and a nearest-neighbor model for improved daily reservoir inflow forecasting. Most of the studies of model combination in ungauged watersheds generate ensemble predictions using multiple rainfall-runoff model parameter sets in order to account for uncertainty stem from model parameters (e.g. McIntyre et al., 2005 ; Randrianasolo et al., 2010). For example, McInyre et al. (2005) proposed an ensemble modeling and model averaging for streamflow prediction in ungauged basins that selects candidate models based on their performance for gauged watersheds and weights them accordingly. In a very few studies multiple structures of models are combined for prediction in ungauged basins (e.g. Goswami et al., 2007 ; Exbrayat et al., 2011) . For example, Exbrayat et al. (2011) combined the outputs of five rainfall-runoff models using a data-fusion and weighting approach for daily runoff prediction at an ungauged basin.

In the current study, the two main categories of regionalization approaches including hydrologic-model-independent (data-driven) and hydrologic-model-dependent models are investigated for continuous daily streamflow regionalization. Since the distance between gauged and ungauged watersheds is identified as a key factor in our previous regionalization studies, it is incorporated in all models to improve the results. In the first category (data-driven approaches) Inverse Distance Weighted and Physical Similarity (IDW-PS) and improved Multilayer Perceptron with IDW-PS (MLP-IDW) and in the second category two lumped conceptual hydrologic models including MAC-HBV (Samuel et al., 2011) and SAC-SMA (Burnash et al., 1973) coupled with IDW-PS for transferring hydrologic models (MAC-IDW and SAC-IDW) parameters, are applied to 90 Ontario watersheds pre-classified in four homogeneous clusters. Finally, to take advantage of the strengths of all models and reduce uncertainty a model combination approach is proposed to improve the regionalization results.

5.3. Study Area and Data

The study area covers 90 watersheds across Ontario (Canada) with various areas ranging from 100 to 100000 km^2 spread in northern, southern and central regions. A full description of the study area can be found in Razavi and Coulibaly (2013b). Two types of meteorological data i.e. gauged and gridded daily precipitation and air temperature are used in this study. Gauged daily precipitation and temperature time series of the closest climate station to the watersheds' centroids were obtained from the Canadian Daily

Climate Data (CDCD), provided by Environment Canada and also 10 km grid precipitation and temperature time series are extracted from interpolated climate data prepared by Natural Resources Canada / Canadian Forest Service (Hutchinson et al. 2009). The daily flow data were obtained from the HYDAT database (Environment Canada, 2004) for the period of 1976-1994 but the lengths of time series are set to

be equal to the days with no missing values of streamflow for 90 watersheds during the whole period which is almost 1246 subsequent days (May 1991-December 1994) to train and validate the MLP-IDW model and also compare the results of all models for subsequent equal days.

5.4. Methodology

Four regionalization approaches investigated in this study including IDW-PS, MLP-IDW, MAC-IDW and SAC-IDW (summarized in Table 5-1) and the model combination approaches described in the following sections, are applied to four hydrologic homogeneous clusters of watersheds. The clusters are identified by Compact Nonlinear Principal Component Analysis (CNLPCA) in a previous study (Razavi and Coulibaly, 2013b) which classifies 90 Ontario watersheds into four clusters with 20 , 17 ,12 and 41 watersheds in each cluster based on their physical attributes such as latitude , longitude , area , elevation , slope and land surface cover.

Table 5-1 Individual regionalization models

Four regionalization models			
IDW-PS	**SAC-IDW**	**MAC-IDW**	**MLP-IDW**
Takes the inverse distance weighted average of daily streamflow values of three most similar gauged watersheds to ungauged ones ("donor" watersheds) inside each cluster.	Takes the inverse distance weighted average of parameters of SAC-SMA model of gauged "donor" watersheds for the ungauged ones inside each cluster to estimate daily streamflow.	Takes the inverse distance weighted average of parameters of MAC-HBV model of gauged "donor" watersheds for the ungauged ones inside each cluster to estimate daily streamflow.	Trains a multilayer perceptron for each ungauged watershed using attributes and climate data of gauged "donor" watersheds inside each cluster and validate the network with inputs from ungauged watershed to estimate daily streamflow.

Hydrologic-model-independent approaches

This category includes approaches which estimate streamflow time series through data-driven techniques rather than hydrologic models .They are IDW-PS and MLP-IDW.

Inverse Distance Weighted and Physical Similarity (IDW-PS)

Inverse Distance Weighted (IDW) is an interpolation technique based on the spatial distance of watersheds. According to this approach the weight gets higher for closer watersheds and less for remote ones. The IDW equation (Shepard, 1968) is used to calculate the weight of other watersheds in a cluster on a specific one as follows:

$$W_i = \frac{(d_i{}^{-2})}{\sum_{i=1}^{n}(d_i{}^{-2})} \qquad \text{Eq. 5-1}$$

Where d_i is the spatial distance between watersheds and is calculated using latitude and longitude of the watersheds' centroid, i indicate a specific watershed while n is the number of total watersheds in the cluster. Physical similarity is a method that identifies the most similar watersheds to a specific one within the cluster in terms of some physical attributes of watersheds. Seven catchment attributes with higher streamflow predictive power are selected among 12 attributes. They are latitude, longitude, percentage of the mean slope, average elevation, and portion of area covered by rooting depth deeper than 150cm, by forest and by glaciofluvial deposits (Samuel et al., 2011). IDW-PS method identifies the three most physically similar and closest gauged watersheds to a specific ungauged one within a cluster and take the inverse distance weighted average of their streamflow time series according to the following equation:

$$Q_j = \sum_{i=1}^{n} w_{ij} Q_i \qquad \text{Eq. 5-2}$$

Where Q_j is the value of daily streamflow of the ungauged watershed and w_{ij} is the weight of gauged watershed i on ungauged watershed j and Q_i is the streamflow value for each gauged "donor" watershed and n is the total number of gauged "donor" watersheds ("donor" implies to the gauged watersheds that their streamflow or model parameters are used in statistical analysis for transferring to ungauged watersheds) which is three in this case. Therefore, in each cluster each watershed is considered as ungauged once and daily streamflow time series are estimated for all watersheds assumed as ungauged within each cluster.

