SENSITIVITY ANALYSIS OF CONVEX RELAXATIONS FOR NONSMOOTH GLOBAL OPTIMIZATION

SENSITIVITY ANALYSIS OF CONVEX RELAXATIONS FOR NONSMOOTH GLOBAL OPTIMIZATION

BY

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Abstract

Nonsmoothness appears in various applications in chemical engineering, including multi-stream heat exchangers, nonsmooth flash calculation, process integration. In terms of numerical approaches, convex/concave relaxations of static and dynamic systems may also exhibit nonsmoothness. These relaxations are used in deterministic methods for global optimization. This thesis presents several new theoretical results for nonsmooth sensitivity analysis, with an emphasis on convex relaxations.

Firstly, the "compass difference" and established ODE results by Pang and Stewart are used to describe a correct subgradient for a nonsmooth dynamic system with two parameters. This sensitivity information can be computed using standard ODE solvers.

Next, this thesis also uses the compass difference to obtain a subgradient for the Tsoukalas-Mitsos convex relaxations of composite functions of two variables.

Lastly, this thesis develops a new general subgradient result for Tsoukalas-Mitsos convex relaxations of composite functions. This result does not limit on the dimensions of input variables. It gives the whole subdifferential of Tsoukalas-Mitsos convex relaxations. Compare to Tsoukalas-Mitsos' previous subdifferential results, it does not require additionally solving a dual optimization problem as well. The new subgradient results are extended to obtain directional derivatives for Tsoukalas-Mitsos convex relaxations. The new subgradient results and directional derivative results are computationally approachable: subgradients in this article can be calculated both by the vector forward AD mode and reverse AD mode. A proof-of-concept implementation in Matlab is discussed.

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Notation, Definitions, and Abbreviations

Notation

$\mathbb{R}^n$	n-dimensional Euclidean space
$\mathbb{Z}$	set of integers
$\mathbb{N}$	set of natural numbers $\{1, 2, \ldots\}$
S, U**, etc.**	sets
I	identity matrix
$\mathbf{cl}S$	closure of set S
$\mathbf{int}S$	interior of set S
$\mathbf{conv}S$	convex hull of S
$\mathbf{x}, \mathbf{y}$	vectors in e.g. $\mathbb{R}^n$
$\mathbf{x}^T$	transposed vector

$\langle \cdot, \cdot \rangle$	Euclidean inner product
$f(x)$	function f, evaluated at x
$\nabla f(x)$	gradient of function f at x
$\partial f(x)$	subdifferential of function f at x
$f'(x; d)$	directional derivative of function f at x in direction d
$\partial_{\mathrm{L}} f(x)$	set of lexicographic subgradients of f at x
max	maximum
min	minimum
sup	supremum
inf	infimum

Abbreviations

NLP	Nonlinear programming
NSO	Nonsmooth optimization
ODE	Ordinary differential equation
KKT	Karush-Kuhn-Tucker optimality conditions
AD	Automatic Differentiation
IVP	Initial value problem

Chapter 1

Introduction

1.1 Background and Goals

1.1.1 Nonsmoothness in Optimization

In this thesis, a smooth function is considered to be a function that is differentiable. Nonsmooth models or functions are continuous but not differentiable everywhere. Nonsmooth optimization (NSO) refers to the "problem of minimizing (or maximizing) functions that are typically not differentiable at their minimizers (maximizers)." (Bagirov *et al.*, 2014) Nonsmoothness appears in applications in chemical engineering. In modelling multi-stream heat exchange for example, nonsmoothness appears when changing thermodynamic phases along the heat exchanger (Watson *et al.*, 2015). In nonideal vapor-liquid equilibrium modelling, inside-out algorithms contain nonsmoothness for flash calculation (Watson *et al.*, 2017). Nonsmoothness also appears in dynamic systems, including campaign continuous pharmaceutical manufacturing (Patrascu and Barton, 2018; Sahlodin and Barton, 2015).

Nonsmoothness also appears in other highly structured problems like neural networks, image denoising (De los Reyes and Schönlieb, 2013) and data mining (Ozögür-Akyüz *et al.*, 2008) etc.

In terms of numerical approaches, convex/concave relaxations of an optimization problem are also a source of nonsmoothness in process system engineering. (McCormick, 1976; Tsoukalas and Mitsos, 2014).

1.1.2 Sensitivity Analysis

Sensitivity analysis aims to describe how a system behaves in response to changes in system parameters. Sensitivity information may be used to construct useful linear approximations that may be employed in optimization methods. Sensitivity information is critical in nonsmooth optimization. For example, a typical subgradient method (Scholtes, 2012, Theorem 2.1) uses a subgradient at each iteration to approximate the optimal solution in nonsmooth convex optimization, so that the overall method converges. Similarly, cutting plane methods, bundle methods and level methods use subgradients at each iteration to form piece-wise linear approximations for minimizing a convex function (Hiriart-Urruty and Lemaréchal, 2013b; Nesterov, 2018). Sensitivity information in nonsmooth optimization typically comprises directional derivatives and subgradients.

1.1.3 Convex Relaxations

An optimization problem is convex if both the objective function and constraints are convex. Several applications involve nonconvexity. For example, in the process control area, hydro power plants' hydroelectric generators have been modeled using nonconvex correlations (Glotić *et al.*, 2014). In gas pipeline operations, nonconvexity also appears in objective functions representing compressors (De los Reyes and Schönlieb, 2013). Nonconvexity of these systems makes them challenge to analyze and simulate.

Convex/concave relaxations are critical in determinstic methods for global optimization. Nonconvex problems are difficult to solve. Convex/concave relaxations can provide useful approximations of global solutions for non-convex problems in acceptable times (Li, 2015). Convex relaxations of functions are also used to provide bounding information to deterministic global optimization methods for nonconvex systems (Horst and Tuy, 2013).

Convex/concave relaxations under/over-estimate the objective function and constraints. Below is a general minimization problem:

$$\begin{aligned} \min_{x\in X} \quad & f(x) \\ \text{s.t.} \quad & g(x) \leq 0 \end{aligned} \tag{1.1.1}$$

where f is an objective function, g is the constraint function and X is a decision set. Both f and g could be nonconvex. In this case, a general form of convex relaxation of the problem (1.1.1) can be established as follows:

$$\begin{aligned} \min_{x\in \bar{X}} \quad & f^{cv}(x) \\ \text{s.t.} \quad & g^{cv}(x) \leq 0 \end{aligned} \tag{1.1.2}$$

where the function f^{cv} is a convex relaxation of f, with $f^{cv}(x) \leq f(x)$ for each x; g^{cv} is convex relaxation of g, with $g^{cv}(x) \leq g(x)$; and $\bar{X}$ is a convex set for which $X \subset \bar{X}$.

A solution of this relaxation (1.1.2) is guaranteed to be a valid lower bound for the unknown global solution of (1.1.1).

One important application of convex relaxations is branch-and-bound methods for global optimization (Falk and Soland, 1969; Horst and Tuy, 2013). This algorithm uses convex relaxations at each iteration to calculate the lower bound in a region (Horst and Tuy, 2013). This method guarantees the location of a global solution for a nonconvex optimization within a certain tolerance. Convex relaxation can also be applied to optimal distributed control (ODC) problems for linear discrete-time deterministic and stochastic systems to obtain global optimal (Fazelnia *et al.*, 2016). Convex relaxation can also be used in optimal power flow (OPF) problems to find a global solution for IEEE benchmark systems by applying semi-definite programming (Madani *et al.*, 2014). This technique is guaranteed to work over acyclic distribution networks.

There are many different types of convex relaxation schemes. For example, α-BB convex relaxations are designed for nonconvex twice-differentiable function. (Adjiman *et al.*, 1998a,b) The α-BB algorithm operates within a branch-and-bound framework. BARON's convex relaxation for factorable problems involve relaxing optimization problems directly (Ryoo and Sahinidis, 1996), and is available as a global optimization solver in GAMS (Sahinidis, 1996). McCormick relaxation (McCormick, 1976; Mitsos *et al.*, 2009; McCormick, 1983) also provides a scheme for computing convex underestimators and concave overestimators for factorable functions which are composed of addition, multiplication, and simple univariate intrinsic functions. Tsoukalas and Mitsos (Tsoukalas and Mitsos, 2014) extend the McCormick relaxation idea to consider general compositions with multivariate outer functions.

1.1.4 Goals

The “compass difference” named by Khan (Khan and Yuan, 2020) provides a way to calculate a subgradient for any scalar-valued bivariate function that is locally Lipschitz continuous and directionally differentiable. The first goal of this study is to use this compass difference to propagate a subgradient in a nonsmooth dynamic system with two parameters.

The second goal is using compass differences to propagate a subgradient for multivariate McCormick relaxations with two variables (Tsoukalas and Mitsos, 2014).

In this thesis, the third goal is to propagate a whole subdifferential set and directional derivatives for multivariate McCormick relaxations, no matter the number of input variables. The new results aim to extend Tsoukalas and Mitsos sensitivity results for multivariate McCormick relaxations (Tsoukalas and Mitsos, 2014). This new subgradient result and directional derivative result can be used with any system that applies multivariate McCormick relaxations.

1.2 Contributions and Structures

This thesis is organized into the following parts:

Chapter 2 introduces basic mathematical notation that will be used in this thesis: including concepts of sets, vector spaces and matrices. Also, some established mathematical concepts that will be used in latter parts are also summarized here, including *directional derivatives* and *subdifferentials*, basic definitions of *local Lipschitz continuity*, compass differences (Khan and Yuan, 2020) and the Tsoukalas-Mitsos convex relaxations (Tsoukalas and Mitsos, 2014) of composite functions.

Chapter 3 and Chapter 4 present new applications of the compass difference. Chapter 3 shows how to use compass differences to describe a correct subgradient for solutions of parametric ordinary differential equations (ODEs) with parameters in $\mathbb{R}^2$. This approach reduces to the classical ODE sensitivity approach of (Hartman, 2002, Section V, Theorem 3.1) when the original ODE is defined in terms of smooth functions. Unlike established methods (Khan and Barton, 2014), this new formulation can be solved by standard ODE solvers.

Chapter 4 uses compass differences and Hogan's Theorem (Hogan, 1973) to obtain a subgradient for the Tsoukalas-Mitsos convex relaxations (Tsoukalas and Mitsos, 2014) of composite functions of two variables. Compared to Tsoukalas-Mitsos' established subdifferential results (Tsoukalas and Mitsos, 2014), it has no need to solve a dual optimization problem.

Chapter 5 develops a new subgradient result for Tsoukalas-Mitsos convex relaxations of composite functions in general. It has no limitation on dimensions of input variables unlike the method if Chapter 4. It can give the whole subdifferential set for Tsoukalas-Mitsos convex relaxations. Compared to Tsoukalas-Mitsos' subdifferential results (Tsoukalas and Mitsos, 2014, Thoerem 4), it no need to additionally solve dual optimization problems. Chapter 5 also extends the new subgradient results to obtain directional derivatives for Tsoukalas-Mitsos convex relaxations. The new subgradient results and directional derivatives results are computationally tractable: subgradients in this article can be calculated both by the vector forward mode and reverse mode of automatic differentiation(AD). This chapter also extends the product-rule and fractional-term applications by Tsoukalas and Mitsos (Tsoukalas and Mitsos,

2014) and gives numerical examples of sensitivity results for both. This new subgradient result for relaxations can be applied to dynamic global optimization. (Song and Khan, 2020)

Chapter 2

Mathematical Background

This section presents mathematical definitions and formulations that will be used in this thesis. This section is aimed to help the reader understand basic concepts that will be used in later part of thesis.

In addition to this section, Chapters 3, 4 and 5 introduce further concepts that are specific to those chapters.

2.1 Notation

Capital letters like Y denotes *sets* (or *matrices*). $X \subset Y$ means that a set X is a subset of Y. $y \in Y$ means y is an element of Y. The convex hull, the interior and the closure of a set $S \subset \mathbb{R}^n$ are denoted as $\operatorname{conv} S$, $\operatorname{int} S$ and $\operatorname{cl} S$, respectively.

$\mathbb{R}$ denotes the set of *real numbers*. $\mathbb{Z}$ denotes the set of *integers*. $\mathbb{N} = \{1, 2, \cdots\}$

denotes the set of *natural numbers*. $\mathbb{R}^n$ denotes the space of *vectors* with real components in n dimensions. eg: $x \in \mathbb{R}^n$ implies

$$x := \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = (x_1, \cdots, x_n),$$

where x_i denotes the i^{th} component of x. Also given vectors $x, y \in \mathbb{R}^n$, $x \leq y$ means $x_i \leq y_i$ for each $i \in \{1, \cdots, n\}$.

$\langle \cdot, \cdot \rangle$ denotes the Euclidean *inner product*. For example, consider two vectors $a, b \in \mathbb{R}^n$; the inner product of these is:

$$\langle a, b \rangle = a^T b := a_1 b_1 + a_2 b_2 + \cdots + a_n b_n \in \mathbb{R}$$

The i^{th} unit coordinate vector in $\mathbb{R}^n$ is denoted as $e_{(i)}$, and components of vectors are indicated using subscripts, e.g. $x_i := \langle e_{(i)}, x \rangle$.

Let V and W be two sets, "$f : V \to W$" means a *function* named f whose *domain* is a set V, and whose codomain is a set W.

In matrix space, $\mathbb{R}^{m \times n}$ denotes the set of *matrices* with m rows and n columns. For example, given $A \in \mathbb{R}^{m \times n}$:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn} \end{bmatrix}$$

where $a_{i,j}$ or a_{ij} denotes the element in the i^{th} row and j^{th} column.

Below are definitions for *Lipschitz continuity* and *lexicographical (L–)smoothness.*

Definition 2.1.1. *(Hiriart-Urruty and Lemaréchal, 2013a, Theorem 3.1.1) A function* $f : X \to \mathbb{R}^m$ *with* $X \subset \mathbb{R}^n$ *is called* Lipschitz continuous, *if there exists a* Lipschitz constant $L \geq 0$ *such that for all* $x, \hat{x} \in X$,

$$||f(x) - f(\hat{x})|| \leq L||x - \hat{x}||,$$

where $|| \cdot ||$ *denotes appropriate norms.*

A function $f : X \to \mathbb{R}^m$ *with* $X \subset \mathbb{R}^n$ *is* locally Lipschitz continuous, *if for any* $x \in X$, *there exist a neighborhood* N *of* x *such that* f *restricted to* N *is Lipschitz continuous.*

Definition 2.1.2. *(Nesterov, 2005b) Consider an open set* $X \subset \mathbb{R}^n$ *and a locally Lipschitz continuous function* $f : X \to \mathbb{R}$. *The function* f *is* lexicographically (L–)smooth *at* $x \in X$ *if the following conditions are satisfied:*

- f *is directionally differentiable at* x,
- *with* $f^{(0)} := f'(x; \cdot)$, *for any collection of vectors* $m_{(1)}, \ldots, m_{(n)} \in \mathbb{R}^n$, *the following inductive sequence of higher-order directional derivatives is well-defined:*

$$f^{(k)} := [f^{(k-1)}]'(m_{(k)}; \cdot), \qquad \text{for each } k \in \{1, 2, \ldots, n\}.$$

If these vectors $m_{(i)}$ *are linearly independent, then* $f^{(n)}$ *is linear, and its constant gradient is called a* lexicographic subgradient *of* f *at* x. *The* lexicographic subdifferential $\partial_{\mathrm{L}} f(x)$ *is the set of all lexicographic subgradients of* f *at* x.

2.2 Convexity

2.2.1 Convex Set

Definition 2.2.1. *A set $S \subset \mathbb{R}^n$ is convex, if for any $x, y \in S$ and all $0 \leq \alpha \leq 1$, it holds that*

$$(\alpha x + (1-\alpha)y) \in S.$$

2.2.2 Convex Function

Definition 2.2.2. *Let $X \subset \mathbb{R}^n$ be a convex set. A function $f : X \to \mathbb{R}$ is convex if for any $x, y \in X$ and all $0 < \alpha < 1$,*

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y). \tag{2.2.1}$$

The function f is said to be strictly convex *when strict inequality holds in* (2.2.1) *if $x \neq y$.*

2.3 Directional Derivatives and Subgradients

The following definitions are standard in nonsmooth analysis (Clarke, 1990).

Definition 2.3.1. *Consider an open set $X \subset \mathbb{R}^n$ and a function $f : X \to \mathbb{R}$. The following limit, if it exists, is the (one-sided)* directional derivative *of f at $x \in X$ in* *the direction* $d \in \mathbb{R}^n$*:*

$$f'(x;d) := \lim_{t\to 0^+} \frac{f(x+td)-f(x)}{t}.$$

If $f'(x;d)$ *exists in* $\mathbb{R}$ *for each* $d \in \mathbb{R}^n$*, then* f *is directionally differentiable at* x*.*

For example, in this thesis $[f^{cv}]'(z;d)$ denotes the directional derivative for a function f^{cv} at z in direction d.

