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# AUTOMATIC DIFFERENTIATION AND THE STEP COMPUTATION IN THE LIMITED MEMORY BFGS METHOD

*Jean Charles Gilbert*<sup>1</sup> and *Jorge Nocedal*<sup>2</sup>

**Abstract.** It is shown that the two-loop recursion for computing the search direction of a limited memory method for optimization can be derived by means of the reverse mode of automatic differentiation applied to an auxiliary function.

## 1. Introduction

The problem of finding efficient procedures for automatically calculating the gradient of a function has recently received much attention [4]. It is known that the *reverse mode* of automatic differentiation can provide the value of the gradient at a cost that is not much greater than that required to evaluate the function.

On the other hand the limited memory BFGS method – an optimization method designed for very large unstructured problems – has recently become popular. This method attempts to mimic the very successful BFGS variable metric method, but without storing matrices. To do this it saves several pairs of vectors  $\{y_i, s_i\}$ ,  $i = 1, \dots, m$  that implicitly define the iteration matrix  $H$ . The search direction of the limited memory method is then computed by  $d = -Hg$ , where  $H$  can be viewed as an approximation of the inverse Hessian of the objective function at the current iterate and  $g$  is the gradient of this function. Since the matrix  $H$  is not formed, but is only represented implicitly by the set of vectors  $\{y_i, s_i\}$ , a formula [6] is required to calculate the product  $Hg$  directly from the vectors  $\{y_i, s_i\}$  and the gradient  $g$ . It turns out that this formula is not unique; one can devise various equivalent expressions, some of which are more economical than others [1]. For unconstrained optimization the most efficient formula for computing  $d$ , given in [6], consists of a two-loop recursion involving the vectors  $\{y_i, s_i\}$  and the gradient  $g$ . In this paper we show that this two-loop recursion can be viewed as an application of the reverse mode of automatic differentiation. Thus, we find a connection between two apparently unrelated subjects: the step computation in a limited memory method and automatic differentiation.

## 2. Adjoint code of a program computing a function

Suppose that a function

$$f : x = (x_1, \dots, x_n) \in \mathbb{R}^n \longrightarrow f(x) \in \mathbb{R}$$

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<sup>1</sup> INRIA, Domaine de Voluceau, Rocquencourt, B.P. 105, 78153 Le Chesnay Cedex (France).

<sup>2</sup> Department of Electrical Engineering and Computer Science, Northwestern University, Evanston IL 60208. This author was supported by the National Science Foundation Grant INT-9101901, and by the Department of Energy Grant DE-FG02-87ER25047.

is computed by a program executing the following sequence of instructions

$$\begin{aligned} &\mathbf{for} \ k := 1 \ \mathbf{to} \ K \ \mathbf{do} \ x_{\mu_k} := \varphi_k(\{x_{P_k}\}); \\ &f := x_N. \end{aligned} \tag{2.1}$$

For convenience, we have denoted by  $x_1, \dots, x_n$  the *independent variables*, with respect to which the gradient of  $f$  is desired, and by  $x_{n+1}, \dots, x_N$  ( $N \geq n$ ) all the other variables used in the program. There is, however, no meaningful ordering in this notation. Instruction  $k$  in (2.1) modifies the variable  $x_{\mu_k}$ ,  $\mu_k \in \{1, \dots, N\}$ , by using an intermediate function  $\varphi_k$  depending on  $\{x_{P_k}\}$ , which is the collection of variables  $x_j$  with indices  $j$  in some subset  $P_k \subset \{1, \dots, N\}$ . After assigning a value to the variable  $x$ , this program will provide the value of  $f(x)$  in the variable  $x_N$ .

It has been shown [8] that the gradient  $\nabla f(x)$  of  $f$  at a given point  $x$  can be evaluated by first executing the original program (2.1), storing some partial derivatives  $\partial\varphi_k/\partial x_j$  for  $j \in P_k$ , and then executing the following *adjoint code*:

$$\begin{aligned} &\mathbf{for} \ i := 1 \ \mathbf{to} \ N - 1 \ \mathbf{do} \ \bar{x}_i := 0; \\ &\bar{x}_N := 1; \\ &\mathbf{for} \ k := K \ \mathbf{down} \ \mathbf{to} \ 1 \ \mathbf{do} \ \{ \\ &\quad \bar{x}_i := \bar{x}_i + \frac{\partial\varphi_k}{\partial x_i} \bar{x}_{\mu_k}, \ \forall i \in P_k \setminus \{\mu_k\}; \\ &\quad \bar{x}_{\mu_k} := \frac{\partial\varphi_k}{\partial x_{\mu_k}} \bar{x}_{\mu_k}; \} \\ &\mathbf{for} \ i := 1 \ \mathbf{to} \ n \ \mathbf{do} \ \frac{\partial f}{\partial x_i} := \bar{x}_i. \end{aligned} \tag{2.2}$$

Here we used the notation  $A \setminus B$  to denote the set of elements that belong to  $A$  but not to  $B$ . The variable  $\bar{x}_i$  is called the *adjoint variable* associated to  $x_i$ . Its value is the current evaluation of the derivative of  $f$  with respect to  $x_i$ . This technique is also called the *reverse mode* of automatic differentiation; see [7], [3], [5] or [2] for an introduction to the subject. Its main advantage is that it computes  $f(x)$  and its gradient  $\nabla f(x)$  in a time  $T(f, \nabla f)$  satisfying

$$T(f, \nabla f) \leq C T(f), \tag{2.3}$$

where  $C$  is some constant and  $T(f)$  is the time to compute  $f(x)$  by algorithm (2.1). When the functions  $\varphi_k$  are restricted to be the ones available in FORTRAN, it is reasonable to bound  $C$  by 5, see [3].