Improved Multi-Layer perceptron (MLP-IDW)

A three layer feed-forward neural network is applied to estimate daily streamflow time series of watersheds in homogenous clusters. The model inputs include: daily precipitation time series, daily temperature time series and seven catchment attributes as used in IDW-PS approach (previous subsection), number of months as logical inputs to account for seasonal variability while model output or target is set to be daily streamflow time series. Tangent sigmoid ("tansig") function was used as transfer function in the hidden layer and a linear transfer function in the output layer. Each network is trained

250 times using Levenberg-Marquat training algorithm with five hidden units and the network with the best performance for training step (gauged watersheds) is selected to account for random weights and bias values and ensure a proper network training. The inputs and target from gauged watersheds are used to train the neural network and then inputs of hypothetical ungauged watershed are used in validation period to estimate streamflow values. The length of streamflow time series for both training (gauged watersheds) and validation (ungauged watersheds) periods are equal to the 1246 subsequent days (May 1991-December 1994). After selecting the gauged "donor" watersheds, catchment attributes and time series of daily precipitation and temperature and the months (logical input) of the gauged watersheds are used as model inputs and their daily streamflow time series are used as model target to train the network. In the validation period the model inputs from ungauged watershed are inputted to the trained network to get the model output or daily streamflow time series. To select the gauged "donor" watersheds for each hypothetical ungauged watershed, three most similar and close watersheds inside each cluster are selected using IDW-PS criterion. IDW-PS is used here because the watersheds which have similar attributes and close location have the most similar network inputs and with more similarity in network inputs, it is expected to achieve better network output. To improve the performance of MLP model, several actions are taken. First, IDW-PS method as described in previous subsection is used to estimate streamflow time series of ungauged watershed for one year to be used as model output in training period while inputs from ungauged watershed i.e. catchment attributes, month as logical input, precipitation, temperature time series are inputted to the network. The performance of the network is assumed to be improved if in the training step the

inputs or part of the inputs of ungauged basin can be presented to the network. As the second improvement action, more accurate climate data i.e. 10km grid climate dataset are used in both training and validation periods. The average of 10 km grid climate data for each watershed is used instead of climate data of the closest meteorological station to the centroid of watersheds. Last, the ensemble averaging approach based on the performance of ensemble networks in the training period is used. Initially, the network for each ungauged watershed was trained 250 times to account for variability in random weights and bias values and the network with best performance in streamflow regionalization for training period or gauged "donor" watersheds in average was selected among multiple trained networks. Since some of the model realizations which have not shown the best performance in the training period but still might produce best results in validation period (for ungauged watershed) are left out , to account for those model realizations an ensemble modeling approach is used to take the weighted average of model outputs which pass a performance threshold in training period. The threshold value is set to be 90 percentile of NSE values which encompass the best 10 percent of all model realizations (the top 25 out of 250). Weights are defined based on NSE values of all 25 best outputs using a linear decreasing function.

Hydrologic-model-dependent methods

Two lumped hydrologic models including MAC-HBV (Samuel et al., 2011) and SAC-SMA (Burnash et al., 1973) are used to estimate daily streamflow in the hypothetical ungauged watersheds within each cluster. The MAC-HBV follows the structure of the HBV model (Bergström, 1976) with modified routing routine following

Seibert (1999) with a simplified Thornwaite formula to account for daily potential evapotranspiration. The model consists of a snow routine, a soil moisture routine, a response function, and a routing routine. Full description of this model can be found in Samuel et al. (2011). The SAC-SMA is widely used by the National Weather Service (NWS) for operational streamflow forecasting and flood warning throughout the United States (VRUGT et al. 2006). This hydrologic model is a conceptual system for modeling the headwater portion of the hydrologic cycle. The first component of the model i.e., rainfall occurring over the basin is considered as falling on two basic areas: the pervious area and impervious area. It consists of a Nash cascade routing method and the same snow component and evapotranspiration calculation methods as used in MAC-HBV are added to this model. The optimized parameters of hydrologic models are transferred from gauged to ungagged watersheds using IDW-PS approach. Each watershed is considered as ungauged once while the three most similar watersheds within the cluster are considered as gauged and optimized model parameters of the selected gauged watersheds are transferred to the ungauged one using IDW averaging method. The optimized parameters using Particle Swarm Optimization (PSO) (Eberhar and Kennedy, 1995) for both SAC-SMA and MAC-HBV are used in this study. In the first experiment, the gauged climate data of the closest station to watersheds' centroid is used for each watershed. To improve the accuracy of results, 10 Km daily gridded climate data are used in the second experiment.

Model combination

To reduce the uncertainty of regionalization results and use all the information provided by different model structures, a weighted averaging approach is used to take the weighted average of model outputs of SAC-IDW, MAC-IDW and MLP-IDW for each time step in the first experiment and all the four models in the second experiment. The weight assigned to model i at time step t ($w_{i,t}$) is determined based on the absolute value of error of each model applied to the gauged "donor" watersheds (in average) at each time step (Li and Sankarasubramanian 2012):

$$w_{i,t} = \frac{1/e_{i,t}}{\sum_{i=1}^{I} e_{i,t}} \qquad \text{Eq. 5-3}$$

Where t is the time step (i.e. day) , i indicates individual models while I is the total number of multiple models and $e_{i,t}$ is the absolute value of error of each model when applied on gauged "donor" watersheds (in average) at each time step. To combine the outputs of the individual models for an ungauged watershed, each basic model i.e. SAC-SMA, MAC-HBV, MLP and IDW-PS is first applied to the gauged "donor" watersheds to estimate daily streamflow and its average error on each day is calculated, then a weight based on this error is assigned to model output for the ungauged watershed on the same day. To apply individual models to each gauged "donor" watershed, SAC-SMA and MAC-HBV used the optimized model parameters of the watershed and MLP is trained with two-third (May1991- Sep. 1993) and validated with one-third (Oct. 1993- Dec. 1994) of data-length of the watershed and IDW-PS took the distance weighted average of the three most similar and close watersheds to the ungauged watershed.