Definition 2.3.2. *Given a convex set* $X \subset \mathbb{R}^n$ *and a convex function* $f : X \to \mathbb{R}$*,* $s \in \mathbb{R}^n$ *is a* subgradient *of* f *at* $x \in X$ *if*

$$f(y) \geq f(x) + \langle s, y-x\rangle, \quad \textit{for each} \quad y \in X$$

The set of all subgradients of f *at* x *is the (convex)* subdifferential $\partial f(x)$*.*

Proposition 2.3.3. *(Scholtes, 2012, Theorem 3.1.1) Consider open sets* $X \subset \mathbb{R}^n$ *and* $Z \subset \mathbb{R}^p$*, and functions* $g : Z \to X$ *and* $f : X \to \mathbb{R}^m$ *that are locally Lipschiz continuous and directionally differentiable at any* $z \in Z$ *and* $x \in X$*. Then the directional derivative at* $z \in Z$ *of the composite function* $f \circ g$ *is*

$$[f \circ g]'(z;d) = f'(g(z); g'(z;d)) \quad \forall d \in \mathbb{R}^p. \tag{2.3.1}$$

2.4 Compass Difference

This section gives a definition of *compass differences* as introduced in (Khan and Yuan, 2020). Directional derivatives form the compass differences. Briefly, the compass differences in two dimension is a subgradient. (Khan and Yuan, 2020)

Definition 2.4.1. *Consider an open set* $X \subset \mathbb{R}^n$ *and a function* $f : X \to \mathbb{R}$ *that is directionally differentiable at* $x \in X$*. The* compass difference *of* f *at* x *is a vector* $\Delta^{\oplus} f(x) := (\Delta_1^{\oplus} f(x), \ldots, \Delta_n^{\oplus} f(x)) \in \mathbb{R}^n$ *for which, for each* $i \in \{1, \ldots, n\}$*,*

$$\Delta_i^{\oplus} f(x) := \frac{1}{2}(f'(x; e_{(i)}) - f'(x; -e_{(i)})).$$

2.4.1 Nonconvex Functions of Two Variables

Proposition 2.4.2. *(Khan and Yuan, 2020, Theorem 3.3) Consider an open set* $X \subset \mathbb{R}^2$ *and a locally Lipschitz continuous function* $f : X \to \mathbb{R}$*. If* f *is differentiable at some* $x \in X$*, then* $\Delta^{\oplus} f(x) \in \partial f(x)$*, with* $\partial f(x)$ *denoting Clarke's generalized gradient (Clarke, 1990), if* f *is nonconvex. Moreover, if* f *is L-smooth at* x *in the sense of (Nesterov, 2005a), then* $\Delta^{\oplus} f(x) \in \mathrm{cl\,conv}\, \partial_{\mathrm{L}} f(x) \subset \partial f(x)$*.*

Proposition 2.4.3. *(Khan and Yuan, 2020, Corollary 3.4) Consider an open set* $X \subset \mathbb{R}^2$*, a locally Lipschitz continuous function* $f : X \to \mathbb{R}$*, and a nonsingular matrix* $V \in \mathbb{R}^{2\times 2}$*. If* f *is directionally differentiable at some* $x \in X$*, and if* $v_{(i)}$ *denotes the* i^{th} *column of* V*, then*

$$\frac{1}{2}(V^{\mathrm{T}})^{-1} \begin{bmatrix} f'(x; v_{(1)}) - f'(x; -v_{(1)}) \\ f'(x; v_{(2)}) - f'(x; -v_{(2)}) \end{bmatrix} \in \partial f(x).$$

2.4.2 Convex Functions of Two Variables

Proposition 2.4.4. *(Khan and Yuan, 2020, Corollary 3.6) Consider an open convex set* $X \subset \mathbb{R}^2$ *and a convex function* $f : X \to \mathbb{R}$*. For each* $x \in X$*,* $\Delta^{\oplus} f(x) \in \partial f(x)$*.*

For convex functions, Clarke's generalized gradient coincides with the subdifferential (Clarke, 1990). All convex functions on open domains in $\mathbb{R}^n$ are L-smooth (Nesterov, 2005b).

2.5 Multivariate McCormick relaxation

McCormick relaxation (McCormick, 1976; Mitsos *et al.*, 2009; McCormick, 1983) provides a scheme for computing convex underestimators and concave overestimators for *factorable functions*. Factorable functions are functions that are well-defined finite compositions of simple intrinsic functions.

Definition 2.5.1. *Consider a set* $X \subset \mathbb{R}^n$*, a function* $h : X \to \mathbb{R}$*, and a convex subset* $C \subset X$*. A function* h^{cv}*:* $C \to \mathbb{R}$ *is a* convex relaxation *of* h *on* C *if* h^{cv} *is convex and* $h^{cv}(x) \leq h(x)$ *for each* $x \in C$*. A function* $h^{cc} : C \to \mathbb{R}$ *is a* concave relaxation *of* h *on* C *if* h^{cc} *is concave and* $h^{cc}(x) \geq h(x)$ *for each* $x \in C$*.*

The convex envelope *of* h *on* C *is the unique convex relaxation of* h *on* C *that dominates all other convex relaxations of* h *on* C*. The* concave envelope *of* h *on* C *is the unique concave relaxation of* h *on* C *that is dominated by all other concave relaxations of* h *on* C *.*

Tsoukalas and Mitsos (Tsoukalas and Mitsos, 2014) give a generalization of McCormick relaxation (McCormick, 1976) for compositions with multivariate outer functions.

Definition 2.5.2. *(Tsoukalas and Mitsos, 2014, Theorem 2) Consider nonempty convex sets* $Z \subset \mathbb{R}^n$ *and* $X_i \subset \mathbb{R}$ *for each* $i \in I = \{1, 2, \ldots, m\}$*, and define* X *as the*

Cartesian product $X_1 \times \cdots \times X_m$. *Consider functions* $F : X \to \mathbb{R}$ *and* $f_i : Z \to x_i$ *for each* $i \in I$, *and suppose the following relaxations exist:*

- *a continuous convex relaxation* $f_i^{cv} : Z \to X_i$ *of* f_i *on* Z *for each* $i \in I$,
- *a continuous concave relaxation* $f_i^{cc} : Z \to X_i$ *of* f_i *on* Z *for each* $i \in I$,
- *a continuous convex relaxation* F^{cv} *of* F *on* X.

Then, the following multivarite McCormick *mapping is a continuous convex relaxation of the composite function* $g : Z \to \mathbb{R} : z \mapsto F(f_1(z), \cdots, f_m(z))$ *on* Z*:*

$$g^{cv}(z) = \min\{F^{cv}(x) \ : \ x \in \mathbb{R}^m, \quad f_i^{cv}(z) \leq x_i \leq f_i^{cc}(z) \quad \forall i \in I\}. \tag{2.5.1}$$

The whole subdifferential for the relaxation of Definition 2.5.2 is computed by Tsoukalas and Mitsos (Tsoukalas and Mitsos, 2014), and involves solving the following dual problem.

Definition 2.5.3. *(Adapted from (Tsoukalas and Mitsos, 2014, Theorem 4)) Consider the same assumptions and notation in Definition 2.5.2. The subdifferential of* g^{cv} *at* $\hat{z}$ *is given by:*

$$\partial g^{cv}(z) = \left\{ \sum_{i=1}^{m} \rho_i^{cv} s_i^{cv} - \rho_i^{cc} s_i^{cc} \middle| \begin{array}{l} (\rho_1^{cv}, \ldots, \rho_m^{cv}, \rho_1^{cc}, \ldots, \rho_m^{cc}) \in \Lambda(\hat{z}), \\ s_i^{cv} \in \partial f_i^{cv}(\hat{z}), s_i^{cc} \in \partial f_i^{cc}(\hat{z}) \quad \forall i = 1, \ldots, m \end{array} \right\}$$

where L *is the following Lagrangian function:*

$$L\left(x, \lambda^{cv}, \lambda^{cc}, \hat{z}\right) = F^{cv}(x) + \sum_{i=1}^{m} \lambda_i^{cv}\left(-x + f_i^{cv}(\hat{z})\right) + \lambda_i^{cc}\left(x - f_i^{cc}(\hat{z})\right)$$
$$\Lambda(\hat{z}) = \underset{(\lambda^{cv}, \lambda^{cc})}{\arg\max} \left\{ \min_{x \in X} L\left(x, \lambda^{cv}, \lambda^{cc}, \hat{z}\right) \right\}.$$

Chapter 3

Sensitivity Analysis for Dynamic Systems Using Compass Difference

This chapter shows how to use directional derivatives to form compass differences of convex functions with two variables to give sensitivity information for parametric ordinary differential equations (ODEs). These compass differences are guaranteed to be subgradients for parametric ODEs' initial value problems. This presented method is easy to implement by standard ODE solvers and can find a subgradient even if ODE right-hand side (RHS) is nonsmooth. This work is already published. (Khan and Yuan, 2020)

3.1 Background

Nonsmooth dynamic process models are often expressed as systems of parametric ordinary differential equations (ODEs). Below is a classic form of parametric ordinary differential equations (ODEs):

Definition 3.1.1. *Consider a system of parametric ordinary differential equations (ODEs), with state variables x and parameters p:*

$$\frac{dx}{dt}(t,p) = f(t,p,x(t,p)), \quad f(t_0,p) = x_0(p)$$

where $x_0(p)$ is the initial value at time $t = 0$.

A description of parametric derivatives for smooth ODEs is summarized by Hartman (Hartman, 2002, Chapter5,Theorem 3.1). This method gives sensitivity information of state variables with respect to uncertain parameters by solving related linear ODEs. This approach requires ODEs' right-hand sides (RHS) to be smooth and to have continuous first order partial derivatives. In a smooth dynamic system, the result in Section 3.4 below reduced to Hartman's result. Hartman's work does not apply to the non-smooth case, but the new result in Section 3.4 below can. The ability to construct sensitivity information for nonsmooth ODEs is important since nonsmoothness widely appears in engineering optimization problems.

Pang and Stewart (Pang and Stewart, 2009, Theorem 11) show that Clarke Jacobian's supersets are linear Newton approximations when a parametric ODE RHS function is semismooth (Clarke, 1990, Theorem 7.4.1). They generate directional derivatives as the unique solution of a related ODE constructed by directionally differentiating the RHS of original parametric ODEs (Pang and Stewart, 2009, Theorem 7). However, linear Newton approximations of a convex function at a domain point can include elements that are not subgradients (Khan and Barton, 2014). Nevertheless, in section 3.4 below, directional derivatives obtained from (Pang and Stewart, 2009, Theorem 7) can be used to form a subgradient as a compass difference.

A description of sensitivity analysis for nonsmooth parametric ODEs was obtained by Khan and Barton (Khan and Barton, 2014, Theorem 4.1 & Theorem 4.2). This description illustrates that Nesterov's lexicographic derivatives (Nesterov, 2005b) can be used to construct a plenary Jacobian element. The plenary Jacobian is a certain superset of Clark's generalized Jacobian (Clarke, 1990, Theorem 7.4.1). They describe this plenary Jacobian element of the unique solution of a nonsmooth parametric ODE system as the unique solution of another ODE system (Khan and Barton, 2014, Theorem 4.2). However, this method cannot generally be implemented with standard ODE solvers, since the RHS functions describing lexicographic derivatives are not always continuous respect to state variables. In the method presented in section 3.4 below, the ODE systems' RHS functions are continuous and so the ODE can be solved by standard ODE solvers.

3.2 Mathematical Background

This section shows how Theorem 7 in (Pang and Stewart, 2009) can be used to get directional derivatives for dynamic systems.

Proposition 3.2.1. *(Pang and Stewart, 2009, Theorem 7) Consider function* $f : \mathbb{R}^n \to \mathbb{R}^n$ *that is locally Lipschitz continuous and directionally differentiable, and an ordinary differential equation (ODE) initial value problem (IVP) formulated as follows:*

$$\frac{d\hat{x}}{dt} = f(\hat{x}), \quad \hat{x}(0) = \hat{p}, \tag{3.2.1}$$

where $\hat{p} \in \mathbb{R}^n$ *is an initial condition. Let* $\hat{x}(t, \hat{p})$ *denote any solution to the ODE (3.2.1) above.*

$\hat{x}'_t((t,\hat{p});(0,\eta))$ is then the unique solution $\hat{y}(t)$ on $[0,T]$ of the ODE below:

$$\frac{d\hat{y}}{dt} = f'(\hat{x}(t,\hat{p});\hat{y}) \quad \hat{y}(0) = \eta. \tag{3.2.2}$$

3.3 Problem Formulation

Assumption 3.3.1. *Consider an ordinary differential equation (ODE) initial value problem (IVP) formulated as follows:*

$$\frac{dx}{dt} = f(x), \quad x(0,p) = x_0(p), \tag{3.3.1}$$

where the right-hand-side (RHS) function $f\colon \mathbb{R}^n \to \mathbb{R}^n$ is directionally differentiable and locally Lipschitz continuous, $x_0\colon \mathbb{R}^2 \to \mathbb{R}^n$ describes the initial value, and $p \in \mathbb{R}^2$ is a parameter. $x(t,p)$ denotes the solution to the ODE (3.3.1) above and is assumed to be exist for all $t \in [0,T]$ where $0 < T$. x_0 is directionally differentiable and locally Lipschiz continuous.

Consider a cost function: $\phi\colon \mathbb{R}^2 \to \mathbb{R}$, for which

$$\phi(p) := g(p, x(T,p)), \tag{3.3.2}$$

where $g\colon \mathbb{R}^2 \times \mathbb{R}^N \to \mathbb{R}$, is locally Lipschitz continuous and directionally differentiable.

The goal of this section is to find a subgradient of the cost function ϕ in Equation (3.3.2) at any given p, where this subgradient is understood to be a element of Clarke's generalized gradient, if ϕ is nonconvex.

3.4 Computing a Subgradient of an ODE Solution

This section shows how to use compass differences to calculate a subgradient of the parametric ODE system (3.3.1). Directional derivatives obtained from Pang and Stewart (Pang and Stewart, 2009, Theorem 7) are used to form this compass difference.

Theorem 3.4.1. *Under Assumption 3.3.1, and using the same notation as Section 3.3, then, consider the following parametric ODE on* $t \in [0, T]$*:*

$$\frac{dy}{dt}(t, d) = f'(x(t, p); y(t, d)) \quad y(0, d) = x_0'(p; d). \tag{3.4.1}$$

This ODE has a unique solution y*, and a subgradient of* ϕ *at* p *in Equation 3.3.2 is*

$$\frac{1}{2}\begin{bmatrix} \phi'(p; (1, 0)) - \phi'(p; (-1, 0)) \\ \phi'(p; (0, 1)) - \phi'(p; (0, -1)) \end{bmatrix}, \tag{3.4.2}$$

where $\phi'(p; d) = g'(p, x(T, p); (d, y(T, d)))$*.*

Proof. This proof proceeds by showing hat the assumptions in Theorem 3.4.1 satisfy all assumptions in Proposition 3.2.1.

Observe that f is locally Lipschitz continuous. Also, Assumption 3.3.1 states (ii), that $x(t, p)$ exists for all $t \in [0, T]$, which satisfies the corresponding assumption in Proposition 3.2.1.

According to (Khan and Barton, 2014, Theorem 4.1), for each $t \in [0, T]$, the function $x_t \equiv x(t, \cdot)$ is well-defined and Lipschitz continuous on a neighborhood of p, with a Lipschitz constant that is in dependent of t. Moreover, x_t is directionally differentiable at p for all $t \in [0, T]$.

The difference between Equation (3.3.1) and the Equation (3.2.1) is that the initial condition of Equation (3.2.1) is a parameter $\hat{p}$ while the the initial condition of Equation (3.3.1) is $x_0(p)$.

By applying the directional derivative chain rule (Scholtes, 2012, Theorem 3.1.1), $x'_T(p;d)$ and $\phi'(p;d)$ become:

$$x'_T(p;d) = \hat{x}'_T(x_0(p); x'_0(p;d)), \tag{3.4.3}$$

$$\phi'(p;d) = g'(p, x(T,p); (d, x'_T(p;d))), \tag{3.4.4}$$

where $x'_0(p;d)$ is the directional derivative of x_0 at p along d, and $\hat{x}'_T(x_0(p); x'_0(p;d))$ is the directional derivative of $\hat{x}_T$ at $x_0(p)$ along the direction $x'_0(p;d)$.

According to Proposition 3.2.1, $\hat{x}'_T(x_0(p); x'_0(p;d))$ is the unique solution of the ODE Equation (3.4.1) at time $t = T$. So $x'_T(p;d) = \hat{x}'_T(x_0(p); x'_0(p;d)) = y(T,d)$. Next, substituting Equation (3.4.4) into (3.4.3), we get

$$\phi'(p;d) = g'(p, x(T,p); (d, y(T,d))). \tag{3.4.5}$$

By using Definition 2.4.1 , the compass difference of ϕ at p is $\Delta^{\oplus}\phi(p)$:

$$\Delta^{\oplus}\phi(p) = \frac{1}{2}\begin{bmatrix} \phi'(p;(1,0)) - \phi'(p;(-1,0)) \\ \phi'(p;(0,1)) - \phi'(p;(0,-1)) \end{bmatrix}, \quad \forall t \in [0,T].$$

Considering Proposition 2.4.2 before, we conclude that $\Delta^{\oplus}\phi(p) \in \partial\phi(p)$.

□

3.5 Case Study

To illustrate computation of the subgradient provided by Theorem 3.4.1, this example describes a Matlab implementation for solving a nonsmooth ODE IVP and calculating a subgradient of $\phi(p)$ by using Theorem 3.4.1. In this case ϕ is convex. Then this subgradient is used to form a subtangent plane of the original function's graph and is tested if the subtangent is correctly below the original function or not. Details can be seen in the text below and Figure 3.1. The ODE solver: ode15s in Matlab is used here.

