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Abstract

A new algorithm is proposed for efficient gradient approximations. It combines the techniques of perturbations, the Broyden update and special iterations. Utilizing this method, powerful gradient-based algorithms for nonlinear optimization of circuits and systems can be effectively employed without calculating exact derivatives.

Introduction

Many powerful algorithms for nonlinear optimization have been developed and applied to circuit design problems, for example, the algorithms for linearly constrained ℓ_1 and minimax optimizations described by Bandler, Kellermann and Madsen [1], [2]. One difficulty in extending their practical applications, however, is that exact gradients of all functions with respect to all variables are usually required. For some applications, either an explicit expression of the exact gradients is not available or the computational labor for evaluating such gradients is prohibitive. Moreover, it is highly desirable to utilize many existing circuit simulation programs which provide only the values of the functions (or responses). In this paper, we propose a new approach to gradient approximation for nonlinear optimization. It is a hybrid method which utilizes parameter perturbations (i.e., finite differencing), the Broyden update [3] and the special iterations of Powell [4]. Finite differencing requires one

additional function evaluation to obtain the gradient with respect to each variable. It is the most reliable but also the most expensive method. The Broyden rank-one formula has been used in conjunction with the special iterations of Powell to update the approximate gradients, see, for example, Madsen [5] and Zuberek [6]. Such an update does not require additional function evaluations but its accuracy may not be satisfactory for some highly nonlinear problems or for a certain stage of the optimization. In our algorithm, parameter perturbations may be used to obtain an initial approximation and to provide regular corrections. The subsequent approximations are updated using the Broyden formula. Special iterations are introduced to improve the performance of the Broyden update. We also propose a modification of the Broyden formula which incorporates the knowledge, if available, of the structure of a Jacobian (e.g., the sparsity of a Jacobian). Such a hybrid method is quite flexible in handling a large variety of problems. An interface is also developed for the gradient approximation module such that it is rather independent of the optimization technique and the circuit simulator. In the following sections, our algorithm is described, implementation of this algorithm in integration with an ℓ_1 and a minimax optimization are illustrated and some test problems are presented.

Method of Perturbations

A nonlinear optimization problem usually involves a set of, say, m nonlinear functions $f_j(\mathbf{x})$, $j = 1, \ldots, m$, where $\mathbf{x} = [x_1 \ldots x_n]^T$ is the vector of n variables.

The first-order derivative of $f_j(\mathbf{x})$ with respect to x_i can be approximated by

$$\frac{\partial f_j(\mathbf{x})}{\partial x_i} \approx \frac{f_j(\mathbf{x} + h\,\mathbf{e}_i) - f_j(\mathbf{x})}{h}, \tag{1}$$

where $\mathbf{e}_i$ is a unit vector and h is the perturbation on x_i. An approximation of the Jacobian

$$\mathbf{G}(\mathbf{x}) \triangleq \left[\frac{\partial \mathbf{f}^T}{\partial \mathbf{x}}\right]^T$$

using perturbations requires $n+1$ evaluations of the functions $\mathbf{f}(\mathbf{x})$.

Broyden Update

Having an approximate Jacobian $\mathbf{G}_k$ at a point $\mathbf{x}_k$ and the function values at $\mathbf{x}_k$ and $\mathbf{x}_k + \mathbf{h}_k$, we can obtain $\mathbf{G}_{k+1}$ using the Broyden rank-one update [3]

$$\mathbf{G}_{k+1} = \mathbf{G}_k + \frac{\mathbf{f}(\mathbf{x}_k + \mathbf{h}_k) - \mathbf{f}(\mathbf{x}_k) - \mathbf{G}_k \mathbf{h}_k}{\mathbf{h}_k^T \mathbf{h}_k} \mathbf{h}_k^T . \tag{2}$$

The new approximation $\mathbf{G}_{k+1}$ provides a linearized model between two points $\mathbf{x}_k$ and $\mathbf{x}_k + \mathbf{h}_k$:

$$\mathbf{f}(\mathbf{x}_k + \mathbf{h}_k) - \mathbf{f}(\mathbf{x}_k) = \mathbf{G}_{k+1} \mathbf{h}_k . \tag{3}$$

Notice that if $\mathbf{x}_k$ and $\mathbf{x}_k + \mathbf{h}_k$ are iterates of optimization the Broyden formula does not require additional function evaluations.

The application of the original Broyden update is not trouble free. As has been observed by Zuberek [6], if some functions are linear in some variables and if the corresponding components of $\mathbf{h}_k$ are nonzero, then the approximation to constant derivatives are updated by nonzero values. We have developed a method where the Broyden formula is applied to each $f_j(\mathbf{x})$ as a single function. Associated with f_j, a weighting vector is defined by

$$\mathbf{w}_k \triangleq [w_{1j} \ \ldots \ w_{nj}]^T , \qquad w_{ij} \geq 0 . \tag{4}$$

The approximation to $\mathbf{f}_j'(\mathbf{x})$ is then updated by

$$(\mathbf{f}_j')_{k+1} = (\mathbf{f}_j')_k + \frac{\mathbf{f}_j(\mathbf{x}_k + \mathbf{h}_k) - \mathbf{f}_j(\mathbf{x}_k) - (\mathbf{f}_j')_k^T \mathbf{h}_k}{\mathbf{q}_{jk}^T \mathbf{h}_k} \mathbf{q}_{jk} , \tag{5}$$

where

$$\mathbf{q}_{jk} \triangleq [w_{1k} \ h_{1k} \ \ldots \ w_{nj} \ h_{nk}]^T . \tag{6}$$

If f_j is linear in x_i, we set $w_{ij} = 0$. In circuit design problems, it may be known that the performance function is linear in or independent of some parameters over certain frequency or time intervals. It can be verified that an approximate Jacobian given by (5) also satisfies equation (3).