Model evaluation criteria

Nash-Sutcliffe Efficiency (NSE) (Nash and Sutcliffe, 1970) and Root Mean Square Error (RMSE) are used to evaluate the model performance in continuous daily streamflow regionalization. NSE is presented in Eq. 5-4 and RMSE in Eq. 5-5:

$$NSE = 1 - \left(\frac{\sum_{i=1}^{N} (Q_{obs} - Q_{sim})^2}{\sum_{i=1}^{N} \left(Qobs - \overline{Q_{obs}}\right)^2} \right) \qquad \text{Eq. 5-4}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (Q_{obs} - Q_{sim})^2}{N}} \qquad \text{Eq. 5-5}$$

Where Q_{sim} and Q_{obs} are the simulated and observed streamflow, respectively, and $\overline{Q}_{obs}$ is the average of observed streamflow values and N is the number of data points.

Uncertainty analysis

The uncertainty analysis in this study focuses on uncertainty associated with the structure of individual regionalization models. Subsequently, it is shown that the combination model of the four individual models which is based on the average of all model outputs is more robust and reliable compared to other models.The uncertainty limits of the combined model as well as individual models can be assessed by generating possible acceptable ensemble outputs of individual models. Four acceptable realizations of each individual model are generated for each watershed assumed as ungauged. The process of generating ensemble outputs for each regionalization model is summarized in Table 5-2. To generate ensemble outputs of SAC-IDW and MAC-IDW, four sets of optimized model parameters of the “donor” gauged watersheds are transferred to ungauged watershed using IDW-PS approach. Parameter sets of each model are optimized in a previous study using optimization algorithms including Particle Swarm Optimization (PSO) (Eberhar and Kennedy, 1995), Shuffle Complex Efficiency (SCE) (Duan et al., 1994) and Non-Sorted Genetic Algorithm II (NSGA II) (Deb et al., 2001) and a Monte Carlo simulation approach. To generate ensemble outputs of MLP-IDW, the four best trained networks among 200 trained networks based on their performance for training period (or gauged “donor” watersheds) in terms of NSE are selected to estimate streamflow for the ungauged watershed. Finally to generate ensembles of IDW-PS model, for each ungauged watershed, the IDW weighted average of streamflow values of four different groups of three gauged “donor” watersheds within each cluster is taken. Therefore, 4×4 (16) estimated hydrographs are generated for each ungauged watershed. The minimum and maximum limits of ensemble hydrographs are considered as uncertainty bounds for each hypothetical ungauged watershed.

Table 5-2 Approaches to generate four ensemble outputs of each regionalization model

Regionalization Model	Ensemble modeling approach
SAC-IDW and MAC-IDW	Transfer the four sets of optimized model parameters by PSO, SCE,NSGA II and Monte Carlo optimization algorithms from gauged “donor” watersheds to the ungauged one and estimate daily streamflow
MLP-IDW	Select the outputs from the best four trained networks among 200 ones based on their performance for the gauged “donor” watersheds
IDW-PS	Take the distance weighted average of streamflow values of four different groups of three gauged “donor” watersheds

5.5. Results and Discussion

IDW-PS and MLP-IDW

IDW-PS is applied to all watersheds of the four clusters assumed as ungauged once. The NSE statistics of this method (Table 5-3) indicate a very good performance of IDW-PS model in average for all clusters of watersheds. MLP-IDW is trained with three similar and close watersheds to each ungauged watershed in each cluster and validated for the ungauged watershed for 1991-1994. As described in Methodology several actions are taken to improve the results of this model. The NSE values of estimated daily streamflow time series using MLP-IDW method before and after the improvement actions are presented in Table 5-3. According to this Table, the performance of the MLP-IDW model is significantly improved after the improvement actions although it can be slightly improved further by using grid climate data or ensemble weighted averaging of outputs. Therefore, it can be assumed that since neural networks learn the pattern of input-target in training period and use the same network to generate output in validation period, using the same type of climate data in both training and validation periods the best performance of model remains the same and since even ensemble weighted averaging could improve the results slightly it can be assumed that the maximum potential performance of the neural network is achieved and the ensemble weighted averaged outputs is taken for further analysis because it yields slightly better results in average for all clusters .

SAC-IDW and MAC-IDW

Comparison of the four regionalization models including SAC-IDW, MAC-IDW, MLP-IDW and IDW-PS (Table 3-3 and

Table 5-4) indicates that in average in all the four clusters IDW-PS outperforms other models. The parameters of the two conceptual hydrologic models i.e. SAC-SMA and MAC-HBV of ungauged basins are estimated using IDW-PS on three most similar watersheds within each cluster. Initially climate data from the closest station to centroid of watersheds are used as models' input. To see if higher accuracy of climate data (i.e. 10 km grid daily climate data) can improve the regionalization results using hydrologic model, average precipitation and temperature time series over all grids inside each watershed are used as model inputs in another experiment. The results of comparison between SAC-IDW and MAC-IDW using climate data of the closest climate station to centroid of watershed and average grid climate data is presented in Table 3-4. According to this Table the performance of MAC-IDW model is almost competitive with SAC-IDW in general and the average value of grid climate data can improve the regionalization results in clusters 3 and 4 using both models and cluster 1 using MAC-IDW. The improved results by using grid climate data are used for further analysis.

Table 5-3 NSE statistics of continuous daily streamflow regionalization using IDW-PS model and MLP-IDW model (1. MLP-IDW model before improvement actions (MLP) 2. Adding IDW-PS simulated streamflow and input from ungauged watershed to training dataset (MLP1) 3. Using average grid climate data (MLP2) 4. Ensemble weighted averaging of outputs (MLP3))

NSE statistics	Cluster 1 (20 basins)					NSE statistics	Cluster 2 (17 basins)				
	IDW-PS	MLP	MLP1	MLP2	MLP3		IDW-PS	MLP	MLP1	MLP2	MLP3
Min	-0.60	-23.7	-0.21	-0.34	-0.14	Min	-0.13	-9.97	0.13	0.13	0.03
Average	0.37	-1.34	0.11	0.14	0.15	Average	0.64	-1.08	0.34	0.35	0.34
Median	0.48	0.11	0.13	0.16	0.14	Median	0.80	-0.13	0.33	0.34	0.36
Max	0.88	0.39	0.53	0.46	0.48	Max	0.95	0.52	0.60	0.55	0.58
NSE statistics	Cluster 3 (12 basins)					NSE statistics	Cluster 4 (41 basins)				
	IDW-PS	MLP	MLP1	MLP2	MLP3		IDW-PS	MLP	MLP1	MLP2	MLP3
Min	-0.36	-2.15	-0.02	-0.10	-0.18	Min	-0.09	-35.5	-0.05	0.10	0.032
Average	0.51	-0.23	0.32	0.32	0.28	Average	0.48	-1.27	0.23	0.24	0.23
Median	0.67	-0.12	0.31	0.33	0.31	Median	0.54	0.08	0.20	0.21	0.19
Max	0.88	0.46	0.64	0.59	0.56	Max	0.77	0.54	0.68	0.65	0.66