Example 3.5.1. *Consider the following ODE IVP instance,* f*:*$\mathbb{R}^3 \rightarrow \mathbb{R}^3$ *,* $x \in \mathbb{R}^3$*,* $p \in \mathbb{R}^2$*:*

$$\frac{dx}{dt} = f(x_1, x_2, x_3), \quad x(0,p) = x_0(p) = \begin{bmatrix} p_1 \\ p_2 \\ p_1 \end{bmatrix} \quad \forall t \in [0,1]$$

$$\frac{dx_1}{dt} = |x_1| + |x_2| + x_3$$

$$\frac{dx_2}{dt} = |x_2|,$$

$$\frac{dx_3}{dt} = x_3$$

$$\phi(p) = g(p, x(T,p)) = x_1(T,p).$$

Using Equation (3.4.1) *and evaluating directional derivatives of* f *by hand, the* *directional derivative of $x(t)$ at p in the direction d can be described by the ODE:*

$$\frac{dy}{dt}(t,d) = f'(x(t,p); y(t,d)), \quad y(0,d) = x_0'(p;d)$$

$$\frac{dy_1}{dt} = \begin{cases} -y_1 - y_2 + y_3, \ \textit{if } x_1 < 0, \ x_2 < 0 \\ -y_1 + y_2 + y_3, \ \textit{if } x_1 < 0, \ x_2 > 0 \\ -y_1 + |y_2| + y_3, \ \textit{if } x_1 < 0, \ x_2 = 0 \\ y_1 - y_2 + y_3, \ \textit{if } x_1 > 0, \ x_2 < 0 \\ y_1 + y_2 + y_3, \ \textit{if } x_1 > 0, \ x_2 > 0 \\ y_1 + |y_2| + y_3, \ \textit{if } x_1 > 0, \ x_2 = 0 \\ |y_1| - y_2 + y_3, \ \textit{if } x_1 = 0, \ x_2 < 0 \\ |y_1| + y_2 + y_3, \ \textit{if } x_1 = 0, \ x_2 > 0 \\ |y_1| + |y_2| + y_3, \ \textit{if } x_1 = 0, \ x_2 = 0 \end{cases}$$

$$\frac{dy_2}{dt} = \begin{cases} y_2, \ \textit{if } x_2 > 0 \\ |y_2|, \ \textit{if } x_2 = 0 \\ -y_2, \ \textit{if } x_2 < 0 \end{cases}$$

$$\frac{dy_3}{dt} = y_3.$$

The directional derivatives at $\bar{p} = \begin{bmatrix} \bar{p_1} \\ \bar{p_2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$, *in direction* $d = (1,0)$, $d = (-1,0)$,$d = (0,1)$ *and* $d = (0,-1)$ *at final time* $t = T = 1$ *were then found by* *solving the coupled ODE systems in x and y in Matlab:*

$$y(T,(1,0)) = \begin{bmatrix} [x_1]'_T(\bar{p};(1,0)) \\ [x_2]'_T(\bar{p};(1,0)) \\ [x_3]'_T(\bar{p};(1,0)) \end{bmatrix} = \begin{bmatrix} 5.4366 \\ 0 \\ 2.7183 \end{bmatrix}$$

$$y(T,(-1,0)) = \begin{bmatrix} [x_1]'_T(\bar{p};(-1,0)) \\ [x_2]'_T(\bar{p};(-1,0)) \\ [x_3]'_T(\bar{p};(-1,0)) \end{bmatrix} = \begin{bmatrix} -1.5431 \\ 0 \\ -2.7183 \end{bmatrix}$$

$$y(T,(0,1)) = \begin{bmatrix} [x_1]'_T(\bar{p};(0,1)) \\ [x_2]'_T(\bar{p};(0,1)) \\ [x_3]'_T(\bar{p};(0,1)) \end{bmatrix} = \begin{bmatrix} 2.7183 \\ 2.7183 \\ 0 \end{bmatrix}$$

$$y(T,(0,-1)) = \begin{bmatrix} [x_1]'_T(\bar{p};(0,-1)) \\ [x_2]'_T(\bar{p};(0,-1)) \\ [x_3]'_T(\bar{p};(0,-1)) \end{bmatrix} = \begin{bmatrix} 1.1751 \\ -0.3679 \\ 0 \end{bmatrix}.$$

The directional derivative for the cost function ϕ becomes:

$$\phi'(\bar{p};d) = g'(\bar{p}, x(T,p);(d, y(T,d))) = [x_1]'_T(\bar{p};d)$$

Then $\phi'(\bar{p};(1,0)) = 5.4316; \phi'(\bar{p};(-1,0)) = -1.5431; \phi'(\bar{p};(0,1)) = 2.7183; \phi'(\bar{p};(0,-1)) = 1.1751.$

By using the Equation (3.4.2), the subgradient of ϕ with initial value $\bar{p}$ at $t = 1$

is:

$$\Delta^{\oplus}\phi(\bar{p}) = \frac{1}{2}\begin{bmatrix} \phi'(\bar{p};(1,0)) - \phi'(\bar{p};(-1,0)) \\ \phi'(\bar{p};(0,1)) - \phi'(\bar{p};(0,-1)) \end{bmatrix} = \begin{bmatrix} 3.4898 \\ 0.7715 \end{bmatrix}, \quad \forall t \in [0,T]$$

The subtangent hyperplane $G(p) : \mathbb{R}^2 \to \mathbb{R}$ *to* $\phi(\bar{p})$ *at* $\bar{p} = \begin{bmatrix} \bar{p_1} \\ \bar{p_2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ *is constructed by* $\Delta^{\oplus}\phi(\bar{p})$*:*

$$G(p) = \phi(\bar{p}) + \Delta^{\oplus}\phi(\bar{p})^T(p - \bar{p})$$

Figure 3.1 shows the cost function ϕ *and its subtangent plane* $G(p)$ *at* $\bar{p_1} = 0, \bar{p_2} = 0$ *and* $T = 1$*.* G *is always below* ϕ *according to the figure. According to the definition of the subgradient (Hiriart-Urruty and Lemaréchal, 2013a, VI, Definition 1.2.1), the subdifferential of function* f *at* x *is the set of vectors* s *satisfying:*

$$f(y) \geq f(x) + < s, y - x >, \quad \forall\, y \in \mathbb{R}^n.$$

Thus, this result says if $\Delta^{\oplus}\phi(\bar{p})$ *is subgradient, then the graph* G *would always be below the graph of the original function* ϕ*. If* $\Delta^{\oplus}\phi(\bar{p})$ *was not a subgradient, the figure would show* G *above or crossing over* ϕ*. Here,* G *is always below* ϕ*. So* $\Delta^{\oplus}\phi(\bar{p})$ *is readily verified to be subgradient of* ϕ*.*

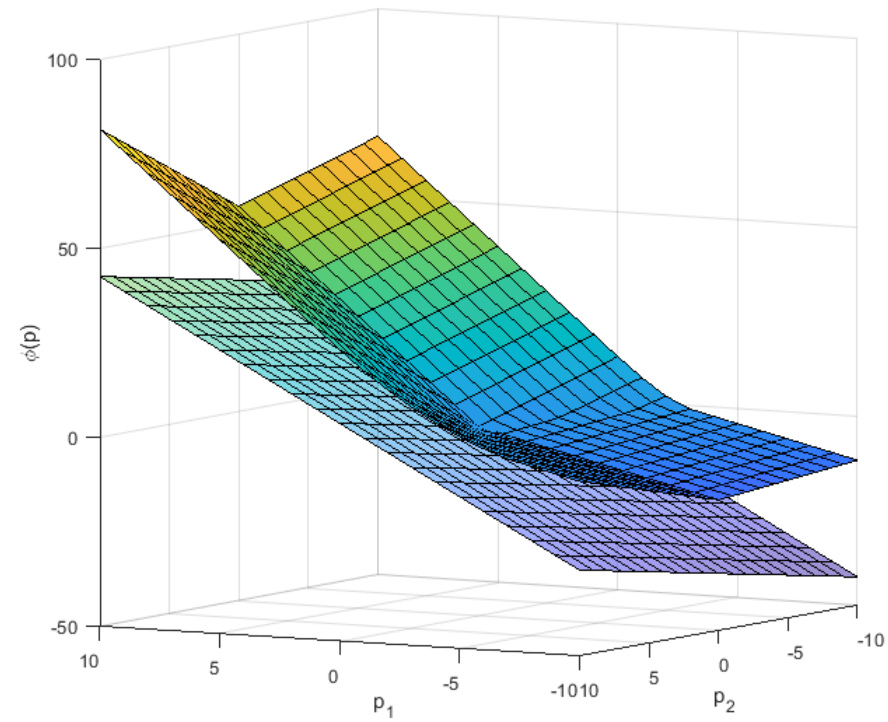

Figure 3.1: The function $\phi : p \mapsto x_1(T, p)$ (top) with $t = T = 1$ and its subtangent plane $G(p)$ (bottom) at $(0, 0)$ on $[-10, 10]^2$.

Chapter 4

Subgradient Propagation for Multivariate McCormick Relaxations of Two Variables

This chapter shows how compass differences (Khan and Yuan, 2020) can be used to obtain a subgradient of the Tsoukalas-Mitsos convex relaxations (Tsoukalas and Mitsos, 2014) of composite functions of two variables. Directional derivatives are obtained here from Hogan's Theorem (Hogan, 1973, Theorem 3). This work has been published in (Khan and Yuan, 2020).

4.1 Background

In addition to the results in Chapter 3. Compass differences also can used to obtain one subgradient for an optimal-value function. Danskin (Danskin, 1966, Thoeorem 1) provided a method to obtain directional derivatives for certain optimal value functions.

Proposition 4.1.1. *(Khan and Yuan, 2020, Proposition 4.8) Consider a compact set $C \subset \mathbb{R}^n$, some open superset Z of C, and a continuously differentiable function $f : \mathbb{R}^2 \times Z \to \mathbb{R}$. Define an optimal-value function $\phi : \mathbb{R}^2 \to \mathbb{R}$ for which*

$$\phi : x \mapsto \min\{f(x, y) : y \in C\}.$$

For some particular $\hat{x} \in \mathbb{R}^2$, define the following:

- *a set $Y := \{\hat{y} \in C : f(\hat{x}, \hat{y}) \leq f(\hat{x}, y), \quad \forall y \in C\}$,*
- *for each $d \in \mathbb{R}^2$, a point $\psi(d) := \min\{\langle d, \nabla_x f(\hat{x}, y)\rangle : y \in Y\}$.*

Then ϕ is locally Lipschitz continuous and directionally differentiable, and

$$\frac{1}{2}\begin{bmatrix}\psi(1,0) - \psi(-1,0) \\ \psi(0,1) - \psi(0,-1)\end{bmatrix}$$

is an element of $\partial\phi(\hat{x})$.

Proof. The optimal-value function ϕ has already been established to be locally Lipschitz continuous (Dempe *et al.*, 2012, Theorem 2.1) and directionally differentiable (Danskin, 1966), with directional derivatives given by $\phi'(\hat{x}; d) = \psi(d)$ for each $d \in \mathbb{R}^2$. The claimed result then follows immediately from Proposition 2.4.2. □

The Tsoukalas-Mitsos convex relaxations (Tsoukalas and Mitsos, 2014) of composite functions 2.5.1 are based entirely on analogous optimal-value functions. This supports the idea that a subgradient of Tsoukalas-Mitsos convex relaxations of two variables can be calculated by applying the compass difference.

4.2 Mathematical Background

This section summarizes Theorem 3 in (Hogan, 1973), which may be used to compute directional derivatives of an optimal-value function.

Assumption 4.2.1. *Consider a convex set* $X \subset \mathbb{R}^p$ *and a set* $Y \subset \mathbb{R}^n$*,* $x \in X$ $y \in Y$*. Consider a function* $f : \mathbb{R}^p \times \mathbb{R}^n \to [-\infty, +\infty]$*, and a function* $g : \mathbb{R}^p \times \mathbb{R}^n \to [-\infty, +\infty]^m$*. Consider the optimal-value problem:*

$$v(y) = \sup f(x, y) \quad \textit{subject to} \quad g(x, y) \leq 0$$

Define an optimal solution set M*,*

$$M(y) = \{x \in X| \quad g(x, y) \leq 0 \quad \textit{and} \quad v(y) \leq f(x, y)\}$$

A point-to-set mapping H *is defined as the set of feasible directions:*

$$H_{(x,y)}(d) \equiv \{w|g(x + \lambda w, y + \lambda d) \leq 0 \textit{ and } x + \lambda w \in X \quad \forall \quad 0 < \lambda \leq \lambda(x, y, d, w)\}.$$

Proposition 4.2.2. *(Hogan, 1973, Theorem 3) Consider the setup of Assumption 4.2.1, and suppose* X *is a nonempty convex set, and that* $-f$ *and* g *are convex on* $X \times Y$*. At* $\bar{y} \in Y$*,* $v(\bar{y})$ *is finite, and* $\hat{x} \in M(\bar{y})$*. Then the directional derivative of* v *at* $\bar{y}$ *in the direction* $d \in \mathbb{R}^n$ *is*

$$v'(y; d) = \sup_{w \in H_{(x,y)}(d)} f'(\hat{x}, \bar{y}; w, d).$$

4.3 Subgradient Computation

This section shows how to use compass differences to calculate a subgradient of multivariate McCormick relaxations in $\mathbb{R}^2$. Directional derivatives obtained from Hogan's Theorem (Hogan, 1973, Theorem 3) are used to form the compass difference.

Definition 4.3.1. *Consider the same set up as Definition 2.5.2. Let* $I = \{1, \cdots, m\}$, *at some specific* $\hat{z} \in Z$, *define the following:*

- *A set* $M(\hat{z}) = \{x \in X|\ g^{cv}(\hat{z}) \geq F^{cv}(x)$ *and* $f_i^{cv}(\hat{z}) \leq x_i \leq f_i^{cc}(\hat{z}) \quad \forall i \in I\}$.
- *A set of feasible direction* $H_{(x,\hat{z})}(d) \equiv \{w | f^{cv}(\hat{z}+\lambda d) \leq x+\lambda w \leq f^{cc}(\hat{z}+\lambda d)$, *and* $x + \lambda w \in X$ *for all sufficient small* $\lambda > 0\}$

Theorem 4.3.2. *Consider the notation in Definition 2.5.2 and the in Definition 4.3.1, when* $Z \subset \mathbb{R}^2$ *and* $X \subset \mathbb{R}^m$ *is a nonempty convex set. At specific* $\hat{z} \in Z$, *and* $\hat{x} \in M(\hat{z})$, *the directional derivative of* g^{cv} *at* $\hat{z}$, *in the direction* $d \in \mathbb{R}^2$ *is:*

$$[g^{cv}]'(\hat{z}; d) = \min_{w \in H_{(\hat{x},\hat{z})}(d)} \{[F^{cv}]'(\hat{x}; w))\} \tag{4.3.1}$$

Then, a subgradient of the function $g^{cv}(\hat{z})$ *is :*

$$\frac{1}{2}\begin{bmatrix} [g^{cv}]'(\hat{z}; (1,0)) - [g^{cv}]'(\hat{z}; (-1,0)) \\ [g^{cv}]'(\hat{z}; (0,1)) - [g^{cv}]'(\hat{z}; (0,-1)) \end{bmatrix}$$

Proof. F^{cv} is convex on x. Define a constrain function for Equation 2.5.1 to be function $k(z,x) = \begin{bmatrix} f^{cv}(z) - x \\ -f^{cc}(z) + x \end{bmatrix}$. Since f^{cv} and $-f^{cc}$ are both convex on z, $f^{cv}(z) - x$

and $-f^{cc}(z) + x$ are convex with respect to (x, z). Then, g^{cv} is directionally differentiable due to Proposition 4.2.2, with its directional derivatives given by Equation (4.3.1).

By using Definition 2.4.1 , the compass difference of $g^{cv}(z)$ is $\Delta^{\oplus} g(z)$, given as follow:

$$\Delta^{\oplus} g(z) = \frac{1}{2} \begin{bmatrix} [g^{cv}]'(\hat{z}; (1, 0)) - [g^{cv}]'(\hat{z}; (-1, 0)) \\ [g^{cv}]'(\hat{z}; (0, 1)) - [g^{cv}]'(\hat{z}; (0, -1)) \end{bmatrix} .$$

Considering Proposition 2.4.2 before, we conclude that $\Delta^{\oplus} g(z) \in \partial g^{cv}(z)$.

□

Chapter 5

Sensitivity Analysis for Multivariate McCormick Relaxations

This section provides a new subgradient result and directional derivative result for Tsoukalas-Mitsos relaxations of composite functions. (Tsoukalas and Mitsos, 2014) This material is intended for publication; a manuscript is currently in preparation (Yuan and Khan, 2020).

5.1 Background

Tsoukalas and Mitsos (Tsoukalas and Mitsos, 2014) provide a "multivariate McCormick" framework for convex/concave relaxations of composition functions. This result can be used to underestimate/overestimate nonconvex problems in global optimization. Tsoukalas and Mitsos also provide subgradients for this multivariate

McCormick relaxation. However, to use this subgradient result, a dual optimization problem must to be solved. In this chapter a new method for computing sensitivity results of multivariate McCormick relaxations is developed. Multivariate McCormick convex relaxations are formulated as nonlinear convex programming problems. Properties of Karush-Kuhn-Tucker (KKT) multipliers and subgradient chain rules are used to get whole subdifferentials of multivariate McCormick relaxations. The advantage of this approach is once the relaxation is evaluated, then all information for tractably calculating the subdifferential is known. There is no need for solving a dual optimization problem.

In essence, the new method obtains sensitivity information for NLP (nonlinear programming). Sensitivity analysis describes how a system behaves in response to changes in system's parameters. Nonsmoothness appears frequently in NLP, since optimal-value functions for NLPs with smooth objectives and constrains are typically nonsmooth (Danskin, 1966). Nonsmooth models are continuous but not differentiable everywhere. Thus, multivariate McCormick relaxations are typically nonsmooth models. Sensitivity information is critical in nonsmooth optimization. For example, a typical subgradient method (Scholtes, 2012, Theorem 2.1) uses a subgradient at each iteration to approximate the optimal solution in nonsmooth convex/concave optimization, so that the overall method converges. Similarly, cutting plane methods, bundle methods and level methods use subgradients at each iteration to form piece-wise linear approximations for minimizing a convex function (Hiriart-Urruty and Lemaréchal, 2013b; Nesterov, 2018). Relevant sensitivity information in this nonsmooth optimization context is considered to be directional derivatives and subgradients.

There are other applicable sensitivity analysis theories for NLP. Stechlinski, Khan and Barton calculate B-subdifferential elements of primal and dual variables in parametric NLP solutions when the active index set is changing. (Stechlinski *et al.*, 2018) In this chapter, however, the whole B-subdifferential is obtained. Danskin gives a way to obtain directional derivatives for optimization problems as the solutions of related optimization problems in a general setting. (Bertsekas, 1997, Proposition B.25) There are special requirements for the objective function in Danskin's theorem: when doing minimization, the objective function must be concave. Due to this constraint, Danskin's theorem cannot apply to evaluating directional derivatives for multivariate McCormick relaxation. Similarly, Hogan's result (Hogan, 1973, Theorem 3) also describes directional derivatives for optimal-value functions. Nevertheless, although the optimal-value functions in this chapter satisfy Hogan's assumptions, our directional derivative results do not appear to follow directly from Hogan's results.

To address this problem, this chapter uses the properties of relationship between subdifferentials and directional derivative (Hiriart-Urruty and Lemaréchal, 2013a) and our new subgradients result to evaluate directional derivatives of multivariate McCormick relaxation.

In terms of optimization of algorithms, Mitsos et al. show that a vector forward mode of AD (Automatic differentiation) can automatically construct convex or affine relaxations of algorithms for global optimization and can also obtain subgradients of classical McCormick relaxations (Mitsos *et al.*, 2009). This implies that the new subgradients in this chapter can be calculated by vector forward AD mode as well since the same subgradient chain rule applied. In Beckers and Nauman also obtain a reverse AD mode for computing subgradients for classical McCormick relaxations. (Beckers *et al.*, 2012) The subgradients in this chapter can also be calculated by reverse AD mode. Additionally, directional derivatives in this paper can be computed by the (non-vector) forward AD.

This chapter extends the product-rule and fractional term applications by Tsoukalas and Mitsos (Tsoukalas and Mitsos, 2014) and gives numerical examples of sensitivity results on both. Also, a case study example provides subgradients to a certain convex envelope (Khajavirad and Sahinidis, 2013, Corollary 1). In terms of future applications, we expect that this new subgradient result for multivariate McCormick relaxation can be applied to dynamic global optimization methods. (Song and Khan, 2020)

This chapter is structured as follows. Section 5.2 summarizes basic mathematical background: including concepts of piecewise differentiable functions. Section 5.3 presents new methods for subgradients propagation for multivariate McCormick relaxations. Section 5.4 demonstrates methods for calculating directional derivatives for multivariate McCormick relaxation in the following cases: the general case; when the objective function is piecewise differentiable; and when the objective function is differentiable. Section 5.5 describes several examples for illustration which are implemented in Matlab.

