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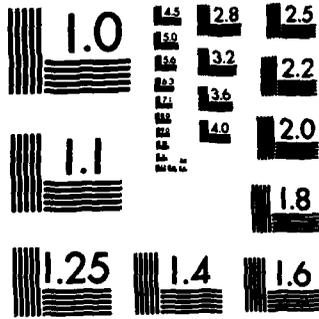
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ABSTRACT (Continue on reverse if necessary and identify by block number)
 This article considers the problem of determining the optimal value and corresponding optimal point of a real function F in m variables. Only function values are given and the computation of derivatives is either not practical or are not available. Many techniques were developed in the last few years which do not use derivatives, however some turn out to be of little practical use when applied to problems in many variables and nonlinear in nature. The main difficulty is slow convergence and early termination of the algorithm. In contrast, methods which use derivatives might converge faster but require instead an immense amount of calculations of large inverse matrices which have first or second partial derivatives. This task is formidable and in many cases impossible to attain. Bremermann (1970) introduced an ingenious and useful optimization algorithm that is guaranteed to converge for polynomials in several variables up to fourth degree. The heart of this method is the use of random directions of search together with a Lagrangian interpolation (CONT.)

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Motivated by the usefulness of random directions it is the purpose of this article to present an algorithm based on the proper use of interpolation schemes; (a) Lagrangian interpolations (such as those in Bremermann's methods); (b) spline approximations with variable nodes; (c) pseudo Newton steps using the spline derivatives (not the function); together with a search procedure along weighted random directions. The directions are chosen to be orthogonal using the Gram Schmidt orthogonalization procedure. This algorithm was extensively used for problem solving in mathematical biology, chemical kinetics, and general dynamical systems.

Perfect line searches along the weighted random directions is not assumed, however, we require monotonicity of the objective function at each successful iteration, in addition close estimates of the optimal point are not required. The method presented has the virtue of being able to solve nonlinear systems in many variables which are very commonly encountered in the area of applied mathematics.

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SPLINE AND WEIGHTED RANDOM
DIRECTIONS METHOD FOR NONLINEAR OPTIMIZATION

J. Milstein

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INTRODUCTION. This article considers the problem of determining the optimal value and corresponding optimal point of a real function F in n variables. Only function values are given and the computation of derivatives is either not practical or are not available. Many techniques were developed in the last few years which do not use derivatives [2] [4] [14] [15], however some turn out to be of little practical use when applied to problems in many variables and nonlinear in nature. The main difficulty is slow convergence and early termination of the algorithm. In contrast, methods which use derivatives might converge faster but require instead an immense amount of calculations of large inverse matrices which have first or second partial derivatives. This task is formidable and in many cases impossible to attain [6] [8]. Bremermann (1970) introduced an ingenious and useful optimization algorithm that is guaranteed to converge for polynomials in several variables up to fourth degree. The heart of this method is the use of random directions of search together with a Lagrangian interpolation scheme. This author, having had extensive experience with this algorithm, found that the method has fast convergence at the early stages and tends to stagnate in the neighborhood of the optimal point [1] [9] [12].

Motivated by the usefulness of random directions it is the purpose of this article to present an algorithm based on the proper use of interpolation schemes; (a) Lagrangian interpolations

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Perfect line searches along the weighted random directions is not assumed, however, we require monotonicity of the objective function at each successful iteration, in addition close estimates of the optimal point are not required. The method presented has the virtue of being able to solve nonlinear systems in many variables which are very commonly encountered in the area of applied mathematics.

THE PROBLEM.

We want to solve the following problem:

$$\min\{F(x) \mid x \in \mathbb{R}_+^n\}.$$

We assume any initial estimate $x^{(0)} \in \mathbb{R}^n$, and for any value $x \in \mathbb{R}^n$ the functional value of F is well defined.

DESCRIPTION OF THE METHOD.