Special Iterations

The Broyden formula updates the approximate gradients along the direction $\mathbf{h}_k$. If the directions of some consecutive steps of optimization are collinear, the Broyden update may

not converge. To cure this problem, Powell [4] suggested the method of "strictly linearly independent directions" generated by special iterations. Unlike an ordinary iteration where a step is taken in order to reduce the objective function, a special iteration is intended to improve the gradient approximation. After every p ordinary iterations the function values are calculated at a point obtained using the formula given by Powell [4] and a Broyden update is applied. We found that $p=2$ is satisfactory, which is also suggested by other authors (see, e.g., [4], [5] and [6]).

Interfacing To Optimization Routines

We have implemented our algorithm in a subroutine which calls a user- written routine (e.g., a simulator) for function values and calculates the approximate gradients required by a gradient-based optimization routine. It has the following features:

1. It is independent of and transparent to the optimizer and the simulator.
2. The user controls how frequently perturbations are used to obtain approximate gradients. between these perturbations the gradient approximation will be updated using the Broyden formula and special iterations.
3. Some sophisticated optimization methods employ distinct stages of optimization. In this case, the user may prescribe different patterns of gradient approximation for different stages. For example, when it is close to a solution, approximate gradients of better accuracy may be desired, which can be achieved by using perturbations more frequently.
4. Any linearity and sparsity present in the sensitivity matrix can be exploited by assigning appropriate weightings to the Broyden update.

Typically, a gradient-based optimizer calls a user's routine when function values and derivatives are needed. A simple interface is to re-direct these calls to a routine which implements gradient approximation. However, it can be made more effective and efficient by suitable modifications to the optimization routine.

1. Assuming that exact derivatives are available, an optimization algorithm usually uses quite restrictive rules for accepting and bounding the increment of an iteration ($\mathbf{h}_k$ in eqn. (2)). These rules should be relaxed when the gradients are only approximate.
2. The optimization algorithm updates the gradients only when an increment (a trial point) is accepted. If we start with a very poor gradient approximation this may lead to a dead cycle. Actually even if a trial point fails, the function values at that point can and should still be used to improve the gradient approximation.

These modifications will not alter the essential body of an optimization algorithm but are necessarily algorithm-dependent.

Numerical Examples

Our method has been applied to two general-purpose algorithms for gradient-based nonlinear optimization. These two algorithms, as described in [1] and [2], employ a 2-stage combined LP and quasi-Newton method to solve linearly constrained ℓ_1 and minimax optimization problems, respectively.

Five problems of ℓ_1 optimization have been tested. The first one, due to Madsen [5], is a data-fitting problem involving 5 variables and 21 functions. The second one is a nonlinear ℓ_1 modelling problem, due to El-Attar [7], of finding a third-order model for a seventh-order system involving 6 variables and 51 functions. The other three examples have been described by Bandler et al. (Example 1, 2 and 5 in [1]).

Three circuit design problems have been solved by minimax optimization. The first two are nominal designs of a 4th-order and a 6th-order multi-cavity microwave filters. For the 4th-order filter, 4 design parameters are taken as variables and the frequency responses are evaluated at 15 sample points. For the 6th-order filter, 6 parameters and 21 sample points are considered. The third example illustrates the problem of optimal centering and tolerancing, as originally described in [8].

These test problems were solved utilizing implementations on a CDC 170/730 system. The results are summarized in Tables 1 and 2. In both tables, the results of two basic cases are compared. In Case 1, parameter perturbations are conducted at every optimization iteration to approximate the gradients. This represents quite a traditional approach to gradient approximation. In Case 2, perturbations are used only for initialization. The subsequent approximations are updated by the Broyden formula and special iterations. Its advantage over Case 1 is clearly shown. The optimization programs employed use a quasi-Newton method to secure fast final convergence when a smooth valley is detected near a solution (namely, Stage 2 of [1] and [2]). The accuracy of the gradient approximation becomes crucial for such iterations. For Case 3 in Table 1, different updating schemes are used for two distinct stages. The approximate gradients are updated by the Broyden formula and special iterations for Stage 1, and perturbations are employed for every Stage 2 iteration where better accuracy is desired. The results show a similar number of function evaluations as Case 2 but the number of iterations is smaller. Such a variant can be achieved very conveniently with the flexibility of our algorithm. Note that this case is not applicable to other examples since no smooth valley is present.

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TABLE 1 ℓ_1 OPTIMIZATION WITH GRADIENT APPROXIMATIONS

Test Problem	Case 1	Case 2	Case 3	Exact Gradients
1	54(9)	32(19)	-	(9)
2	105(15)	63(40)	-	(11)
3	71(17)	65(48)	54(24)	(13)
4	98(32)	54(43)	58(26)	(53)
5	89(17)	51(38)	54(26)	(17)

TABLE 2 MINIMAX OPTIMIZATION WITH GRADIENT APPROXIMATIONS

Test Problem	Case 1	Case 2	Exact Gradients
1	59(11)	30(18)	(14)
2	83(11)	66(41)	(11)
3	30(6)	13(7)	(6)

Comments: The entries are the number of function evaluations. The entries in parentheses are the number of optimization iterations. Case 1: perturbations are used at every iteration for gradient approximations. Case 2: perturbations are used only for the first iteration to initialize the approximation. Case 3: perturbations are used for the first iteration and every Stage 2 iteration (when close to a solution).