5.2 Mathematical Background

Definition 5.2.1. *For any $\sigma \in \mathbb{R}$, let σ^+ denote $\sigma^+ = \max(0, \sigma)$, and let σ^- denote $\sigma^- = \min(0, -\sigma)$. Observe that $[-\sigma]^+ = \sigma^-$, and $[-\sigma]^- = \sigma^+$ for each $\sigma \in \mathbb{R}$.*

5.2.1 Piecewise Differentiable Functions

This section shows a definition of piecewise differentiable functions and the associated set of essentially active indices. This will be used in Section 5.4 as one of the cases.

Definition 5.2.2. *(Scholtes, 2012, Chapter 4.1) Given a open set $X \subset \mathbb{R}^n$, consider a function $F : X \to \mathbb{R}^m$. This function F is called piecewise differentiable (PC^1) at $x_0 \in X$, if there exists a neighborhood $U \subset X$ of x_0 and a finite collection of C^1 selection functions: $f_j : X \to \mathbb{R}^n, j = 1, \cdots, k$, such that F is continuous on U, and if $F(x) \in \{f_1(x), ..., f_k(x)\}$ for every $x \in U$.*

The essentially active indices of F at x_0 are:

$$I_F^e(x_0) = \{j \in \{1, \ldots, k\} | x_0 \in \text{cl}(\text{int}\{x \in U | f(x) = f_j(x)\})\}. \tag{5.2.1}$$

The essentially active functions F^e of F at x_0 are:

$$F^e(x_0) = \{f_j \mid j \in I_F^e(x_0)\}$$

Scholtes (Scholtes, 2012) shows that $I_F^e(x_0)$ is always nonempty.

Lemma 5.2.3. *Consider a closed convex set $X \subset \mathbb{R}^m$, a PC^1-function $F : X \to \mathbb{R}$ and a convex continuous function $c : \mathbb{R}^m \to \mathbb{R}^n$. Then, at point a $x_0 \in X$:*

$$\max\{c(\sigma) : \sigma \in \partial F(x_0)\} = \max\{c(\sigma) : \sigma \in \partial f^*(x_0), f^* \in F^e(x_0)\}. \tag{5.2.2}$$

Proof. The function F is piecewise differentiable. From (Scholtes, 2012, Proposition

4.3.1), the subdifferential of F at x is:

$$\partial F(x) = conv\{\nabla f_j(x) | j \in I_F^e(x)\},$$

where ∇ denotes the gradient.

The mapping $\sigma \in \mathbb{R}^m \mapsto c(\sigma)$ is convex. The feasible set of the first NLP in equation (5.2.2) ($\partial F(x)$) is convex. Through a result (Rockafellar, 1970, Corollary 32.3.2) concerning concave minimization and convex maximization: some extreme point of $\partial F(x)$ is a maximum for the first optimization problem (5.2.2).

Through Definition 5.2.2, the function F involves active selection function in F^e at x_0. So

$$\max\{c(\sigma) : \sigma \in \partial F(x_0)\} = \max\{c(\sigma) : \sigma \in \partial f^*(x_0), f^* \in F^e(x_0)\}.$$

□

5.3 Subgradient Characterization

Lemma 5.3.1. *Let $X \subset \mathbb{R}^m$ and $C \subset \mathbb{R}^m$ be nonempty compact convex sets, and define a set $\Phi := \{(\phi^{cv}, \phi^{cc}) : \phi^{cv} \in C, -\phi^{cc} \in C, \phi^{cv} \leq -\phi^{cc}\}$. Consider a continuous convex function $F^{cv} : X \to \mathbb{R}$ and a function $h : \Phi \to \mathbb{R}$, for which*

$$h(\phi^{cv}, \phi^{cc}) = \min\{F^{cv}(x) : -x \leq -\phi^{cv}, x \leq -\phi^{cc}\}. \tag{5.3.1}$$

Let $\hat{x}$ be an optimal solution of the right-hand-side optimization problem in Equation (5.3.1). Let $I = \{1, 2 \cdots, m\}$. The subdifferential of h at $(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \in \Phi$ is given *by:*

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) = \left\{ \begin{bmatrix} \sigma^+ + a \\ \sigma^- + a \end{bmatrix} : \sigma \in \ \partial F^{cv}(\hat{x}); a \in \mathbb{R}^m, a \geq 0, \right. \\ \left. a_i = 0 \textit{ whenever } \hat{\phi}_i^{cv} \neq -\hat{\phi}_i^{cc}, \textit{ for any } i \in I \right\} \tag{5.3.2}$$

Proof. The Lagrangian L for the right-hand-side optimization problem in Equation (5.3.1) is:

$$L(x, \mu) = F^{cv}(x) + \sum_{i=1}^{m} (\mu_i^{cv}(-x_i + \phi_i^{cv}) + \mu_i^{cc}(x_i + \phi_i^{cc})), \tag{5.3.3}$$

where $X \subset \mathbb{R}^m$ and multipliers $\mu^{cv}, \mu^{cc} \in \mathbb{R}^m$. Let $M(x)$ denote the associated set of Lagrange multipliers (μ^{cv}, μ^{cc}).

According to (Hiriart-Urruty and Lemaréchal, 2013a, §VII Propositions 3.1.1 & 3.1.4), $\hat{x}$ is an optimal solution of the right-hand-side optimization problem in Equation (5.3.1), so it also minimizes $L(\cdot, \mu^{cv}, \mu^{cc})$ in Equation (5.3.3).

Since the NLP in (5.3.1) is convex and is linearly constrained, the Karush-Kuhn-Tucker (KKT) optimality conditions are necessary and sufficient for optimality. $\hat{x}$ solves (5.3.1), thus, $\hat{x}$ also satisfies the nonsmooth KKT condition (Hiriart-Urruty and Lemaréchal, 2013a, §VII. Theorem 2.1.4). So there exist $\sigma \in \partial F^{cv}(\hat{x})$ and $\mu^{cv}, \mu^{cc} \in \mathbb{R}^m$ for which:

$$\begin{aligned} &\sigma + \sum_{i=1}^{m} (-\mu_i^{cv} + \mu_i^{cc}) = 0 \\ &\mu_i^{cv} \geq 0, \mu_i^{cc} \geq 0 \\ &\mu_i^{cv}(-\hat{x}_i + \phi_i^{cv}) = 0, \quad \mu_i^{cc}(\hat{x}_i + \phi_i^{cc}) = 0 \text{ for } i = 1, \ldots, m. \end{aligned} \tag{5.3.4}$$

Consider a function $P : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ and $(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \in \Phi$, for which, for each $w, y \in \mathbb{R}^m$

$$P(w, y) = \inf\{F^{cv}(x) : \hat{\phi}^{cv} - x \leq w, \hat{\phi}^{cc} + x \leq y\}. \tag{5.3.5}$$

P is convex. According to (Hiriart-Urruty and Lemaréchal, 2013a, §VII. 3.3), then $P(0, 0) = h(\hat{\phi}^{cv}, \hat{\phi}^{cc})$.

According to (Hiriart-Urruty and Lemaréchal, 2013a, §VII. Theorem 3.3.2), any multipliers $\mu^{cv}, \mu^{cc} \in M(\hat{x})$ satisfy: for each $w, y \in \mathbb{R}^m$ it holds that

$$P(w, y) \geq P(0, 0) - \mu^{cv} w - \mu^{cc} y,$$

and so, by (Hiriart-Urruty and Lemaréchal, 2013a, §VI. Definition 1.2.1),

$$\begin{bmatrix} -\mu^{cv} \\ -\mu^{cc} \end{bmatrix} \in \partial P(0, 0). \tag{5.3.6}$$

Since $\hat{\phi}^{cv} - \hat{x} \leq \hat{\phi}^{cv} - \phi^{cv}$ and $\hat{\phi}^{cc} + \hat{x} \leq \hat{\phi}^{cc} - \phi^{cc}$, by substituting Equation (5.3.1) into (5.3.5), the result is:

$$h(\phi^{cv}, \phi^{cc}) \equiv P(\hat{\phi}^{cv} - \phi^{cv}, \hat{\phi}^{cc} - \phi^{cc}).$$

According to (Bertsekas, 1997, Theorem 2.9.9), the subdifferential for h at any

(ϕ^{cv}, ϕ^{cc}) is then:

$$\partial h(\phi^{cv}, \phi^{cc}) = \{-\nu : \quad \nu \in \partial P(\hat{\phi}^{cv} - \phi^{cv}, \hat{\phi}^{cc} - \phi^{cc})\}$$

Thus, the subdifferential for h at $(\hat{\phi}^{cv}, \hat{\phi}^{cc})$ is:

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) = \{-\nu : \quad \nu \in \partial P(0, 0)\} \tag{5.3.7}$$

Equations (5.3.6) and (5.3.7) together yield

$$\begin{bmatrix} \mu^{cv} \\ \mu^{cc} \end{bmatrix} \in \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}),$$

which also means,

$$M(\hat{x}) \subset \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}), \tag{5.3.8}$$

We have already verified that if $\begin{bmatrix} \mu^{cv} \\ \mu^{cc} \end{bmatrix} \in M(\hat{x})$, then $M(\hat{x}) \subset \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc})$. For the converse, first assume $\begin{bmatrix} \mu^{cv} \\ \mu^{cc} \end{bmatrix} \in \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc})$, and we wish to show that $\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \subset M(\hat{x})$. Then, for any $(\phi^{cv}, \phi^{cc}) \in \Phi$,

$$h(\phi^{cv}, \phi^{cc}) \geq h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) + \mu^{cv}(\phi^{cv} - \hat{\phi}^{cv}) + \mu^{cc}(\phi^{cc} - \hat{\phi}^{cc}). \tag{5.3.9}$$

Since $h(\phi^{cv}, \phi^{cc}) \equiv P(\hat{\phi}^{cv} - \phi^{cv}, \hat{\phi}^{cc} - \phi^{cc})$ and $h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \equiv P(0, 0)$, with the substitutions $w = \hat{\phi}^{cv} - \phi^{cv}$ and $y = \hat{\phi}^{cc} - \phi^{cc}$ for each $w, y \in \mathbb{R}^m$, Equation (5.3.9) becomes:

$$P(w, y) \geq P(0, 0) - \mu^{cv} w - \mu^{cc} y,$$

which means,

$$\begin{bmatrix} -\mu^{cv} \\ -\mu^{cc} \end{bmatrix} \in \partial P(0, 0).$$

According to (Hiriart-Urruty and Lemaréchal, 2013a, §VI. Theorems 3.3.2 & 3.3.3) $\partial P(0,0) = -M(\hat{x})$. So $\begin{bmatrix} \mu^{cv} \\ \mu^{cc} \end{bmatrix}$ are multipliers of the primal optimization problem in (5.3.4): and so $\begin{bmatrix} \mu^{cv} \\ \mu^{cc} \end{bmatrix} \in M(\hat{x})$. This means

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \subset M(\hat{x}) \tag{5.3.10}$$

Thus, by (5.3.8) and (5.3.10), $\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \subset \partial M(\hat{x})$ and $M(\hat{x}) \subset \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc})$, and so:

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) = M(\hat{x}) \tag{5.3.11}$$

The next step is using the KKT conditions (5.3.4) to evaluate the multipliers (μ^{cv}, μ^{cc}). For any $\sigma \in \partial F^{cv}(\hat{x})$, then at the point $(\hat{\phi}^{cv}, \hat{\phi}^{cc})$, the multipliers of the

NLP (5.3.1) satisfy:

$$\sigma_i + (-\mu_i^{cv} + \mu_i^{cc}) = 0,$$
$$\mu_i^{cv} \geq 0, \mu_i^{cc} \geq 0,$$
$$\mu_i^{cv}(-\hat{x}_i + \hat{\phi}_i^{cv}) = 0, \quad \mu_i^{cc}(\hat{x}_i + \hat{\phi}_i^{cc}) = 0 \text{ for } i = 1, \dots, m.$$

Since $\hat{\phi}^{cv} \leq \hat{x} \leq -\hat{\phi}^{cc}$, using the equations above, we may evaluate (μ^{cv}, μ^{cc}) in three separate cases (for each $i \in I = \{1, \cdots, m\}$):

- Case I: Suppose $\hat{\phi}_i^{cv} < x_i$. Then, because $\mu_i^{cv}(-\hat{x}_i + \hat{\phi}_i^{cv}) = 0$, we can conclude $\mu_i^{cv} = 0$. Moreover, $\sigma_i + (-\mu_i^{cv} + \mu_i^{cc}) = 0$ implies $\mu_i^{cc} = -\sigma_i$; Also $\mu_i^{cv} \geq 0$ implies $\sigma_i \leq 0$. Lastly, due to $\mu_i^{cc}(\hat{x}_i + \hat{\phi}_i^{cc}) = 0$, so $x_i = -\hat{\phi}_i^{cc}$.
- Case II: Suppose $x_i < -\hat{\phi}_i^{cc}$. Following similar arguments as Case I, we can conclude that $\mu_i^{cc} = 0$, $\mu_i^{cv} = \sigma_i$, $\sigma_i \geq 0$ and $x_i = \hat{\phi}_i^{cv}$.
- Case III: Suppose $\hat{\phi}_i^{cv} = \hat{x}_i = -\hat{\phi}_i^{cc}$. This case is continued below.

In case I,II,

$$\mu_i^{cv} = \sigma_i^+$$
$$\text{and} \quad \mu_i^{cc} = \sigma_i^-$$

If these case hold for all $i \in I$, then, by Definition 5.2.1, the corresponding subdifferential of h is

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) = \left\{ \begin{bmatrix} \sigma^+ \\ \sigma^- \end{bmatrix} : \sigma \in \partial F^{cv}(\hat{x}) \right\}.$$

The special Case III (if $\hat{\phi}_i^{cv} = x_i = -\hat{\phi}_i^{cc}$), according to KKT conditions (5.3.4), μ_i^{cv}, μ_i^{cc} for any $i \in I$ satisfy:

$$\begin{aligned} \mu_i^{cv} - \mu_i^{cc} &= \sigma_i, \\ \mu_i^{cv} \geq 0, \mu_i^{cc} &\geq 0 \end{aligned} \tag{5.3.12}$$

Equation (5.3.12) has infinitely many solutions μ_i^{cv}/μ_i^{cc}. Assume for any $i \in I$, $\mu_i^{cv} = \sigma_i^+ + a_i$ and $\mu_i^{cc} = \sigma_i^- + b_i$, where $a \in R^m$, $b \in R^m$ are unknowns. Equation (5.3.12) implies:

$$\begin{aligned} \sigma_i^+ + a_i - \sigma_i^- - b_i &= \sigma_i \\ \sigma_i^+ + a_i \geq 0, \sigma_i^- + b_i &\geq 0. \end{aligned} \tag{5.3.13}$$

Next, we determine the value of a_i and b_i by looking at the signs of σ_i

For any $i \in I$, if $\sigma_i \geq 0$, then $\sigma_i^+ = \sigma_i$ and $\sigma_i^- = 0$, Equation (5.3.13) becomes

$$\begin{aligned} \sigma_i + a_i - 0 - b_i &= \sigma_i \\ \sigma_i + a_i \geq 0, b_i &\geq 0. \end{aligned}$$

This implies $a_i = b_i$, and both $a_i \geq 0, b_i \geq 0$.

For any $i \in I$, if $\sigma_i < 0$, then $\sigma_i^+ = 0$ and $\sigma_i^- = -\sigma_i$, Equation (5.3.13) becomes

$$\begin{aligned} 0 + a_i + \sigma_i - b_i &= \sigma_i \\ a_i \geq 0, -\sigma_i + b_i &\geq 0. \end{aligned}$$

This also implies $a_i = b_i$, and both $a_i \geq 0, b_i \geq 0$.

In general, for any $i \in I$, no matter the sign of σ_i is in Case III, always $a_i = b_i$ and $a_i \geq 0$.

So collecting all these cases, the subdifferential of h is given by Equation (5.3.2).

□

Theorem 5.3.2. *Consider the sets and functions from Definition 2.5.2. Let $\hat{x}$ denote an optimal solution of the right-hand-side optimization problem in Equation (2.5.1), and let $I = \{1, 2 \cdots, m\}$.*

The subdifferential of g^{cv} at $z \in Z$ is given by:

$$\begin{aligned}\partial g^{cv}(z) = \Big\{ \sum_{i=1}^{m} [(\sigma_i^+ + a_i)v_{(i)} - (\sigma_i^- + a_i)w_{(i)}] : \sigma \in \ \partial F^{cv}(\hat{x});\ v_{(i)} \in \partial f_i^{cv}(z), \\ w_{(i)} \in \partial f_i^{cc}(z) \quad \forall i \in I, a \in \mathbb{R}^m, a \geq 0; \\ \textit{if } f_i^{cv}(z) \neq f_i^{cc}(z), \textit{then } a_i = 0,\ \textit{for any } i \in I \Big\}\end{aligned} \tag{5.3.14}$$

Proof. Consider Equation (2.5.1) in Definition 2.5.2 and Equation (5.3.1), and observe that

$$g^{cv}(z) \equiv h(f_1^{cv}(z), \cdots, f_m^{cv}(z), -f_1^{cc}(z), \cdots, -f_m^{cc}(z))$$

From the convexity of F^{cv} in Equation (2.5.1), the function h is increasing and convex as a perturbation function of a convex problem. (Boyd and Vandenberghe, 2004) Moreover,

$$\partial[-f_i^{cc}](z) = \{w : -w \in \partial f_i^{cc}(z)\}.$$

By applying (Tsoukalas and Mitsos, 2014, Lemma 1) and Lemma 5.3.1, the subdifferential of g^{cv} becomes Equation (5.3.14).

□

Corollary 5.3.3. *Consider the setup of Theorem 5.3.2. If any one of the following conditions hold, $g^{cv}(z)$ is differentiable:*

- *All of F^{cv}, f^{cv}, f^{cc} are differentiable.*
- *For all $i \in I$, $\partial f_i^{cv}(z) = 0$ and $\partial f_i^{cc}(z) = 0$.*
- *All elements in $\partial F^{cv}(\hat{x})$ are 0.*
- *All elements in $\partial F^{cv}(\hat{x})$ are smaller than 0, and for all $i \in I$ $\partial f_i^{cc}(z) = 0$.*
- *All elements in $\partial F^{cv}(\hat{x})$ are greater than 0, and for all $i \in I$ $\partial f_i^{cv}(z) = 0$.*

5.4 Directional Derivatives

This section shows how to compute directional derivatives for multivariate McCormick relaxations (Tsoukalas and Mitsos, 2014). Several cases will be discussed: the general case under the same setup as Theorem 5.3.2; when the objective function is piecewise differentiable; and when the objective function is differentiable.