Table 5-4 NSE statistics of regionalization results using MAC-IDW and SAC-IDW with climate data from center station (Cent) and average gridded climate data (Aveg) in four clusters of watersheds

	Cluster 1 (20 basins)				Cluster 2 (17 basins)			
NSE statistics	MAC-IDW		SAC-IDW		MAC-IDW		SAC-IDW	
	Cent	Aveg	Cent	Aveg	Cent	Aveg	Cent	Aveg
Min	-0.68	-0.55	-0.69	-0.86	-0.12	-0.13	-0.15	-0.02
Mean	0.30	0.36	0.37	0.28	0.56	0.52	0.57	0.50
Median	0.33	0.43	0.45	0.32	0.61	0.62	0.62	0.51
Max	0.77	0.78	0.74	0.72	0.83	0.79	0.73	0.70
	Cluster 3 (12 basins)				Cluster 4 (41 basins)			
NSE statistics	MAC-IDW		SAC-IDW		MAC-IDW		SAC-IDW	
	Cent	Aveg	Cent	Aveg	Cent	Aveg	Cent	Aveg
Min	0.19	0.04	-0.24	-0.11	0.12	0.06	-0.09	0.09
Mean	0.42	0.54	0.37	0.50	0.54	0.58	0.48	0.56
Median	0.44	0.57	0.46	0.57	0.58	0.61	0.54	0.60
Max	0.61	0.76	0.64	0.71	0.81	0.84	0.77	0.80

Comparison of the individual regionalization models and model combination

The performance of individual models for different regions is analysed . Table 5-5 summarizes the performance of the models in different clusters along with specific characteristics and the slope of flow duration curve (high/low: Q5/Q95) of the majority of watersheds in each clusters. For example MLP-IDW and IDW-PS reach their best performance in clusters 2 and 3, while SAC-IDW and MAC-IDW reach their best performance in groups 4 and 2, and in cluster 1 MAC-IDW and IDW-PS perform better compared to other models. It can be concluded that in large northern watersheds with low Q5/Q95, MAC-IDW and IDW-PS perform better than other models while in small southern watersheds with high Q5/Q95, SAC-IDW and MAC-IDW perform better than data-driven models and in watersheds with low elevation, small forest area and moderate Q5/Q95 data-driven models i.e. MLP-IDW and IDW-PS performs better compared to other watersheds.

Table 5-5 Models with best performance and some governing characteristics of each cluster

Clusters	**Best models**	**Q5/Q95**	**Specific characteristics**
C1 (20 basins)	MAC-IDW , IDW-PS	Low	Large northern watersheds
C2 (17 basins)	MLP-IDW, IDW-PS	Moderate	Low elevation
C3 (12 basins)	MLP-IDW, IDW-PS	Moderate	Small forest area
C4 (41 basins)	SAC-IDW , MAC-IDW	High	Small southern watersheds

To take advantage of the strengths of each model, the outputs of individual models are combined based on their performance for gauged watersheds for each time step using weighted averaging approach. Weight of each model is specified based on its average absolute error for gauged “donor” watersheds at the same time step (day) using Eq. (3). First the outputs of the three poorer models i.e. SAC-IDW, MAC-IDW and MLP-IDW are combined to see if that can compete with IDW-PS. Table 5-1. a and b present number of basins with NSE values greater than 0.5 and less than 0.1 and

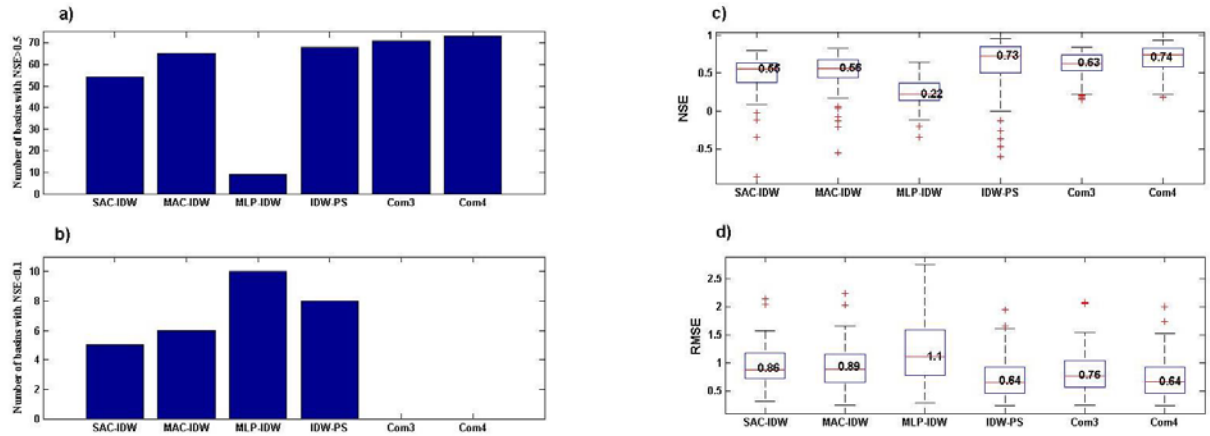

Figure 5-1. c and d present the boxplots of NSE and RMSE values for all the 90 watersheds using individual regionalization and the combined models. It can be seen that with combined models, no watershed has NSE value less than 0.1, while most of them produce NSE value greater than 0.5. The median and mean values of NSE and RMSE are higher and lower respectively for the IDW-PS and combined model of four individual models, but the box plots indicate less outliers for combined model compared to IDW-PS and other models.