### 3. Application to the L-BFGS method

In a typical iteration of the limited memory BFGS method (L-BFGS), one is given a symmetric and positive definite matrix  $H_0$  and  $m$  pairs of vectors  $\{y_0, s_0\}, \dots, \{y_{m-1}, s_{m-1}\}$ , where  $m$  is some integer. Each of these pairs satisfies the condition  $\rho_i \equiv (y_i^\top s_i)^{-1} > 0$ . The matrix  $H_0$  is then updated  $m$  times using the BFGS formula, i.e., for  $i = 0, \dots, m-1$ :

$$H_{i+1} = V_i^\top H_i V_i + \rho_i s_i s_i^\top, \tag{3.1}$$

where

$$V_i = I - \rho_i y_i s_i^\top; \tag{3.2}$$

see [6]. The resulting matrix,  $H_m$ , is then used to compute the search direction

$$d = -H_m g,$$

where  $g$  is the current value of the gradient of the objective function.

To interpret this step computation in terms of automatic differentiation, we need to express  $H_m g$  as the gradient of a real-valued function. A natural candidate for this is

$$f_m(g) = \frac{1}{2} g^\top H_m g,$$

since, due to the symmetry of  $H_m$ ,  $\nabla_g f_m(g)$  is precisely  $H_m g$ . From (3.1) we find that  $f_m(\cdot)$  can easily be expressed in terms of  $f_{m-1}(\cdot)$ :

$$f_m(g) = f_{m-1}(V_{m-1} g) + \frac{\rho_{m-1}}{2} (s_{m-1}^\top g)^2.$$

Therefore, if we define

$$q_m = g, \quad q_{i-1} = V_{i-1} q_i \quad \text{for } i = m, \dots, 1, \quad (3.3)$$

we find by induction that

$$f_m(g) = f_0(q_0) + \sum_{i=0}^{m-1} \frac{\rho_i}{2} (s_i^\top q_{i+1})^2.$$

Using this formula, the computation of  $f_m(g)$  can be performed by the following algorithm. We assume that the scalars  $\rho_i$  have been computed beforehand, and to save storage, we place all the  $q_i$  in the same vector  $q$ . Recall that the vectors  $q_i$  are updated by (3.3), where the matrices  $V_i$  are defined by (3.2).

$$\begin{aligned} & f := 0; \\ & q := g; \\ & \mathbf{for } i := m - 1 \mathbf{ down to } 0 \mathbf{ do } \{ \\ & \quad \alpha_i := s_i^\top q; \\ & \quad f := f + \frac{\rho_i}{2} \alpha_i^2; \\ & \quad q := q - \rho_i \alpha_i y_i; \} \\ & f := f + \frac{1}{2} q^\top H_0 q. \end{aligned} \quad (3.4)$$

The product  $H_m g$  will now be computed by the adjoint code of (3.4). Let  $\bar{f}$ ,  $\bar{q}$ ,  $\bar{\alpha}_0$ ,  $\dots$ ,  $\bar{\alpha}_{m-1}$  be the adjoint variables corresponding to  $f$ ,  $q$ ,  $\alpha_0$ ,  $\dots$ ,  $\alpha_{m-1}$ . The adjoint code is obtained by writing the adjoint instructions corresponding to the instructions in (3.4), in the reverse order of execution. After the initialization of the adjoint variables,

$$\bar{f} := 1; \quad \bar{q} := 0; \quad \bar{\alpha}_0 := 0; \dots; \bar{\alpha}_{m-1} := 0,$$

the code continues as follows:

$$\begin{aligned}
& \bar{q} := H_0 q; \\
& \mathbf{for} \ i := 0 \ \mathbf{to} \ m - 1 \ \mathbf{do} \ \{ \\
& \quad \bar{\alpha}_i := \bar{\alpha}_i - \rho_i y_i^\top \bar{q}; \\
& \quad \bar{\alpha}_i := \bar{\alpha}_i + \rho_i \alpha_i \bar{f}; \\
& \quad \bar{q} := \bar{q} + \bar{\alpha}_i s_i; \\
& \quad \bar{\alpha}_i := 0; \} \\
& \bar{g} := \bar{q}; \\
& \bar{q} := 0; \\
& \bar{f} := 0.
\end{aligned} \tag{3.5}$$

We now combine (3.4) and (3.5), omitting those instructions needed only for the evaluation of  $f$  (since we are only interested in  $H_m g$ ). To save space in the adjoint portion of the code, we store all values of  $\bar{\alpha}_i$  in the same location  $\beta$  and the values of  $\bar{q}$  in the location of  $q$ . After deleting all unnecessary instructions we obtain

$$\begin{aligned}
& q := g; \\
& \mathbf{for} \ i := m - 1 \ \mathbf{down\ to} \ 0 \ \mathbf{do} \ \{ \\
& \quad \alpha_i := s_i^\top q; \\
& \quad q := q - \rho_i \alpha_i y_i; \} \\
& q := H_0 q; \\
& \mathbf{for} \ i := 0 \ \mathbf{to} \ m - 1 \ \mathbf{do} \ \{ \\
& \quad \beta := \rho_i (\alpha_i - y_i^\top q); \\
& \quad q := q + \beta s_i; \}.
\end{aligned} \tag{3.6}$$

The value of  $H_m g$  is placed in the vector  $q$ . Algorithm (3.6) is identical to the 2-loop formula used for the computation of the search direction in the L-BFGS method [6].

This derivation shows why algorithm (3.6) is efficient: it is based on the compact algorithm (3.4) computing  $f_m$ , and on the reverse mode of automatic differentiation, which is known to be very efficient.

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