Lemma 5.4.1. *Consider the setup of Lemma 5.3.1. Let $\hat{x}$ be an optimal solution of the right-hand-side optimization problem in Equation (5.3.1). Let $I = \{1, 2 \cdots, m\}$. The directional derivative of h at a point $(\hat{\phi}^{cv}, \hat{\phi}^{cc}) \in \Phi$ in the direction (d_1, d_2), for $d_1 \in \mathbb{R}^m$ and $d_2 \in \mathbb{R}^m$, is:*

$$h'((\hat{\phi}^{cv}, \hat{\phi}^{cc}); (d_1, d_2)) = \max \left\{ \sum_{i=1}^{m} \sigma_i^+ d_{1,i} + \sigma_i^- d_{2,i} : \ \sigma \in \partial F^{cv}(\hat{x}) \right\}. \tag{5.4.1}$$

provided that, if $\hat{\phi}_i^{cv} = -\hat{\phi}_i^{cc}$ for any $i \in I$, then an additional requirement needs to be satisfied: $d_{1,i} + d_{2,i} \leq 0$.

Proof. From (Hiriart-Urruty and Lemaréchal, 2013a, Remark 4.1.6), in which directional directive and subdifferentials are related, the directional derivative of h in Equation (5.3.1) becomes:

$$h'((\hat{\phi}^{cv}, \hat{\phi}^{cc}); (d_1, d_2)) = \max\left\{\langle \psi^+, d_1\rangle + \langle \psi^-, d_2\rangle : \begin{bmatrix} \psi^+ \\ \psi^- \end{bmatrix} \in \partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc})\right\} \quad (5.4.2)$$

From Lemma 5.3.1, we know

$$\partial h(\hat{\phi}^{cv}, \hat{\phi}^{cc}) = \left\{ \begin{bmatrix} \sigma^+ + a \\ \sigma^- + a \end{bmatrix} : \sigma \in \ \partial F^{cv}(\hat{x}); a \in \mathbb{R}^m, a \geq 0, \right.$$
$$\left. a_i = 0 \text{ whenever } \hat{\phi}_i^{cv} \neq -\hat{\phi}_i^{cc}, \text{ for any } i \in I \right\},$$

so for each $i \in I$, $\psi_i^+ = \sigma_i^+ + a_i$ and $\psi_i^- = \sigma_i^- + a_i$, $a_i \geq 0$.

Equation (5.4.2) becomes

$$h'((\hat{\phi}^{cv}, \hat{\phi}^{cc}); (d_1, d_2)) = \max_{\sigma \in \partial F^{cv}(\hat{x})} \left\{ \sum_{i=1}^{m} \sigma_i^+ d_{1,i} + \sigma_i^- d_{2,i} + (d_{1,i} + d_{2,i}) a_i : a \in \mathbb{R}^m, a \geq 0, \right.$$
$$\left. a_i = 0 \text{ whenever } \hat{\phi}_i^{cv} \neq -\hat{\phi}_i^{cc}, \text{ for any } i \in I \right\}. \quad (5.4.3)$$

If $\hat{\phi_i^{cv}} = -\hat{\phi_i^{cc}}$ for any $i \in I$, due to the feasible direction of h, $d_{1,i} + d_{2,i} \leq 0$. To maximize term $(d_{1,i} + d_{2,i})a_i$ for any $i \in I$, then $a_i = 0$, Equation (5.4.3) becomes

$$h'((\hat{\phi}^{cv}, \hat{\phi}^{cc}); (d_1, d_2)) = \max\left\{ \sum_{i=1}^{m} \sigma_i^+ d_{1,i} + \sigma_i^- d_{2,i} : \ \sigma \in \partial F^{cv}(\hat{x}) \right\}.$$

□

Theorem 5.4.2. *Consider the setup of Theorem 5.3.2. Define* $c_i = [f_i^{cv}]'(z;d),\ d_i = [f_i^{cc}]'(z;d) \quad \forall i \in I$. *The directional derivative of* g *at* z *in the direction* $d \in \mathbb{R}^n$ *is:*

$$[g^{cv}]'(z;d) = \max\left\{\sum_{i=1}^{m}(\sigma_i^+ c_i - \sigma_i^- d_i) :\ \sigma \in \partial F^{cv}(\hat{x})\right\}. \tag{5.4.4}$$

where we require that, if $f_i^{cv}(z) = f_i^{cc}(z)$ *for any* $i \in I$, *then* $c_i + d_i \leq 0$.

Proof. The result follows from Definition 5.2.1, Lemma 5.4.1 and the chain rule (Scholtes, 2012, Theorem 3.1.1):

$$g^{cv}(z) = h(f^{cv}(z), -f^{cc}(z))$$

According to the directional derivative chain rule (Scholtes, 2012, Theorem 3.1.1)

$$\begin{aligned}[g^{cv}]'(z;d) &= h'(f^{cv}(z), -f^{cc}(z); [f^{cv}]'(z;d), -[f^{cc}]'(z;d)) \\ &= \max\left\{\sum_{i=1}^{m}(\sigma_i^+[f_i^{cv}]'(z;d) - \sigma_i^-[f_i^{cc}]'(z;d)) : \sigma \in \partial F^{cv}(\hat{x})\right\}.\end{aligned}$$

□

Corollary 5.4.3. *Consider the setup of Theorem 5.4.2, and suppose that* F^{cv} *is piecewise differentiable. Define* $c_i = [f_i^{cv}]'(z;d),\ d_i = [f_i^{cc}]'(z;d) \quad \forall i \in I$. *Also let* $F^e(\hat{x})$ *be the essential active function of* F^{cv} *at* $\hat{x}$.

The directional derivative of g *at* z *in direction* $d \in \mathbb{R}^n$ *is:*

$$[g^{cv}]'(z;d) = \max\left\{\sum_{i=1}^{m}(\sigma_i^+ c_i - \sigma_i^- d_i) : \quad \sigma \in \partial f^*(\hat{x}), f^* \in F^e(\hat{x})\right\}.$$

Proof. Since the mapping: $\sigma \in \mathbb{R}^m \longmapsto \sum_{i=1}^{m}(\sigma_i^+ c_i - \sigma_i^- d_i)$ is both convex and concave.

The result follows from Theorem 5.4.2 and Lemma 5.2.3 □

Corollary 5.4.4. *Consider the setup of Theorem 5.4.2, and suppose that* F^{cv} , f^{cv} *and* f^{cc} *are differentiable. Define* $\sigma = \nabla F^{cv}(\hat{x})$; $v_{(i)} = \nabla f_i^{cv}(z)$ *and* $w_{(i)} = \nabla f_i^{cc}(z)$ $\forall i \in I$ *and also define a direction* $d \in \mathbb{R}^n$. *The gradient of* g^{cv} *at* z *is:*

$$\nabla g^{cv}(z) = \sum_{i=1}^{m} (\sigma_i^+ v_{(i)} - \sigma_i^- w_{(i)}). \tag{5.4.5}$$

Proof. The result follows from Theorem 5.4.2.

Define $v_{(i)} = \nabla f_i^{cv}(z)$, $w_{(i)} = \nabla f_i^{cc}(z) \quad \forall i \in I$, then, for any $d \in \mathbb{R}^n$ $[f_i^{cv}]'(z;d) = \langle v_{(i)}, d\rangle$ and $[f_i^{cc}]'(z;d) = \langle w_{(i)}, d\rangle$. Since $\sigma = \nabla F^{cv}(\hat{x})$, the directional derivative of g^{cv} in direction d becomes

$$\begin{aligned} [g^{cv}]'(z;d) &= \max \left\{ \sum_{i=1}^{m} (\sigma_i^+ \langle v_{(i)}, d\rangle - \sigma_i^- \langle w_{(i)}, d\rangle) : \ \sigma \in \partial F^{cv}(\hat{x}) \right\} \\ &= \sum_{i=1}^{m} (\sigma_i^+ \langle v_{(i)}, d\rangle - \sigma_i^- \langle w_{(i)}, d\rangle) \end{aligned}$$

Since all of F^{cv}, $f^{cv}(z)$ and $f^{cc}(z)$ are differentiable , due to Corollary 5.3.3, g^{cv} is differentiable: $\langle \nabla g^{cv}(z), d\rangle = [g^{cv}]'(z;d)$.

□

5.5 Examples

5.5.1 Directional Derivative Computation

Product Rule

In this section, Theorem 5.4.2 and Corollary 5.4.3 will be used to provide directional derivatives for bilinear products of functions described by (Tsoukalas and Mitsos, 2014, Corollary 5). All assumptions here are the same as (Tsoukalas and Mitsos, 2014, Corollary 5). Consider the function $mult(x_1, x_2) = x_1x_2$. The convex/concave envelopes of $mult(x_1, x_2)$ on the domain $[x_1^L, x_1^U] \times [x_2^L, x_2^U]$ by (Al-Khayyal and Falk, 1983; McCormick, 1976) are:

$$mult^{cv}(x_1, x_2) = max\{x_2^U x_1 + x_1^U x_2 - x_1^U x_2^U, x_2^L x_1 + x_1^L x_2 - x_1^L x_2^L\}$$
$$mult^{cc}(x_1, x_2) = min\{x_2^L x_1 + x_1^U x_2 - x_1^U x_2^L, x_2^U x_1 + x_1^L x_2 - x_1^L x_2^U\}$$

Consider a nonempty convex set $Z \in \mathbb{R}^n$. Let $g(z) = mult(f_1(z), f_2(z))$, with $f_1 : Z \to \mathbb{R}$, $f_2 : Z \to \mathbb{R}$. Also f_i^L, f_i^U denote lower and upper bounds for f_i on Z, and let f_i^{cv},f_i^{cc} be convex and concave relaxation of f_i on Z. Then, the Tsoukalas-Mitsos convex relaxation of g on Z is:

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} & \max\left\{f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U, f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L\right\} \\ \text{s.t.} \quad & f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z}). \end{aligned}$$

Example 5.5.1. *Consider* $g(z) = mult(f_1(z), f_2(z)) = f_1(z)f_2(z)$ *with* $f_1(z) = (z +$

$1)^2$ *and* $f_2(z) = (z-1)^6 + 1$ *on* $Z = [0, 2] \in \mathbb{R}$. *Bounds of* f_i *on* Z *are calculated by hand to be* $f_1^L = 1, f_1^U = 9$, $f_2^L = 1$ *and* $f_2^U = 2$. *The following functions are relaxations of* f_i *in* Z*:*

$$f_1^{cv}(z) = (z+1)^2, \quad f_1^{cc}(z) = 1 + 4z$$
$$f_2^{cv}(z) = (z-1)^6 + 1, \quad f_2^{cc}(z) = 2$$

The multivariate McCormick relaxation of $g(z)$ *by Definition 2.5.2 becomes*

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{x_i \in \left[f_i^L, f_i^U\right]} & F^{cv}(x) \\ s.t. \quad & f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z}) \end{aligned} \tag{5.5.1}$$

with

$$\begin{aligned} F^{cv}(x) &= \max\left\{Q_1(x), Q_2(x)\right\}, \\ \textit{where} \quad Q_1(x) &= f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U = 2x_1 + 9x_2 - 18 \\ Q_2(x) &= f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L = x_1 + x_2 - 1 \end{aligned}$$

To calculate $g^{cv}(z)$, *the optimization problem* (5.5.1) *is expressed as an LP below* *and solved in Matlab using the LP solver 'linprog':*

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{\substack{x_i \in [f_i^L, f_i^U]; \\ t \in \mathbb{R}}} \quad & t \\ s.t. \quad & f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U \le t \\ & f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L \le t \\ & f_1^{cv}(\mathbf{z}) \le x_1 \le f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \le x_2 \le f_2^{cc}(\mathbf{z}) \end{aligned} \tag{5.5.2}$$

F^{cv} is a piecewise differentiable function, and Figure 5.1 shows g^{cv} is also a nonsmooth function. In this case, the directional derivative of g^{cv} at the point $z = \hat{z} = 1.75$ will be tested to illustrate Corollary 5.4.3, since this is a nonsmooth point of g^{cv}. In two direction $d_1 = 1$ and $d_2 = -1$ will be found in this example.

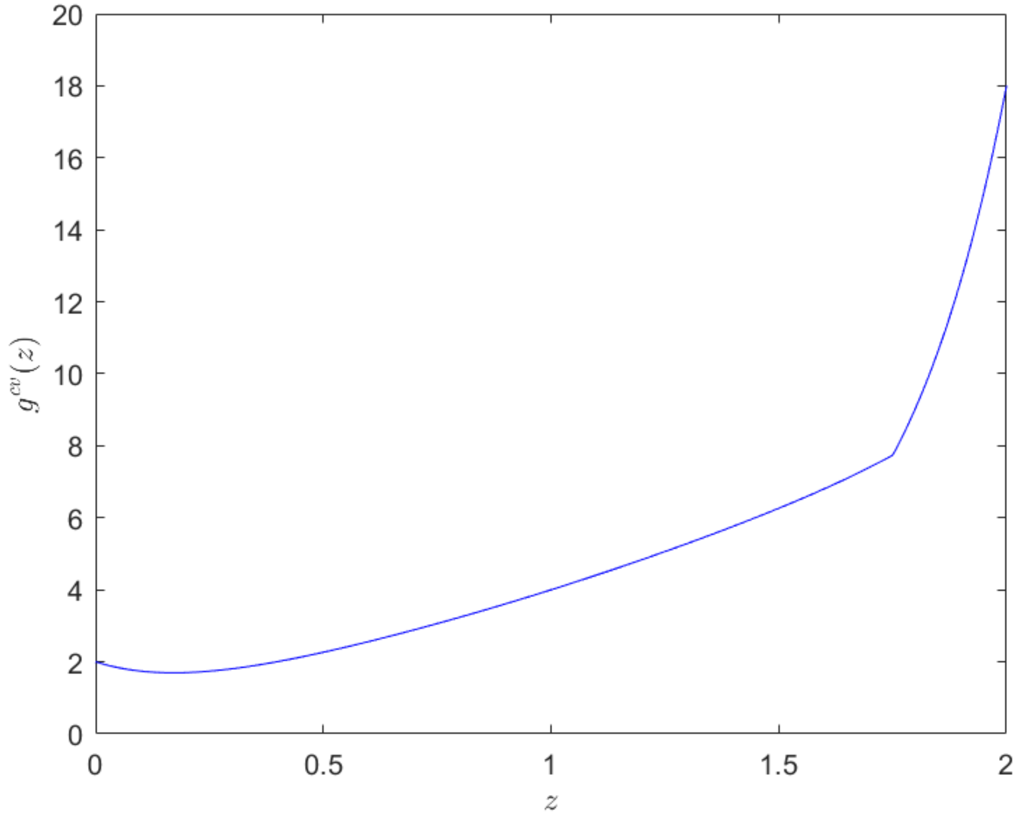

Figure 5.1: The relaxation $g^{cv}(z)$ on $z = [0, 2]$ in example 5.5.1.

At point $z = \hat{z} = 1.75$, $g^{cv}(\hat{z}) = 7.7405$, *the optimal solution of* (5.5.1) *is* $\hat{x}_1 = 7.5626$, $\hat{x}_2 = 1.1780$. Q_1 *and* Q_2 *are essentially active function of* $F^{cv}(\hat{x}_1, \hat{x}_2)$. *According to Definition 5.2.2, the essentially active functions of* F^{cv} *at* $\hat{x}$ *are:*

$$F^e(\hat{x}_1, \hat{x}_2) = \{Q_1, Q_2\}$$

The partial derivatives of Q_1 Q_2 *at* $(\hat{x}_1, \hat{x}_2)$ *are* $\frac{\partial Q_1}{\partial \hat{x}_1} = 2$, $\frac{\partial Q_1}{\partial \hat{x}_2} = 9$, $\frac{\partial Q_2}{\partial \hat{x}_1} = 1$ *and*

$\frac{\partial Q_2}{\partial \hat{x}_2} = 1$. *According to Lemma 5.2.3, the subdifferential of* F^{cv} *at* $\hat{x}$ *is*

$$\begin{aligned}\partial F^{cv}(\hat{x}) &= conv\{\nabla f_j(\hat{x}) | j \in I^e_{F^{cv}}(\hat{x})\} \\ &= conv\{\nabla Q_1(\hat{x}), \nabla Q_2(\hat{x})\}.\end{aligned}$$

Define $v_{(i)} = \nabla f_i^{cv}(z)$, $w_{(i)} = \nabla f_i^{cc}(z) \quad \forall i \in I$, *at* $z = \hat{z} = 1.75 = 1.75$, $v_{(1)} = (2\hat{z}+2)$, $v_{(2)} = 6(\hat{z}-1)^5$, $w_{(1)} = 4$ *and* $w_{(2)} = 0$. *Let* $a_i \equiv [f_i^{cv}]'(\hat{z}; d) = \langle v_{(i)}, d\rangle$, $b_i \equiv [f_i^{cc}]'(\hat{z}; d) = \langle w_{(i)}, d\rangle$ *for all* $i \in I$.

Applying Corollary 5.4.3, the directional derivative of g^{cv} *at* $\hat{z} = 1.75$ *in direction* $d_1 = 1$ *becomes:*

$$[g^{cv}]'(z; d) = \max\left\{\sum_{i=1}^{m}(\sigma_i^+ c_i - \sigma_i^- d_i) : \quad \sigma \in \partial f^*(\hat{x}), f^* \in F^e(\hat{x})\right\} = 23.8125.$$

The directional derivative of g^{cv} *at* $\hat{z} = 1.75$ *in direction* $d_2 = -1$ *becomes:*

$$[g^{cv}]'(z; d) = \max\left\{\sum_{i=1}^{m}(\sigma_i^+ c_i - \sigma_i^- d_i) : \quad \sigma \in \partial f^*(\hat{x}), f^* \in F^e(\hat{x})\right\} = -6.9238.$$

In Figure 5.2 below, on $T = [0, 0.2]$, *the solid blue line is* $g^{cv}(\hat{z} + td_1)$ *plotted against* t *when* $\hat{z} = 1.75$ *and* $d_1 = 1$ *are fixed.*

The dotted red line $V : \mathbb{R} \to \mathbb{R}$ *shows an affine function constructed with slope* $[g^{cv}]'(\hat{z}; d_1)$ *when* $\hat{z} = 1.75$ *and the direction* $d_1 = 1$ *are fixed:*

$$V(t) = g^{cv}(\hat{z} + td_1) + [g^{cv}]'(\hat{z}; d_1)(t - 0).$$

Here $[g^{cv}]'(\hat{z}; d_1)$ *is the slope of* $V(t)$.