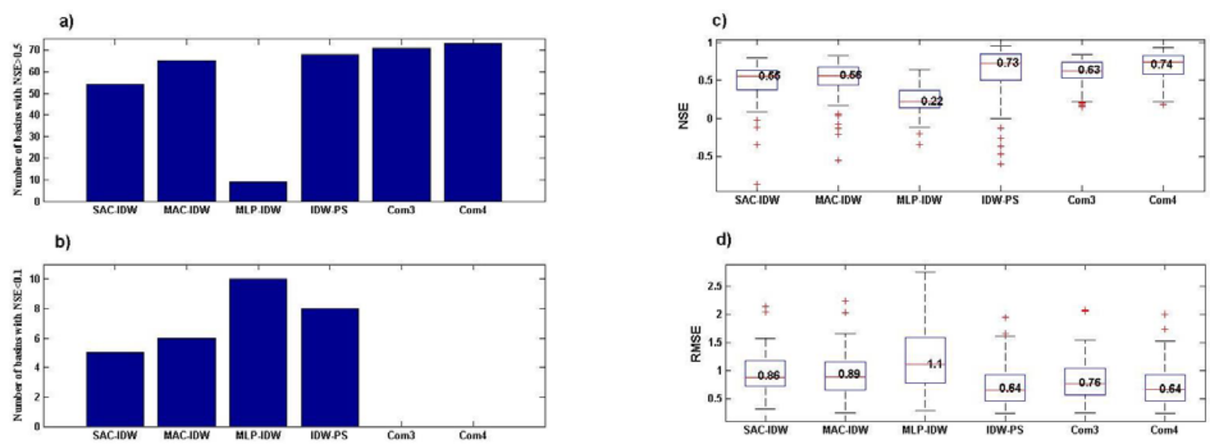

Figure 5-1 Boxplots of NSE and RMSE value of daily streamflow regionalization results using: SAC-IDW, MAC-IDW, MLP-IDW, IDW-PS and combination models of the first three (Com3) and combination of the four models (Com4)

Therefore, the combination of four individual models is more robust compared to individual models. Scatterplots of observed vs simulated daily flow using individual regionalization models along with their combination models for all the 90 watersheds (Figure 5-2) reveal the performance of each model in low, high and mean daily flow regionalization. It can be seen that when the daily flow gets higher the distance between points and observed vs simulated line gets higher for all single models which indicates higher errors. However, for the combined models and IDW-PS, points are spread around the observed vs. simulated line more evenly in general. MAC-IDW indicates lower error for low flows compared to SAC-IDW and MLP-IDW, while SAC-IDW indicates less correlation of errors for high flows compared to the two other models.

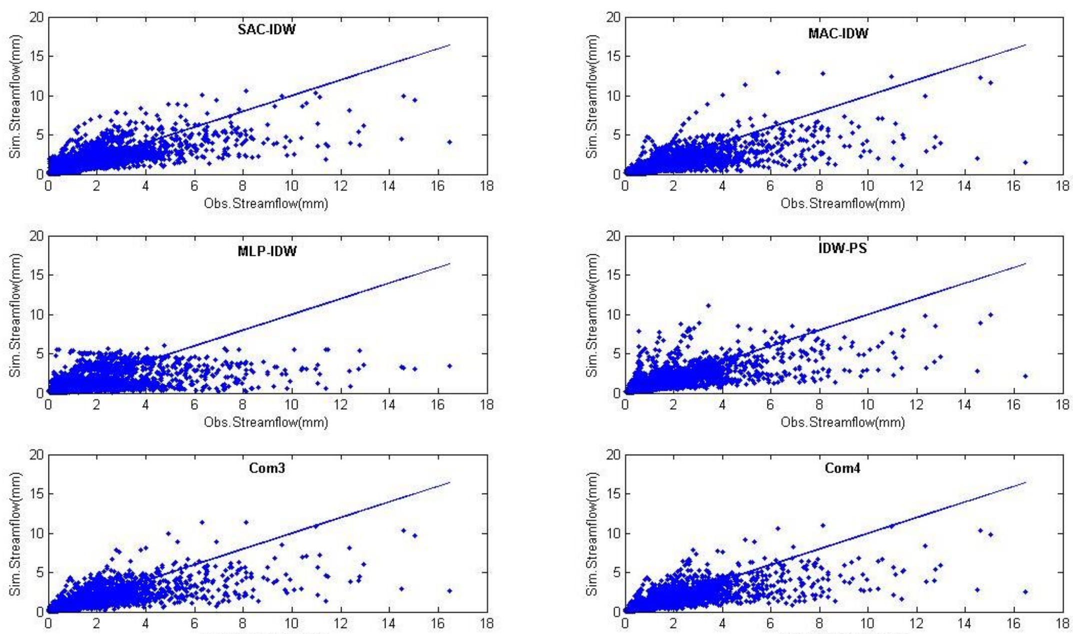

Figure 5-2 Scatterplots of observed vs. simulated daily streamflow for all the 90 watersheds using individual regionalization models and combination of the first three and all the four models

To visualize the performance of each model for individual watersheds, the spatial distribution of NSE values using the four regionalization models for all 90 watersheds across Ontario are presented in Figure 5-3 and Figure 5-3. The spatial distribution of NSE values for IDW-PS (Figure 5-4a) reveals that in about 10% of the watersheds, the performance of this method is very poor while for other watersheds it is very good and just in one watershed it is in the middle (or average) level. It can be seen (Figure 5-4a) that in northern large basins and in few central watersheds, IDW-PS has a poor performance while it reveals a very good performance in small dense southern watersheds. Comparison of this map with the spatial distribution of NSE values using the remaining three regionalization models (Figure 5-3) demonstrates that those ones can perform better than IDW-PS in some cases while each one has a different level of performance. This is apparent for three specified watersheds (in Figure 5-3) which have different sizes and are spread in northern, central and southern regions. Furthermore, it can be seen that for a nested watershed in northern area (04CB001 , Figure 5-4a.) only MAC-IDW model has a satisfactory performance and for the large northern watershed (04CC001) MLP-IDW has the best performance. Figure 5-4 b shows the spatial distribution of NSE values for combination of four models. It can be seen that the combined output of three regionalization models can compete with IDW-PS, and for those watersheds where IDW-PS has a poor performance the combined model can perform better. In the next step, the outputs of IDW-PS are combined with the outputs of other individual models. The spatial distribution of NSE values using combination of the four models is presented in Figure 5-4 C. Comparison of this map with IDW-PS and the combination of the three other models indicates that the combination of the four models can improve regionalization performance in general and this combination model does not reveal a poor performance in any of the watersheds.