In the definition of the directional derivative given by Definition 2.3.1,

$$f'(x;d) = \lim_{t \to 0} \frac{f(x+td) - f(x)}{t}$$

Then the directional derivative of f *at* x *is the slope of the tangent line at* $t = 0$ *in* $f(x+td) vs\ t$ *when* x *and* d *are fixed.*

Figure 5.2 shows that the graph of V *is always below* $g^{cv}(\hat{z} + td_1)$ *and is tangent to* $g^{cv}(\hat{z} + td_1)$ *at* $t = 0$*. Then,* $[g^{cv}]'(\hat{z}; d_1)$ *is verified to be the directional derivative of* g^{cv} *at* $\hat{z}$ *in direction* d_1*.*

Similar to $T = [0, 0.2]$*, in Figure 5.3, the solid blue line shows* $g^{cv}(\hat{z} + td_2)$ *plotted against* t *when* $\hat{z} = 1.75$ *and direction* $d_2 = -1$ *are fixed.*

The red dotted line $W(t) : \mathbb{R} \to \mathbb{R}$ *in Figure 5.3 is constructed by* $[g^{cv}]'(\hat{z}; d_2)$ *when* $\hat{z} = 1.75$ *and* $d_2 = -1$ *are fixed:*

$$W(t) = g^{cv}(\hat{z} + td_2) + g'^{cv}(\hat{z}; d_2)(t - 0)$$

here $[g^{cv}]'(\hat{z}; d_2)$ *is the slope of* $W(t)$*.*

The graph of $W(t)$ *is also tangent to* $g^{cv}(\hat{z} + td_2)$ *at* $t = 0$*. It is thus verified to be the directional derivative of* g^{cv} *at* $\hat{z}$ *in direction* d_2*.*

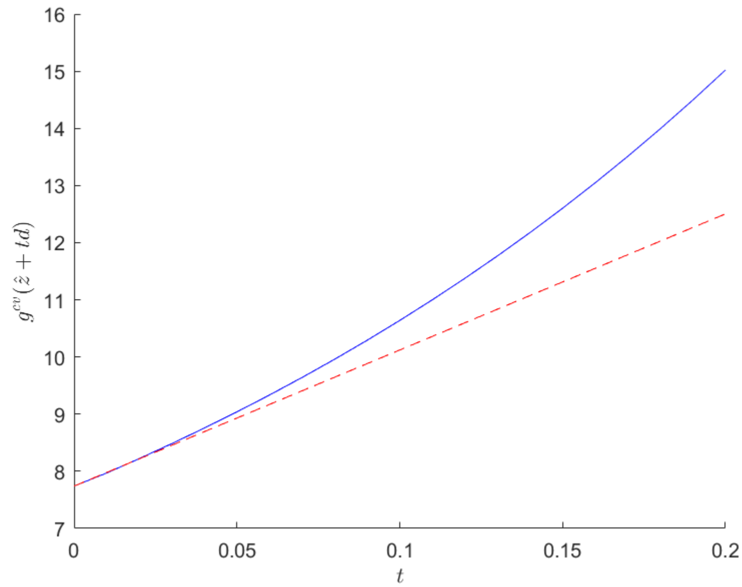

Figure 5.2: At fixed $\hat{z} = 1.75$, the relaxation $g^{cv}(\hat{z} + td_1)$ in Example 5.5.1 with $d_1 = 1$ on $T = [0, 0.2]$ (top). Tangent line $V(t)$ (bottom) is constructed by directional derivative $[g^{cv}]'(\hat{z}; d_1)$

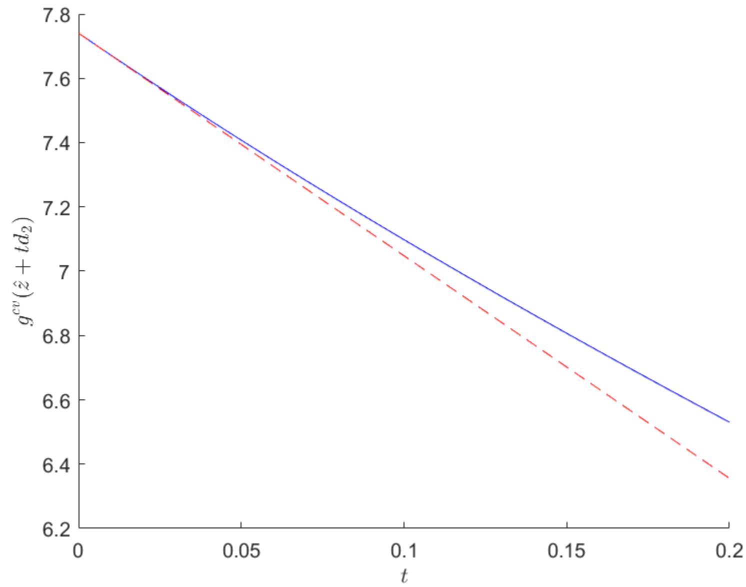

Figure 5.3: At fixed $\hat{z} = 1.75$, the relaxation $g^{cv}(\hat{z} + td_2)$ in Example 5.5.1 with $d_2 = -1$ on $T = [0, 0.2]$ (top). Tangent line $W(t)$ (bottom) is constructed by the directional derivative $[g^{cv}]'(\hat{z}; d_2)$.

5.5.2 Subgradient

Product Rule

In this section, Theorem 5.3.2 will be used to provide subgradients of relaxations of bilinear products of functions same as in Section 5.5.1. The two examples involve two and three variables, respectively. These two examples are smooth functions, which shows Theorem 5.3.2 is valid for computing gradients for smooth functions.

Example 5.5.2. *Consider* $g(z) = mult(f_1(z), f_2(z)) = f_1(z)f_2(z)$ *with* $f_1(z) = (z + 1)^2$ *and* $f_2(z) = (z - 1)^6 + 1$ *on* $Z = [0, 1] \subset \mathbb{R}$. *Bounds of* f_i *calculated by hand are*

$f_1^L = 1, f_1^U = 4$ *and* $f_2^L = 1, f_2^U = 2$. *Convex and concave relaxations of* f_i *are:*

$$f_1^{cv}(z) = (z+1)^2, \quad f_1^{cc}(z) = 1 + 3z$$
$$f_2^{cv}(z) = (z-1)^6 + 1, \quad f_2^{cc}(z) = 2 - z$$

The multivariate McCormick relaxation of g^{cv} *according to Definition 2.5.2 is*

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} & F^{cv}(x) \\ s.t. \quad & f_1^{cv}(\mathbf{z}) \le x_1 \le f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \le x_2 \le f_2^{cc}(\mathbf{z}) \end{aligned} \tag{5.5.3}$$

with

$$\begin{aligned} F^{cv}(x) &= \max\{Q_1(x), Q_2(x)\} \\ \text{where} \quad Q_1(x) &= f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U \\ Q_2(x) &= f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L \end{aligned}$$

To evaluate g^{cv}, *the optimization problem* (5.5.3) *is expressed as an LP below and* *calculated in Matlab using 'linprog'. This is shown in Figure 1:*

$$
\begin{aligned}
g^{cv}(\mathbf{z}) = \min_{\substack{x_i \in [f_i^L, f_i^U];\\ t\in\mathbb{R}}} \quad & t \\
s.t. \quad & f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U \leq t \\
& f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L \leq t \\
& f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z}) \\
& f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z})
\end{aligned}
\tag{5.5.4}
$$

In order to calculate a subgradient of g^{cv} at z using Equation (5.3.14) *in Theorem 5.3.2, then elements of $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ and $\partial F_i^{cv}(\hat{x})$ need to be known. $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ are easily to be calculated by hand in this case:*

$$
\begin{aligned}
v_1 = 2z + 2; &\quad v_1 \in \partial f_1^{cv}(z) \\
w_1 = 3; &\quad w_1 \in \partial f_1^{cc}(z) \\
v_2 = 6(z+1)^5; &\quad v_2 \in \partial f_2^{cv}(z) \\
w_2 = -1; &\quad w_2 \in \partial f_2^{cc}(z)
\end{aligned}
$$

Now, $F^{cv}(\hat{x}) = \max\{Q_1(\hat{x}), Q_2(\hat{x})\}$, Q_1 and Q_2 are both affine functions, and the difference between them is $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = x_1 + 3x_2 - 7$. Two cases can be considered when describing some $\sigma \in \partial F^{cv}(\hat{x})$:

- *if $\triangle Q(\hat{x}) \geq 0$,then $F^{cv}(\hat{x}) = Q_1(\hat{x})$ and we may choose $\sigma \in \partial Q_1(\hat{x})$, so $\sigma = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$*

- *if* $\triangle Q(\hat{x}) < 0$,*then* $F^{cv}(\hat{x}) = Q_2(\hat{x})$ *and* $\sigma \in \partial Q_2(\hat{x})$: $\sigma = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

We now compute a subgradient of g^{cv} *at the point* $\hat{z} = 0.5$*: The optimal solution of* (5.5.4) *is* $g^{cv}(\hat{z}) = 2.2656$ *and* $\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} 2.2500 \\ 1.0156 \end{bmatrix}$*, which was computed in Matlab, and*

$$v_1 = 2\hat{z} + 2 = 3$$
$$w_1 = 3$$
$$v_2 = 6(\hat{z} - 1)^5 = -0.1875$$
$$w_2 = -1$$

Here, $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = \hat{x}_1 + 3\hat{x}_2 - 7 = -1.7032 < 0$*, so in Theorem 5.3.2, we may choose* $\sigma \in \partial Q_1(\hat{x})$*; so* $\sigma = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$*. Then by using Definition 5.2.1 ,* σ^+, σ^- *becomes:*

$$\sigma^+ = \begin{bmatrix} 1 \\ 1 \end{bmatrix}; \sigma^- = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since $f_i^{cv}(\hat{z}) \neq f_i^{cv}(\hat{z})$ *for each* $i \in I$, $a_i = 0$ *for all* $i \in I$.

A subgradient of g^{cv} *at* $\hat{z} = 0.5$ *by Equation* (5.3.14) *is*

$$\sum_{i=1}^{2}(\sigma_i^+ v_i - \sigma_i^- w_i) = 2.8125 =: s$$
$$s \in \partial g^{cv}(\hat{z})$$

Then, the tangent function $K(z) : \mathbb{R} \to \mathbb{R}$ *to* g^{cv} *at* $\hat{z} = 0.5$ *is constructed using this subgradient* s*:*

$$K(z) = g^{cv}(z) + s(z - \hat{z})$$

Figure 5.4 shows the orignal product $g(z) = (z+1)^2((z-1)^6+1)$ *and its convex relaxation* g^{cv} *on* $Z = [0, 1]$*.* $K(z)$ *is evidently the tangent line of* g^{cv} *at* $\hat{z} = 0.5$ *and is always below* g^{cv}*. According to Definition 2.3.2, the subdifferential of function* f *at* x *is set of vectors* s *satisfying:*

$$f(y) \geq f(x) + \langle s, y - x \rangle, \quad \forall\ y \in \mathbb{R}^n.$$

Thus, this result says: if s *is subgradient, then* K *would always below original function* g^{cv}*. If* s *is not subgradient,* K *would lie above or cross over* g^{cv}*. Here, the graph of* K *is always below* g^{cv}*. So* s *is readily verified to be a subgradient of* g^{cv} *at* $\hat{z}$*.*

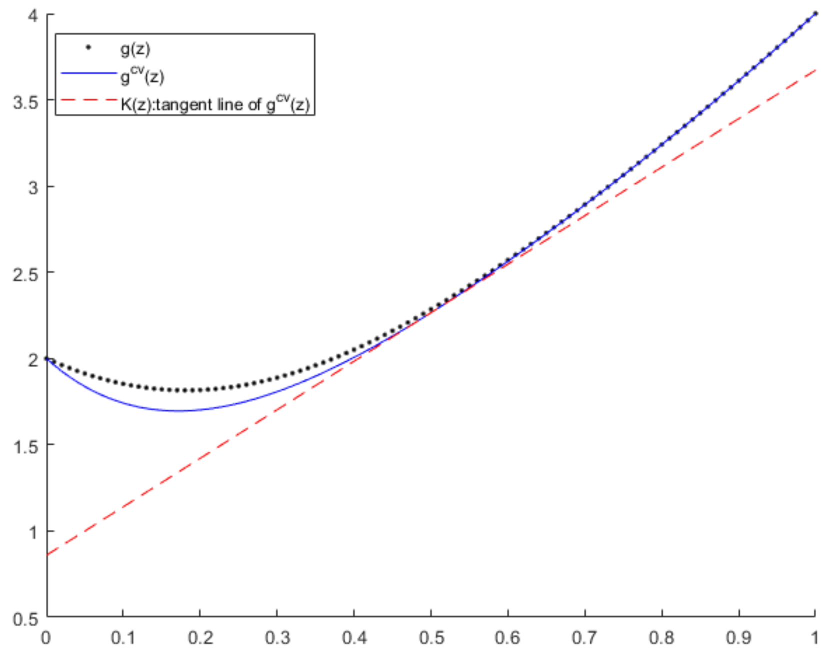

Figure 5.4: Plot of $g(z) = (z+1)^2((z-1)^6+1)$ from Example 5.5.2 and its convex relaxation $g^{cv}(z)$ on $Z = [0,1]$. $K(z)$ is the tangent line of g^{cv} at $\hat{z} = 0.5$, constructed using the computed subgradient

Example 5.5.3. *Consider* $g(z) = mult(f_1(z), f_2(z))$ *with* $f_1(z) = z_1^2 - z_2^2 + 1$ *and* $f_2(z) = (z_1 - 1)^6 + z_2 + 1$ *on* $Z = [0,1] \subset \mathbb{R}^2$*. BoundS of* f_i *calculated by hand are* $f_1^L = 0, f_1^U = 2$ *and* $f_2^L = 1, f_2^U = 3$*. Convex and concave relaxations of each* f_i *are:*

$$f_1^{cv}(z) = z_1^2 + z_2^2 - 2, \quad f_1^{cc}(z) = 3z_1 + 3z_2 + 2$$

$$f_2^{cv}(z) = (z_1 - 1)^6 + z_2 + 1, \quad f_2^{cc}(z) = 2 - z_1 + z_2.$$

As in Example 5.5.2, the multivariate McCormick relaxation of g *by Definition*

2.5.2 is

$$g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} F^{cv}(x)$$
$$s.t. \quad f_1^{cv}(\mathbf{z}) \le x_1 \le f_1^{cc}(\mathbf{z}) \tag{5.5.5}$$
$$f_2^{cv}(\mathbf{z}) \le x_2 \le f_2^{cc}(\mathbf{z})$$

with

$$F^{cv}(x) = \max\{Q_1(x), Q_2(x)\}$$
$$\textit{where} \quad Q_1(x) = f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U$$
$$Q_2(x) = f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L.$$

To evaluate the $g^{cv}(z)$, the optimization problem Equation (5.5.5) *is expressed as an LP below and solved in Matlab using 'linprog' which can be seen in Figure 5.5:*

$$g^{cv}(\mathbf{z}) = \min_{\substack{x_i \in [f_i^L, f_i^U];\\ t \in \mathbb{R}}} \quad t$$
$$s.t. \quad f_2^U x_1 + f_1^U x_2 - f_1^U f_2^U \le t$$
$$f_2^L x_1 + f_1^L x_2 - f_1^L f_2^L \le t \tag{5.5.6}$$
$$f_1^{cv}(\mathbf{z}) \le x_1 \le f_1^{cc}(\mathbf{z})$$
$$f_2^{cv}(\mathbf{z}) \le x_2 \le f_2^{cc}(\mathbf{z})$$

In order to calculate a subgradient of $g^{cv}(z)$ using Equation (5.3.14) *in Theorem 5.3.2, we do the following.*

Set:

$$v = \begin{bmatrix} \frac{\partial f_1^{cv}}{\partial z_1}(z) & \frac{\partial f_1^{cv}}{\partial z_2}(z) \\ \frac{\partial f_2^{cv}}{\partial z_1}(z) & \frac{\partial f_2^{cv}}{\partial z_2}(z) \end{bmatrix} = \begin{bmatrix} 2z_1 & 2z_2 \\ 6(z_1-5)^5 & 1 \end{bmatrix}$$

$$w = \begin{bmatrix} \frac{\partial f_1^{cc}}{\partial z_1}(z) & \frac{\partial f_1^{cc}}{\partial z_2}(z) \\ \frac{\partial f_2^{cc}}{\partial z_1}(z) & \frac{\partial f_2^{cc}}{\partial z_2}(z) \end{bmatrix} = \begin{bmatrix} 3 & 3 \\ -1 & 1 \end{bmatrix}.$$

Now, $F^{cv}(\hat{x}) = \max\{Q_1(\hat{x}), Q_2(\hat{x})\}$, *where* Q_1 *and* Q_2 *are affine functions, so the difference between them is* $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = (f_2^U - f_2^L)\hat{x}_1 + (f_1^U - f_1^L)\hat{x}_2 - (f_1^U f_2^U - f_1^L f_2^L) = 2\hat{x}_1 + 2\hat{x}_2 - 6$. *Two cases can be considered when describing some* $\sigma \in \partial F^{cv}(\hat{x})$*:*

- *if* $\triangle Q(\hat{x}) \geq 0$*,then* $F^{cv}(\hat{x}) = Q_1(\hat{x})$ *and we may choose* $\sigma \in \partial Q_1(\hat{x})$*, so* $\sigma = \begin{bmatrix} f_2^U \\ f_1^U \end{bmatrix}$
- *if* $\triangle Q(\hat{x}) < 0$*,then* $F^{cv}(\hat{x}) = Q_2(\hat{x})$ *and* $\sigma \in \partial Q_2(\hat{x})$ *is valid, so* $\sigma = \begin{bmatrix} f_2^L \\ f_1^L \end{bmatrix}$

We now compute a the subgradient of g^{cv} *at point* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$*: The optimal solution of* (5.5.6) *is* $g^{cv}(\hat{z}) = -1.5$ *and* $\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} -1.5 \\ 1.5168 \end{bmatrix}$ *which was computed in*

Matlab, and

$$v = \begin{bmatrix} 1 & 1 \\ -0.1875 & 1 \end{bmatrix}$$

$$w = \begin{bmatrix} 3 & 3 \\ -1 & 1 \end{bmatrix}.$$

Here, $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = 2\hat{x}_1 + 2\hat{x}_2 - 6 = -5.9664 < 0$, *so in Theorem 5.3.2 we may choose* $\sigma \in \partial Q_1(\hat{x})$*; so* $\sigma = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. *Then by using Definition 5.2.1 ,* σ^+, σ^- *becomes:*

$$\sigma^+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \sigma^- = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since $f_i^{cv}(\hat{z}) \neq f_i^{cv}(\hat{z})$ *for each* i, $a_i = 0$ *for all* $i \in I$.

By Equation (5.3.14), *the subgradient of* g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *is*

$$\begin{bmatrix} \sum_{i=1}^{2}(\sigma_i^+ v_{i,1} - \sigma_i^- w_{i,1}) \\ \sum_{i=1}^{2}(\sigma_i^+ v_{i,2} - \sigma_i^- w_{i,2}) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} =: s$$

$$s \in \partial g^{cv}(\hat{z})$$

Then, the subtangent function $M : \mathbb{R}^2 \to \mathbb{R}^2$ *to* g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *is constructed* *using subgradient s:*

$$M(z) = g^{cv}(z) + s^T(z - \hat{z}).$$

Figure 5.5 shows the original product rule $g(z) = (z_1^2 - z_2^2 + 1)((z_1 - 1)^6 + z_2 + 1)$ *on* $Z = [0,1] \times [0,1]$ *and its convex relaxation* g^{cv}*.* M *is evidently a subtangent plane of* g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *and is always below* g^{cv}*. Same as Example 5.5.2, according to (Hiriart-Urruty and Lemaréchal, 2013a, §VI, Definition 1.2.1), the graph of* M *is always below* g^{cv}*, so* s *is readily verified to be a subgradient of* g^{cv} *at* $\hat{z}$*.*

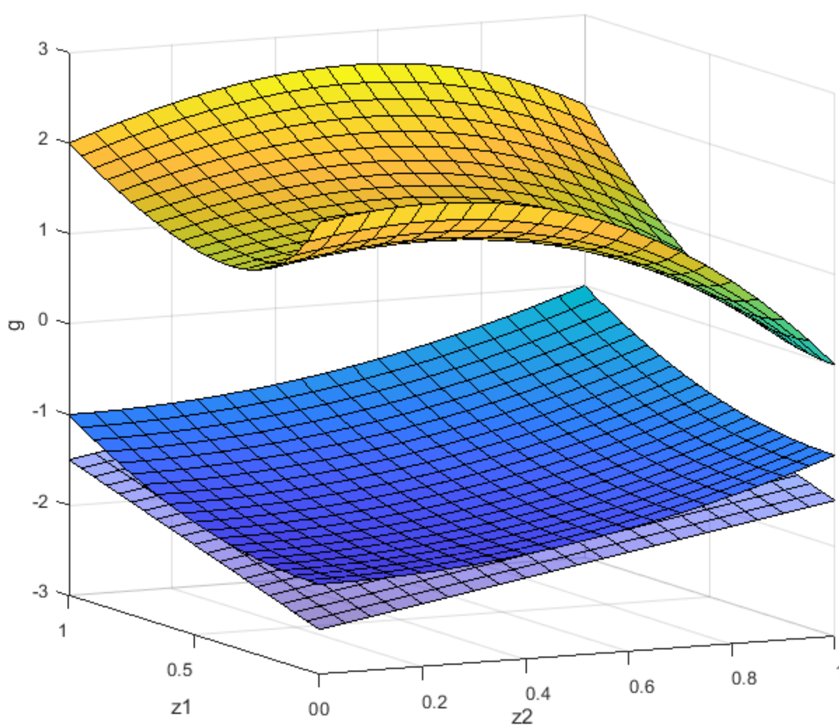

Figure 5.5: Top: Plot of $g(z) = (z_1^2 - z_2^2 + 1)((z_1 - 1)^6 + z_2 + 1)$ from Example 5.5.3 on $Z = [0,1] \times [0,1]$; Middle: convex relaxation g^{cv} of g. Bottom: M is subtangent plane of g^{cv} at $\hat{z} = [0.5, 0.5]$, constructed using obtained subgradient.

Fractional Terms

In this section, Theorem 5.3.2 will be used to compute a subgradient for bilinear fraction terms considered in (Tsoukalas and Mitsos, 2014, Corollary 6). All assumptions are the same as (Tsoukalas and Mitsos, 2014, Corollary 6). The two examples invilve two and three variables, respectively. These two examples' relaxations are nonsmooth functions, which shows Theorem 5.3.2 is valid for computing subgradients for nonsmooth functions.

Consider the function $div(x_1, x_2) = \frac{x_1}{x_2}$. A convex relaxation of $div(x_1, x_2)$ on the domain $[x_1^L, x_1^U] \times [x_2^L, x_2^U]$ (Tsoukalas and Mitsos, 2014, Equation 30) is:

$$div^{cv}(x_1, x_2) = max\{\frac{x_1}{x_2^U} + \frac{x_1^L}{x_2} - \frac{x_1^L}{x_2^U}, \frac{x_1}{x_2^L} + \frac{x_1^U}{x_2} - \frac{x_1^U}{x_2^L}\}$$

Let $g(z) = div(f_1(z), f_2(z))$, with $f_1 : Z \subset \mathbb{R}^n \to \mathbb{R}$, $f_2 : Z \subset \mathbb{R}^n \to \mathbb{R}$. Let f_i^L, f_i^U denote lower and upper bounds for f_i, and let f_i^{cv},f_i^{cc} be convex and concave relaxations of f_i on Z. Then:

$$\begin{aligned} g^{cv}(z) = \min_{x_i \in \left[f_i^L, f_i^U\right]} & \max\left\{\frac{x_1}{f_2^U} + \frac{f_1^L}{x_2} - \frac{f_1^L}{f_2^U}, \frac{x_1}{f_2^L} + \frac{f_1^U}{x_2} - \frac{f_1^U}{f_2^L}\right\} \\ \text{s.t.} \quad & f_1^{cv}(\mathbf{z}) \le x_1 \le f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \le x_2 \le f_2^{cc}(\mathbf{z}) \end{aligned}$$

is a convex relaxation of g on Z.

Let $F^{cv}(x) \equiv \max\left\{\frac{x_1}{f_2^U} + \frac{f_1^L}{x_2} - \frac{f_1^L}{f_2^U}, \frac{x_1}{f_2^L} + \frac{f_1^U}{x_2} - \frac{f_1^U}{f_2^L}\right\}$ for $x \in \mathbb{R}^2$. By Theorem 5.3.2, the subdifferential of g at z becomes:

$$\partial g^{cv}(z) = \Big\{ \sum_{i=1}^{m} [(\sigma_i^{+} + a_i) v_{(i)} - (\sigma_i^{-} + a_i) w_{(i)}] : \sigma \in \ \partial F^{cv}(\hat{x});\ v_{(i)} \in \partial f_i^{cv}(z),$$
$$w_{(i)} \in \partial f_i^{cc}(z) \quad \forall i \in I, a \in \mathbb{R}^m, a \geq 0;\ \text{if } f_i^{cv}(z) \neq f_i^{cc}(z), \text{then } a_i = 0,\ \text{for any } i \in I \Big\}$$

where $\hat{x}$ denotes one of the optimal solutions of the right-hand-side optimization problem of defining $g^{cv}(z)$.

Example 5.5.4. *Consider* $g(z) = div(f_1(z), f_2(z)) = \frac{f_1(z)}{f_2(z)}$ *with* $f_1(z) = (z+1)^2$ *and* $f_2(z) = (z-1)^6 + 1$ *on* $Z = [0, 1] \subset \mathbb{R}$. *Bounds of* f_i *on* Z *calculated by hand are* $f_1^L = 1, f_1^U = 4$ *and* $f_2^L = 1, f_2^U = 2$. *Convex and concave relaxations of* f_i *on* Z *are:*

$$f_1^{cv}(z) = (z+1)^2, \quad f_1^{cc}(z) = 1 + 3z$$
$$f_2^{cv}(z) = (z-1)^6 + 1, \quad f_2^{cc}(z) = 2 - z$$

The multivariate McCormick relaxation of g *on* Z *by Definition 2.5.2 is*

$$g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} F^{cv}(x)$$
$$s.t. \quad f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z})$$
$$f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z})$$

with

$$\begin{aligned} F^{cv}(x) &= \max\{Q_1(x), Q_2(x)\} \\ \textit{where} \quad Q_1(x) &= \frac{x_1}{f_2^U} + \frac{f_1^L}{x_2} - \frac{f_1^L}{f_2^U} \\ Q_2(x) &= \frac{x_1}{f_2^L} + \frac{f_1^U}{x_2} - \frac{f_1^U}{f_2^L} \end{aligned}$$

To calculate $g^{cv}(z)$ above, since both f_1^L and f_2^L are greater than 0, then, $x_1 = f_1^{cv}, x_2 = f_2^{cc}$. So, if $Q_1(x) \geq Q_2(x)$, then $g^{cv}(z) = Q_1(x)$. If $Q_1(x) \leq Q_2(x)$, then $g^{cv}(z) = Q_2(x)$.

In order to calculate a subgradient of g^{cv} using Equation (5.3.14) *in Theorem 5.3.2, and $\sigma \in \partial F^{cv}(\hat{x})$ and $v_i \in \partial f_i^{cv}(z)$, $w_i \in \partial f_i^{cc}(z)$ for all $i \in I$, then, $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ and $\partial F_i^{cv}(\hat{x})$ need to be known. $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ are easily calculated by hand in this case:*

$$\begin{aligned} v_1 &\in \partial f_1^{cv}(z); \quad v_1 = 2z + 2 \\ w_1 &\in \partial f_1^{cc}(z); \quad w_1 = 3 \\ v_2 &\in \partial f_2^{cv}(z); \quad v_2 = 6(z-1)^5 \\ w_2 &\in \partial f_2^{cc}(z); \quad w_2 = -1 \end{aligned}$$

Now, $F^{cv}(\hat{x}) = \max\{Q_1(\hat{x}), Q_2(\hat{x})\}$, $Q_1(\hat{x})$ and $Q_2(\hat{x})$ are both function in terms of x, the difference between them is $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x})$. Two cases can be considered separately to choose some $\sigma \in \partial F^{cv}(\hat{x})$:

- *if $\triangle Q(\hat{x}) \geq 0$, then $F^{cv}(\hat{x}) = Q_1(\hat{x})$ and we may choose $\sigma \in \partial Q_1(\hat{x})$, so $\sigma =$*

$$\begin{bmatrix} \frac{1}{f_2^U} \\ -\frac{f_1^L}{\hat{x}_2^2} \end{bmatrix}$$

- *if* $\triangle Q(\hat{x}) < 0$, *then* $F^{cv}(\hat{x}) = Q_2(\hat{x})$ *and we may choose* $\sigma \in \partial Q_2(\hat{x})$, *so* $\sigma = \begin{bmatrix} \frac{1}{f_2^L} \\ -\frac{f_1^U}{\hat{x}_2^2} \end{bmatrix}$

Now, we find a subgradient of g^{cv} *at the point* $\hat{z} = 0.5$*: In Matlab,* $g^{cv}(\hat{z}) = 1.2917$ *was computed to be* $\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} 2.25 \\ 1.5 \end{bmatrix}$, *with*

$$v_1 = 2\hat{z} + 2 = 3$$
$$w_1 = 3$$
$$v_2 = 6(\hat{z} - 1)^5 = -0.1875$$
$$w_2 = -1$$

$\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = 0.375 > 0$, *so we may choose* $\sigma \in \partial Q_1(\hat{x})$, *so* $\sigma = \begin{bmatrix} 0.5 \\ -0.4444 \end{bmatrix}$. *Then by using Definition 5.2.1 ,* σ^+, σ^- *becomes:*

$$\sigma^+ = \begin{bmatrix} 0.5 \\ 0 \end{bmatrix}; \sigma^- = \begin{bmatrix} 0 \\ 0.4444 \end{bmatrix}$$

Since $f_i^{cv}(\hat{z}) \neq f_i^{cv}(\hat{z})$ *for each* i, $a_i = 0$ *for all* $i \in I$.

A subgradient of g^{cv} at $\hat{z} = 0.5$ is then

$$\sum_{i=1}^{2}(\sigma_i^+ v_i - \sigma_i^- w_i) = 1.9444 =: s$$
$$s \in \partial g^{cv}(\hat{z})$$

Then, a tangent line $R(z) : \mathbb{R} \to \mathbb{R}$ to g^{cv} at $\hat{z} = 0.5$ in Figure 5.6 and $\hat{z} = 0.63$ in Figure 5.7 are constructed with s:

$$R(z) = g^{cv}(z) + s(z - \hat{z})$$

Figure 5.6 and 5.7 show the original function $g(z) = \frac{(z+1)^2}{(z-1)^6+1}$ and its convex relaxation g^{cv} on $Z = [0, 1]$. $R(z)$ is the tangent line of g^{cv} at $\hat{z} = 0.5, \hat{z} = 0.63$ constructed with the new subgradient and is always below $g^{cv}(z)$. According to definition of subgradient Definition 2.3.2, the subdifferential of function f at x is set of vectors s satisfying:

$$f(y) \geq f(x) + \langle s, y - x\rangle, \quad \forall\ y \in \mathbb{R}^n.$$

Thus, this result says: if s is subgradient, if and only if the graph of R is below the original function g^{cv}. Here, R is always below g^{cv}. So s is readily verified to be a subgradient of g^{cv} at $\hat{x}$.

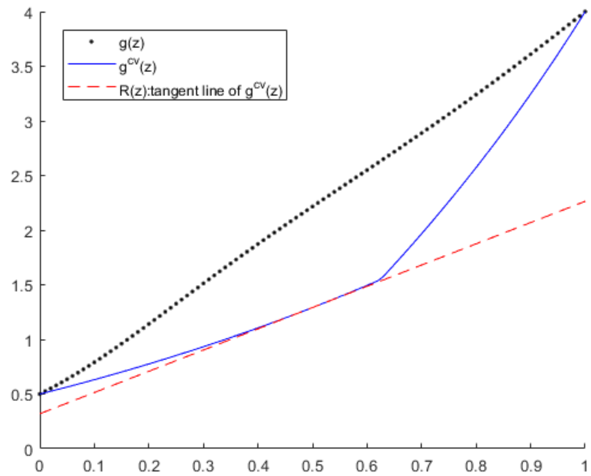

Figure 5.6: Plot of $g(z) = \frac{(z+1)^2}{(z-1)^6+1}$ and its convex relaxation $g^{cv}(z)$ on $Z = [0, 1]$ in Example 5.5.4. $R(z)$ is a subtangent line of g^{cv} at $\hat{z} = 0.5$.

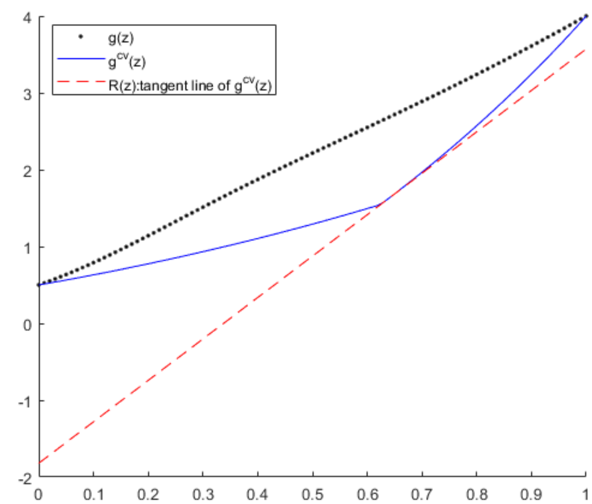

Figure 5.7: Plot $g(z) = \frac{(z+1)^2}{(z-1)^6+1}$ and its convex relaxation $g^{cv}(z)$ on $Z = [0, 1]$ in Example 5.5.4. $R(z)$ is a subtangent line of g^{cv} at $\hat{z} = 0.63$.

Example 5.5.5. *Consider* $g(z) = div(f_1(z), f_2(z)) = \frac{f_1(z)}{f_2(z)}$ *with* $f_1(z) = z_1^2 - z_2^2 + 1$ *and* $f_2(z) = (z_1 - 1)^6 + z_2 + 1$ *on* $Z = [0, 1] \times [0, 1]$*:* $Z \in \mathbb{R}^2$*. Bounds of* f_i *calculated* *by hand are* $f_1^L = 0, f_1^U = 2$ *and* $f_2^L = 1, f_2^U = 3$. *Convex and concave relaxations of* f_i *on* Z *are:*

$$f_1^{cv}(z) = z_1^2 - z_2 + 1, \quad f_1^{cc}(z) = -z_2^2 + z_1 + 1$$
$$f_2^{cv}(z) = (z_1 - 1)^6 + z_2 + 1, \quad f_2^{cc}(z) = 2 - z_1 + z_2.$$

In Example 5.5.2, the multivariate McCormick relaxation of g *by Definition 2.5.2 becomes*

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} & F^{cv}(x) \\ s.t. \quad & f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z}) \end{aligned} \tag{5.5.7}$$

with

$$\begin{aligned} F^{cv}(x) &= \max\{Q_1(x), Q_2(x)\} \\ \text{where} \quad Q_1(x) &= \frac{x_1}{f_2^U} + \frac{f_1^L}{x_2} - \frac{f_1^L}{f_2^U} \\ Q_2(x) &= \frac{x_1}{f_2^L} + \frac{f_1^U}{x_2} - \frac{f_1^U}{f_2^L} \end{aligned}$$

To calculate $g^{cv}(z)$ *above, since both* f_1^L *and* f_2^L *are greater than 0, then,* $x_1 = f_1^{cv}(z), x_2 = f_2^{cc}(z)$. *If* $Q_1(x) \geq Q_2(x)$, *then* $g^{cv}(z) = Q_1(x)$. *If* $Q_1(x) \leq Q_2(x)$, *then* $g^{cv}(z) = Q_2(x)$.