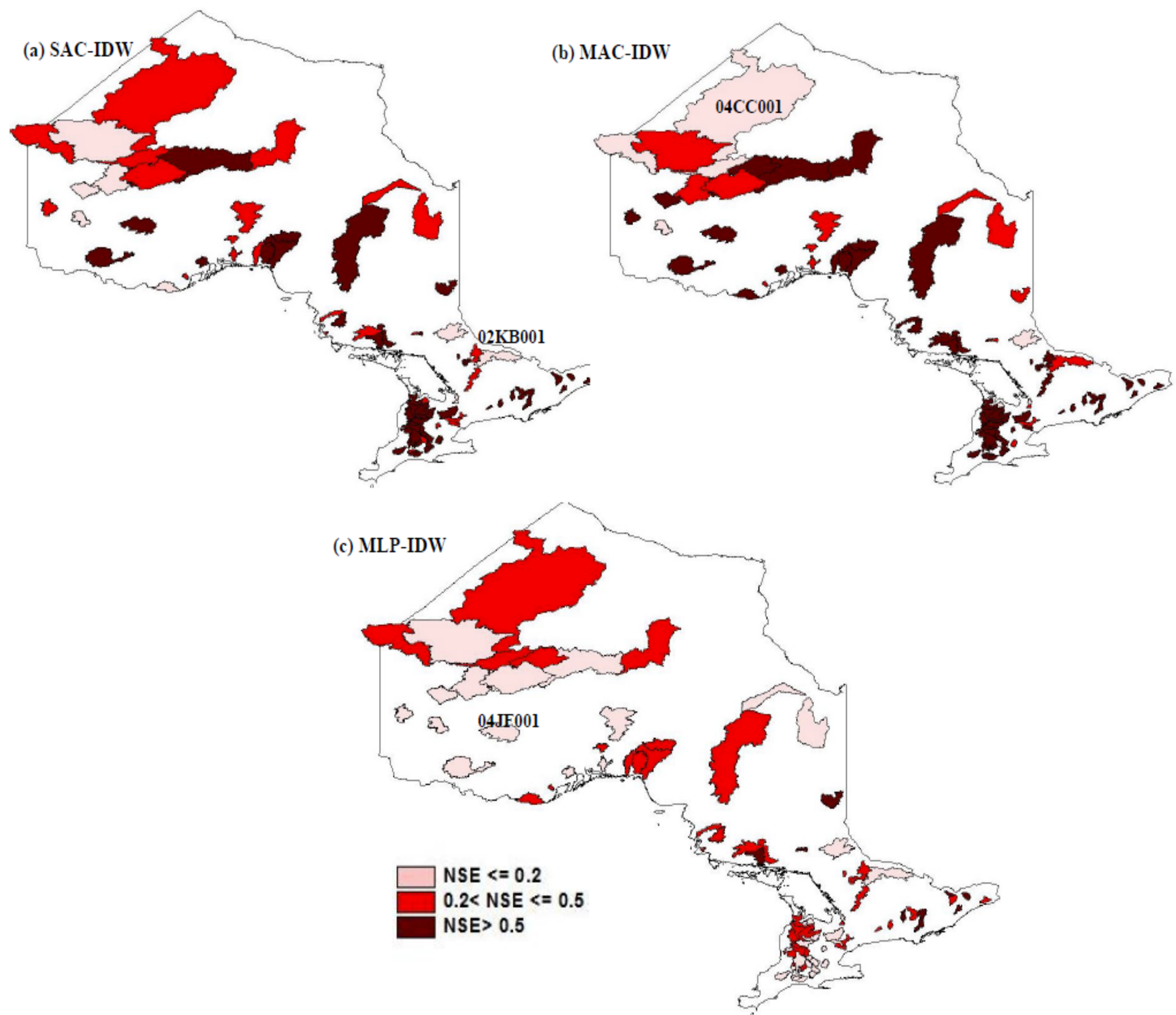

Figure 5-3 Spatial distribution of NSE values for daily streamflow regionalization models : (a) SAC-IDW, (b) MAC-IDW (c) MLP-IDW over Ontario watersheds (unscaled maps)

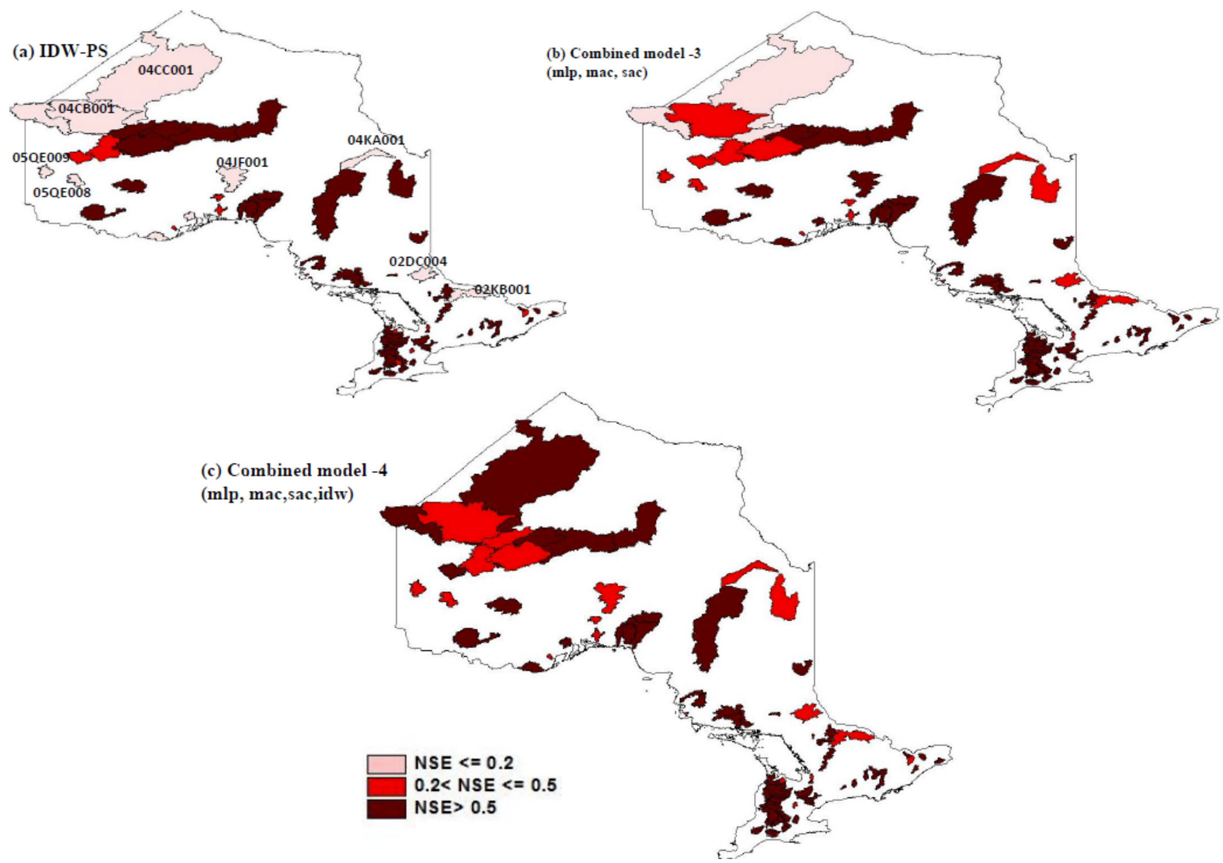

Figure 5-4 Spatial distribution of NSE values for daily streamflow regionalization models: (a) IDW-PS (b) combined model of three models (MLP-IDW, MAC-IDW and SAC-IDW) (c) combined model of all the four models (unscaled maps)

Uncertainty Analysis Results

The uncertainty bounds of all 90 watersheds are estimated using 16 possible acceptable ensemble outputs of the four individual regionalization models. Since the ensemble outputs are generated using possible acceptable results of individual models it can be assumed that the combined model might fluctuate in this range. The uncertainty bounds of estimated daily streamflow for three basins selected earlier (specified in figure 5-1) are presented in Figure 5-5. This graph shows the observed and estimated hydrographs of three sample watersheds using the combination of four models along with estimated uncertainty bounds. In general, this figure shows that for the three sample watersheds with various sizes in various regions of Ontario, the confidence limits of the combination model encompass the observed hydrograph.

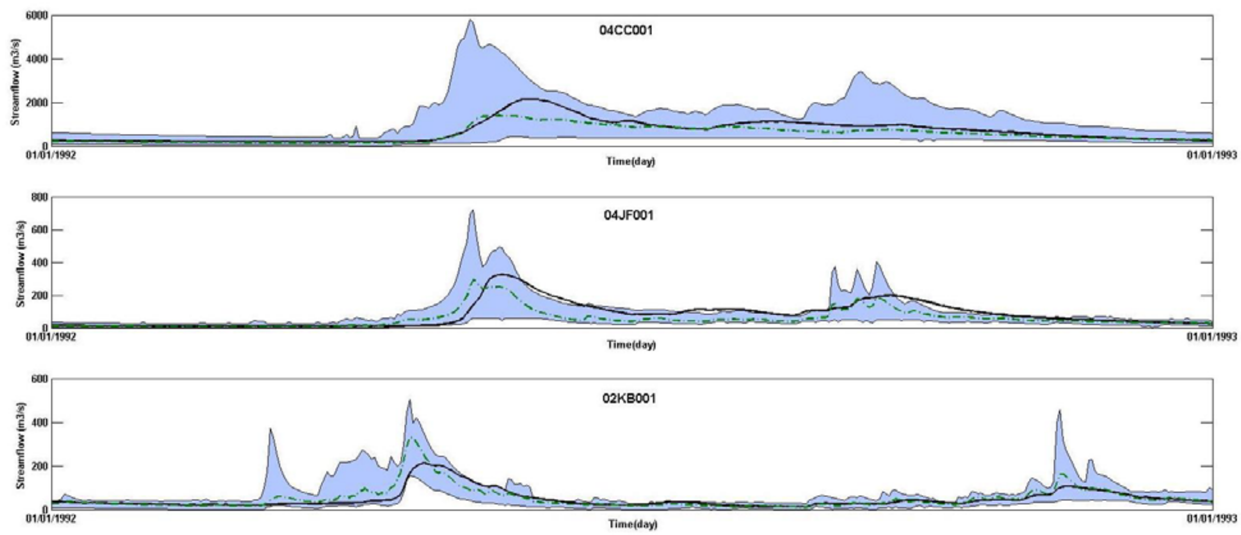

Figure 5-5 Uncertainty limits of continuous daily stream flow regionalization (shades), observed (solid line) and estimated hydrograph using combination of four individual regionalization models (dashed line)

5.6. Summary and Conclusions

In this study four regionalization models including SAC-IDW, MAC-IDW, MLP-IDW and IDW-PS are applied to four clusters of 90 pre-classified Ontario watersheds. The comparison of the four regionalization models indicates that IDW-PS outperforms other models for almost 90 percent of the watersheds and MLP-IDW indicates the poorest performance for most of the watersheds. However, for large northern watersheds with low Q5/Q95, MLP-IDW can reach a satisfactory performance. MAC-IDW and

SAC-IDW outperform other models for small southern watersheds with high Q5/Q95. Furthermore, for daily low and high flow regionalization each model has different performance. For example SAC-IDW has better performance for high flows compared to low flows, while MAC-IDW performs better for low flows. The results of this study indicates that although MLP-IDW model has a relatively poor performance in general, and IDW-PS outperforms other models in most of the watersheds, a combination of the four models can significantly improve the performance of continuous streamflow regionalization. The combination of the four models performs satisfactory for all of the watersheds while individual models indicate poor performance for some of them. The study results suggest that the combination of structurally different models can offer a robust model for continuous streamflow prediction in ungauged basins.