In order to calculate a subgradient of g^{cv} *at* z *using Equation 5.3.14 in Theorem 5.3.2, we proceed similar by Example 5.5.2:*

$$v = \begin{bmatrix} \frac{\partial f_1^{cv}}{\partial z_1}(z) & \frac{\partial f_1^{cv}}{\partial z_2}(z) \\ \frac{\partial f_2^{cv}}{\partial z_1}(z) & \frac{\partial f_2^{cv}}{\partial z_2}(z) \end{bmatrix} = \begin{bmatrix} 2z_1 & -1 \\ 6(z_1-5)^5 & 1 \end{bmatrix}$$

$$w = \begin{bmatrix} \frac{\partial f_1^{cc}}{\partial z_1}(z) & \frac{\partial f_1^{cc}}{\partial z_2}(z) \\ \frac{\partial f_2^{cc}}{\partial z_1}(z) & \frac{\partial f_2^{cc}}{\partial z_2}(z) \end{bmatrix} = \begin{bmatrix} 1 & -2z_2 \\ -1 & 1 \end{bmatrix}.$$

Now, $F^{cv}(\hat{x}) = \max\{Q_1(\hat{x}), Q_2(\hat{x})\}$, $Q_1(\hat{x})$ and $Q_2(\hat{x})$ are both functions in terms of x, the difference between them is $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x})$. Two cases can be considered to determine some $\sigma \in \partial F^{cv}(\hat{x})$:

- *if $\triangle Q(\hat{x}) \geq 0$,then $F^{cv}(\hat{x}) = Q_1(\hat{x})$ and $\sigma \in \partial Q_1(\hat{x})$: $\sigma = \begin{bmatrix} \frac{1}{f_2^U} \\ -\frac{f_1^L}{\hat{x}_2^2} \end{bmatrix}$*
- *if $\triangle Q(\hat{x}) < 0$,then $F^{cv}(\hat{x}) = Q_2(\hat{x})$ and $\sigma \in \partial Q_2(\hat{x})$: $\sigma = \begin{bmatrix} \frac{1}{f_2^L} \\ -\frac{f_1^U}{\hat{x}_2^2} \end{bmatrix}$*

We now compute a subgradient of g^{cv} at the point $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$: The optimal solution of (5.5.7) is $g^{cv}(\hat{z}) = 0.25$ and $\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} 0.75 \\ 2 \end{bmatrix}$, which was computed in Matlab, and

$$v = \begin{bmatrix} 1 & -1 \\ -0.1875 & 1 \end{bmatrix}$$

$$w = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

Here, $\triangle Q(\hat{x}) = Q_1(\hat{x}) - Q_2(\hat{x}) = 0.5 > 0$*, so in Theorem 5.3.2, we may choose* $\sigma \in \partial Q_1(\hat{x})$*, so* $\sigma = \begin{bmatrix} 0.3333 \\ 0 \end{bmatrix}$*. Then by using Definition 5.2.1 ,* σ^+, σ^- *becomes:*

$$\sigma^+ = \begin{bmatrix} 0.3333 \\ 0 \end{bmatrix}; \sigma^- = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since $f_i^{cv}(\hat{z}) \neq f_i^{cv}(\hat{z})$ *for each* i*,* $a_i = 0$ *for all* $i \in I$*.*

A subgradient of g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *is*

$$\begin{bmatrix} \sum_{i=1}^{2}(\sigma_i^+ v_{i,1} - \sigma_i^- w_{i,1}) \\ \sum_{i=1}^{2}(\sigma_i^+ v_{i,2} - \sigma_i^- w_{i,2}) \end{bmatrix} = \begin{bmatrix} 0.3333 \\ -0.3333 \end{bmatrix} =: s.$$

Then, the subtangent function $L : \mathbb{R}^2 \to \mathbb{R}^2$ *to* g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *is constructed using this subgradient* s*:*

$$L(z) = g^{cv}(z) + s^T(z - \hat{z}).$$

Figure 5.8 shows the original function $g(z) = \frac{z_1^2 - z_2^2 + 1}{(z_1 - 1)^6 + z_2 + 1}$ *on* $Z = [0, 1] \times [0, 1]$ *and its convex relaxation* g^{cv}*.* L *is evidently the subtangent plane of* g^{cv} *at* $\hat{z} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}$ *and is always below* $g^{cv}(z)$*. The corresponding subtangent plane* $L(z) : \mathbb{R}^2 \to \mathbb{R}^2$ *to*

$g^{cv}(z)$ *at* $\hat{z} = \begin{bmatrix} 0.6 \\ 0.2 \end{bmatrix}$ *is shown in Figure 5.9. As in Example 5.5.2, according to Definition 2.3.2,* L *is always below* g^{cv}*, so* s *is readily verified to be a subgradient of* g^{cv} *at* $\hat{z}$*.*

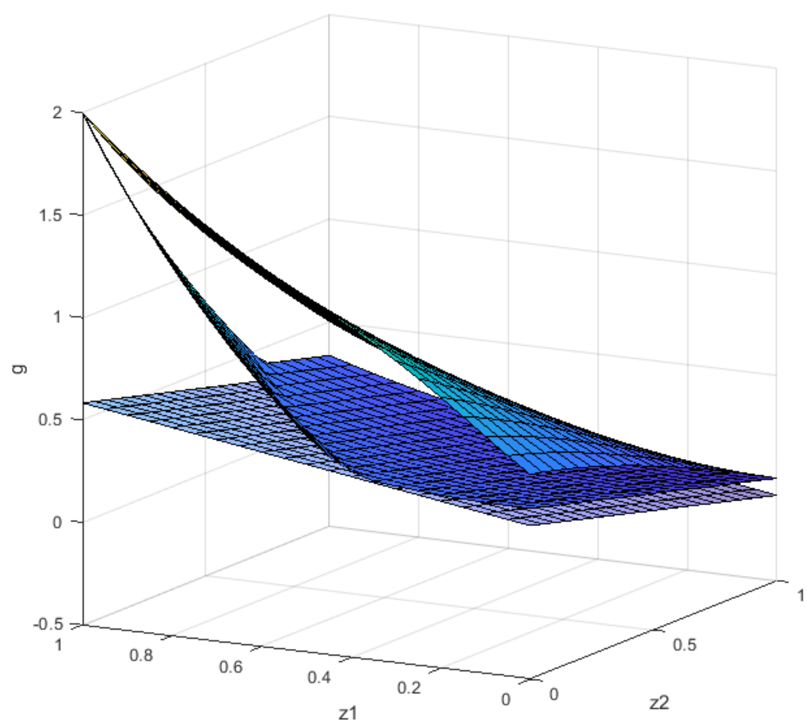

Figure 5.8: Top: plot of $g(z) = \frac{z_1^2 - z_2^2 + 1}{(z_1-1)^6 + z_2 + 1}$ on $Z = [0,1] \times [0,1]$ from Example 5.5.5; Middle: convex relaxation g^{cv} of g. Bottom: L is the subtangent plane of g^{cv} at $\hat{z} = [0.5, 0.5]$ constructed using obtained subgradient.

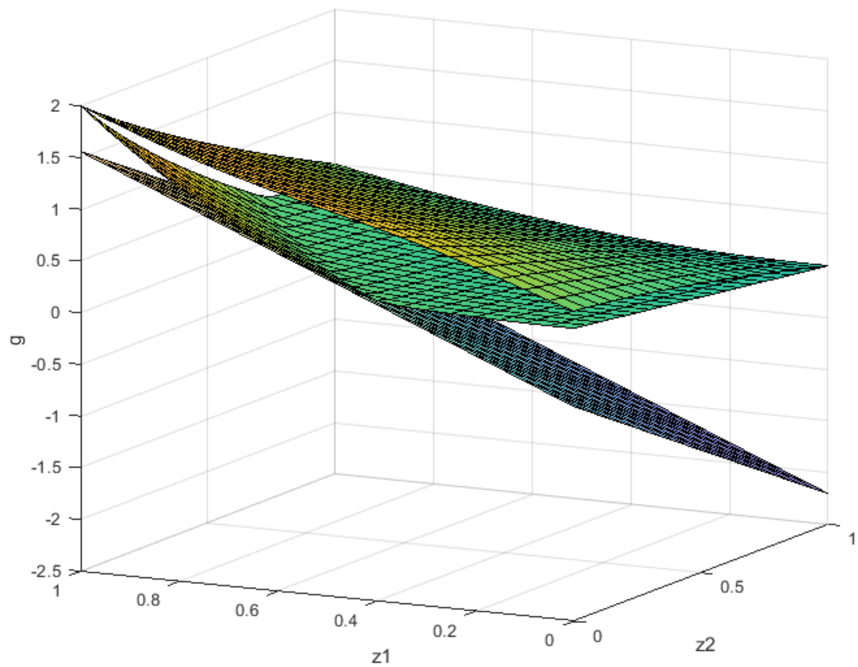

Figure 5.9: Top: Plot of $g(z) = \frac{z_1^2 - z_2^2 + 1}{(z_1-1)^6 + z_2 + 1}$ on $Z = [0,1] \times [0,1]$ from Example 5.5.5; Middle: convex relaxation g^{cv} of g. Bottom: L is the subtangent plane of g^{cv} at $\hat{z} = [0.6, 0.2]$ constructed using obtained subgradient.

Convex Envelope

In this section, Theorem 5.3.2 will be used to provide a subgradient for a nontrivial convex envelope (Khajavirad and Sahinidis, 2013, Corollary 1). Consider the function $F = \frac{\sqrt{x_2}}{x_1^2}$, for $x_1 \in [-2, -1]$ and $x_2 \in [1, 4]$. The convex envelope $F^{cv}(x)$ can be expressed as below (Khajavirad and Sahinidis, 2013, Example 1) :

$$F^{cv}(x) = \begin{cases} \frac{(4-x_2)^3}{3(3x_1+2x_2-2)^2} + \frac{x_2-1}{6}, & \text{if } -2 \leq x_1 \leq -0.14x_2 - 1.45 \\ \frac{(0.09x_2+0.9)^3}{x_1^2}, & \text{if } -0.14x_2 - 1.45 \leq x_1 \leq -0.09x_2 - 0.9 \\ \frac{2(x_2-1)^3}{3(3x_1-x_2+4)^2} + \frac{4-x_2}{3}, & \text{if } -0.09x_2 - 0.9 \leq x_1 \leq -1.0 \end{cases} \tag{5.5.8}$$

Example 5.5.6. *Consider* $g(z) = \frac{\sqrt{f_2(z)}}{f_1(z)^2}$ *with* $f_1(z) = z - 2$ *and* $f_2(z) = z^3 + 2z + 1$ *on* $Z = [0, 1] \subset \mathbb{R}$*. Bounds of* f_i *calculated by hand are* $f_1^L = -2, f_1^U = -1$ *and* $f_2^L = 1, f_2^U = 4$*. Convex and concave relaxations of* f_i *on* Z *are:*

$$f_1^{cv}(z) = z - 2, \quad f_1^{cc}(z) = z - 1$$

$$f_2^{cv}(z) = z^3 + 2z + 1, \quad f_2^{cc}(z) = 3z + 1$$

The multivariate McCormick relaxation of g *according to 2.5.2 is*

$$\begin{aligned} g^{cv}(\mathbf{z}) = \min_{x_i \in [f_i^L, f_i^U]} & F^{cv}(x) \\ s.t. \quad & f_1^{cv}(\mathbf{z}) \leq x_1 \leq f_1^{cc}(\mathbf{z}) \\ & f_2^{cv}(\mathbf{z}) \leq x_2 \leq f_2^{cc}(\mathbf{z}) \end{aligned} \tag{5.5.9}$$

where $F^{cv}(x)$ *is the same in equation* (5.5.8)*.*

In order to calculate a subgradient of g^{cv} *at* z *using Equation* (5.3.14) *in Theorem 5.3.2,then elements of* $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ *and* $\partial F_i^{cv}(\hat{x})$ *need to be known.* $\partial f_i^{cv}(z), \partial f_i^{cv}(z)$ *are easily calculated by hand in this case:*

$$v_1 = 1; \quad v_1 \in \partial f_1^{cv}(z)$$

$$w_1 = 1; \quad w_1 \in \partial f_1^{cc}(z)$$

$$v_2 = 3z^2 + 2; \quad v_2 \in \partial f_2^{cv}(z)$$

$$w_2 = 3; \quad w_2 \in \partial f_2^{cc}(z)$$

These cases below can be considered when describing some $\sigma \in \partial F^{cv}(\hat{x})$:

- *if $-2 \leq x_1 \leq -0.14x_2 - 1.45$, then $\sigma = \begin{bmatrix} \frac{2(x_2-4)^3}{(3x_1+2x_2-2)^3} \\ -\frac{4(4-x_2)^3}{3(3x_1+2x_2-2)^3} - \frac{(4-x_2)^2}{(3x_1+2x_2-2)^2} + \frac{1}{6} \end{bmatrix}$*
- *if $-0.14x_2 - 1.45 \leq x_1 \leq -0.09x_2 - 0.9$, then $\sigma = \begin{bmatrix} -\frac{0.001458(x_2-10)^3}{x_1^3} \\ \frac{0.002187(x_2-10)^2}{x_1^2} \end{bmatrix}$*
- *if $-0.09x_2 - 0.9 \leq x_1 \leq -1.0$, then $\sigma = \begin{bmatrix} -\frac{4(x_2-1)^3}{(3x_1-x_2+4)^3} \\ \frac{4(x_2-1)^3}{3(3x_1-x_2+4)^3} + \frac{2(x_2-1)^2}{(3x_1-x_2+4)^2} - \frac{1}{3} \end{bmatrix}$*

We now compute a subgradient of g^{cv} at point $\hat{z} = 0.5$: The optimal solution of (5.5.9) is $g^{cv}(\hat{z}) = 0.5776$ and $\hat{x} = \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} -1.5 \\ 2.125 \end{bmatrix}$, which was computed in Matlab, and

$$v_1 = 1$$

$$w_1 = 1$$

$$v_2 = 2.75$$

$$w_2 = -3,$$

$so\sigma = \begin{bmatrix} 0.7701 \\ 0.1429 \end{bmatrix}.$

Then by using Definition 5.2.1 , σ^+, σ^- becomes:

$$\sigma^+ = \begin{bmatrix} 0.7701 \\ 0.1429 \end{bmatrix}; \sigma^- = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Since $f_i^{cv}(\hat{z}) \neq f_i^{cv}(\hat{z})$ for each i, $a_i = 0$ for all $i \in I$.

A subgradient of g^{cv} at $\hat{z} = 0.5$ is

$$\sum_{i=1}^{2} (\sigma_i^+ v_i - \sigma_i^- w_i) = 1.1630 =: s,$$

$$s \in \partial g^{cv}(\hat{z})$$

Then, the tangent function $O : \mathbb{R} \rightarrow \mathbb{R}$ to g^{cv} at $\hat{z} = 0.5$ in Figure 5.10 is constructed using this subgradient s:

$$O(z) = g^{cv}(z) + s(z - \hat{z})$$

Figure 5.10 shows the original function $g(z) = \frac{\sqrt{z^3+2z+1}}{(z-2)^2}$ and its convex relaxation g^{cv} on $Z = [0, 1]$. $O(z)$ is tangent line of $g^{cv}(z)$ at $\hat{z} = 0.5$ and is always below $g^{cv}(z)$. According to Definition 2.3.2, the subdifferential of the function f at x is set of vectors s satisfying:

$$f(y) \geq f(x) + \langle s, y - x \rangle, \quad \forall\ y \in \mathbb{R}^n.$$

Thus, this result says: if s is a subgradient, then O would always be below original *function g^{cv}. If s is not a subgradient, O would lie above or cross over g^{cv}. Here, O is always below g^{cv}. Here, the graph of O is always below g^{cv}. So s is readily verified to be a subgradient of g^{cv} at $\hat{z}$.*

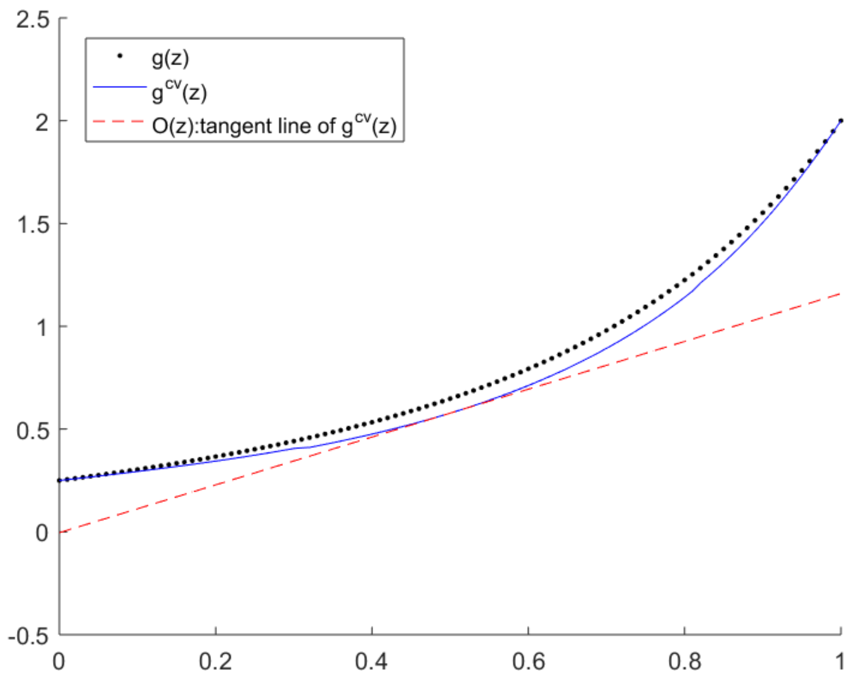

Figure 5.10: Plot of $g(z) = \frac{\sqrt{z^3+2z+1}}{(z-2)^2}$ from Example 5.5.6 and its convex relaxation $g^{cv}(z)$ on $Z = [0, 1]$. $O(z)$ is the tangent line of g^{cv} at $\hat{z} = 0.5$ constructed using the computed subgradient.

Chapter 6

Conclusion and Future Work

This chapter summarizes the contributions of the entire study and suggests avenues for future research.

6.1 Conclusion

In this thesis, several new theoretical results for nonsmooth sensitivity analysis are developed.

Chapter 3 uses compass differences and extends Pang and Stewart's directional derivative result (Pang and Stewart, 2009, Theorem 11) to describe a correct subgradient for nonsmooth dynamic system in $\mathbb{R}^2$ in Theorem 3.4.1. It is computationally inexpensive and can be computed by standard ODE solvers.

In chapter 4, compass differences are used to give a subgradient for certain optimal-value functions in $\mathbb{R}^2$, including Tsoukalas-Mitsos convex relaxations (Tsoukalas and Mitsos, 2014). Its limitations are: this result cannot apply to functions more than three variables; comparing to the new subgradient result Theorem 5.3.2 in chapter 5, it can just get a subgradient instead of the whole subdifferential set.

Chapter 5 develops a new subgradient result, Theorem 5.3.2, for Tsoukalas-Mitsos convex relaxations of composite function. This new result has no limitation on dimensions of input variables. It can give the whole subdifferential set of the Tsoukalas-Mitsos convex relaxations. Compared to Tsoukalas-Mitsos' previous subdifferential results (Tsoukalas and Mitsos, 2014, Theorem 4), it has no need to solve a dual optimization problem as well. This chapter also extends the new subgradient results to obtain directional derivatives for Tsoukalas-Mitsos convex relaxations in Theorem 5.4.2. The new subgradient results and directional derivatives results are both computational approachable.

6.2 Future Work

In the future, we expect that the new subgradient result can be applied in nonsmooth dynamic system.

A particular application for this new subgradient result is the computation of subgradients for convex relaxations solutions of the parametric ODE which is in preparation (Song and Khan, 2020). A typical ODE system is shown in Definition 3.1.1. As in (Song and Khan, 2020), this may be accomplished by solving an auxiliary ODE based on subgradients of relaxations of f, with these subgradients computed using this new subgradient Theorem 5.3.2.

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