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Chapter 6 : Conclusions and Recommendations

6.1. Conclusions

The research work presented in this PhD thesis covers an important issue in the management of water resources. Streamflow estimation/prediction in ungauged basins is required for water resources management purposes such as water allocation, long-term watershed planning, industrial and domestic water supply and flood prediction. The scope of this research is to present a reliable and effective methodology for streamflow prediction in ungauged basins. The main conclusions of the thesis can be summarized as follows:

6.1.1. Streamflow regionalization approaches

- Continuous streamflow regionalization can be carried out through hydrologic model dependent and hydrologic model-independent approaches.
- Studies on hydrologic model-dependent methods in arid to warm temperate climate (e.g. Australia) indicate that physical similarity and spatial proximity appears to be the best approach, while in warm temperate (most European countries) regression-based methods have been preferred. Similarly, in cold and snowy climate (e.g. Canada) spatial proximity and physical similarity approaches seem to outperform other hydrologic model-dependent methods.
- The HBV and IHACRES are the most frequently used hydrologic models.
- Among the hydrologic model-independent methods, linear and nonlinear regression methods have performed well in warm temperate regions (e.g. European countries) while in cold and snowy climate (e.g. Canada) and warm humid climate (e.g. Brazil) scaling relationships have shown good performance.

6.1.2. Watershed Classification

- Proposed nonlinear classification techniques i.e. SOM, NLPCA and Compact-NLPCA on both watershed attributes and daily streamflow series were consistently superior to PCA in terms of identifying hydrologically homogenous clusters of Ontario watersheds.
- The superior performance of NLPCA based on watershed attributes suggests its potential for the classification of ungauged watersheds.
- Watershed classification results using SOM, NLPCA and CNLPCA based on watershed attributes indicated distinct patterns of FDC slope, timing of event flows (annual hydrograph) shape, and dominant physical attributes in each cluster.
- The proposed nonlinear classification methods based on attributes can potentially improve the performance of streamflow regionalization in ungauged watersheds.

6.1.3. Nonlinear streamflow regionalization applied on classified watersheds

- The MLP model is very competitive with the IDW (identified as the best regionalization method in the study area) while the more complicated types of neural networks, CPN and SVR, become competitive when they are applied on classified watersheds.
- The combination of watershed classification technique, regionalization technique and hydrologic model, affects the performance of daily streamflow, baseflow and peakflow regionalization substantially.

- MAC-HBV as hydrologic model coupled with CPN as regionalization technique in combination with NLPCA or SOM as classification technique reveals a clear improvement in daily streamflow, baseflow and peakflow regionalization.
- In general nonlinear data-driven techniques are more likely to improve the performance of daily streamflow regionalization after watershed classification in basins with high FDC's slope (Q95/Q5) , less area covered by forest , more area covered by rapid drainage and glaciodeposits, monthly low flow in March and spring snowmelt peak flow in May/June .
- Neural networks as dynamic nonlinear methods are capable to account for non-stationarity due to urbanization and climate change in the hydrological modelling of ungauged watersheds.

6.1.4. Improving streamflow prediction by multi-model combination

- The investigated streamflow regionalization models which lie in the two categories of regionalization approaches i.e. hydrologic-model-independent and hydrologic model dependent including IDW-PS, MLP-IDW, SAC-IDW and MAC-IDW indicate potentially good performance for different Ontario watersheds .
- Different structure of regionalization models result in different performance of daily streamflow regionalization. For example, SAC-IDW has better performance for high flows compared to low flows, while MAC-IDW performs better for low flows.

- Although MLP-IDW has a relatively poor performance in general, and IDW-PS outperforms other models in most of the watersheds, a combination of the four models can significantly improve the performance of continuous streamflow regionalization.
- IDW-PS outperforms other models for almost 90 percent of the watersheds and MLP-IDW indicates the poorest performance for most of the watersheds.
- In large northern watersheds with low Q5/Q95, MLP-IDW can reach a satisfactory performance while MAC-IDW and SAC-IDW outperform other models for small southern watersheds with high Q5/Q95.
- The combination of the four models performs satisfactory for all of the watersheds while individual models indicate poor performance for some of them.
- The combination of structurally different models can offer a robust model for continuous streamflow prediction in ungauged basins.

6.2. Recommendations for future research

Future research should focus on issues which can increase the reliability of estimation in ungauged basins. Climate change along with changes in land use and land cover due to human activities cause nonstationarity in streamflow time series which is generally overlooked by most regionalization methods that assume stationarity. Thus, estimating uncertainty in streamflow estimation/prediction in ungauged basins using regionalization techniques remains a challenging research topic. In the current research, neural networks have been emerged to be able to account for nonstationary hydrological time series modeling, thus, investigation of different types of neural networks in watershed classification and streamflow regionalization as well as their combination with hydrologic models in future studies in regions with different climate pattern and watershed attributes is suggested to further explore the possibility of improvement in hydrologic predictions in ungauged watersheds.

Hydrologic ensemble modeling can account for uncertainties in streamflow estimation/prediction. It has emerged as a prediction tool in hydrology particularly during the last decade (Hydrologic Ensemble Predictions Experiment (HEPEX) initiated in 2004 (www.hepex.org)). Ensemble estimations/predictions of streamflow time series can be used as an indication of uncertainty in hydrologic predictions and can also improve the reliability of hydrologic modeling. Ensemble streamflow predictions in hydrology have been generated using multiple climatological input data (e.g. He et al. 2009), multiple sets of hydrologic model parameter sets (e.g., McIntyre et al 2005, Seibert and Beven (2009)) or multiple rainfall-runoff model structures (e.g. Velezque et. al 2011). Evaluation methods for Ensemble Prediction Systems (EPS) are either deterministic or probabilistic. To evaluate the ensemble predictions, bias, variance and covariance of ensembles need to be considered. Deterministic approaches evaluate a weighted or simple average of model outputs while probabilistic approaches are based on the joint distribution of forecasts and observations. Probabilistic approaches consider all model realizations. Criteria which are usually used to evaluate the ensemble realizations include some scores adopted from meteorology such as Brier Score (Jolliffe and Stephensen 2003), continuous ranked probability score (Brown 1974), ignorance score (Roulston and Smit 2002) and cost/loss function (Laio and Tamea (2007)), rank histogram approach which measures the tendency of model to over or under estimate (Regimbeau et al.

(2007)). Finally, probabilistic models for streamflow estimation/prediction in ungauged basins are highly recommended as future research direction.

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