(1) A set of linearly independent vectors is formed, one of which is a random vector $R = (r_1, \dots, r_n)$. That is, we take the standard basis

$$e_k = (0, \dots, 1, 0, \dots, 0) \quad (1 \text{ at the } k \text{ place}).$$

We look for the entry of R having the highest value, say it appears in the j^{th} position. Now we form the set of vectors

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$$\begin{cases} e_k = (0, \dots, 1, 0, \dots, 0) & k \neq j \\ e_j = (r, \dots, r_m) & k = j \end{cases}$$

R is a random vector whose components (r, \dots, r_n) are independently generated from a Gaussian distribution.

(2) We use the Gram-Schmidt orthogonalization procedure to obtain a set of orthogonal vectors $v^{(1)}, \dots, v^{(n)}$, such that $\langle v^{(i)}, v^{(j)} \rangle = 0$, for $i \neq j$.

(3) A matrix D is constructed such that

$$D = \begin{pmatrix} (x_1^0)^{-\frac{1}{2}} & & & 0 \\ & (x_2^0)^{-\frac{1}{2}} & & \\ & & \ddots & \\ 0 & & & (x_n^0)^{-\frac{1}{2}} \end{pmatrix} = P_0^{-\frac{1}{2}}$$

If $x_i^{(0)} \leq 0$ set $x_i^{(0)} = 1$, for any i .

The diagonal elements of D are precisely the elements of $x^{(0)} = (x_1^{(0)}, \dots, x_n^{(0)})$.

(4) Define the random vectors

$$w^{(i)} = [P^{-\frac{1}{2}}]^{(i)} v^{(i)} \quad i = 0, 1, \dots, n$$

(5) Choose the random directions $w^{(1)}$ as the first direction of search.

(6) A set of functional values $\{F_j\}_{j=1}^5$ is obtained by evaluating F at equidistant collinear points $y_1 = x^{(0)} + 2w^{(1)}$; $y_2 = x^{(0)} + w^{(1)}$; $y_3 = x^{(0)}$; $y_4 = x^{(0)} - w^{(1)}$; and $y_5 = x^{(0)} - 2w^{(1)}$.

(7) The cubic spline $S(\lambda) \in C^2[y_i, y_{i+1}]$, $1 \leq i \leq 4$, approximates the function F restricted to the line $x^{(0)} + \lambda w^{(1)}$.

(8) The roots of $S'(\lambda) = 0$ are found. There are from 8 to 1 possible real roots, λ_l , $l = 1, \dots, 8$.

(9) Determine the minimum functional value among $F[x^{(0)} + \lambda_l w^{(1)}]$, $l = 1, \dots, 8$. Denote the vector which corresponds to this minimum by $x^{(1)} = x^{(0)} + \lambda_m w^{(1)}$. This vector is the new approximation to the minimum.

(10) If $F[x^{(1)}] > F[x^{(0)}]$ we generate a new approximation to F by using a four degree Lagrangian interpolation such as the one used in Bremermann's scheme.

(11) For any successful step, i.e. $F[x^{(i)}] < F[x^{(i-1)}]$, perform a pseudo Newton random step

$$x^{(n)} = x^{(n-1)} - \frac{F[x^{(n-1)}]}{S'(\lambda_m)}$$

(12) Terminate the search if

- (1) $F \leq \epsilon_1$ and $\|x^{(j)} - x^{(j-1)}\| \leq \epsilon_2$
 ϵ_1, ϵ_2 are pre-assigned tolerances

or

- (2) A predetermined number of iterations have been executed.

ANALYSIS OF THE ALGORITHM.

One of the main features of this method is the nature of the random direction. In what follows we will analyze the search directions and their properties.

DEFINITION Two vectors $w^{(i)}$ and $w^{(j)}$, $i \neq j$, are said to be duals with respect to the product $(P^{(j)} P^{(i)})$ of two diagonal matrices $P^{(i)}$ and $P^{(j)}$ having positive entries if

$$w^{(i)T} (P^{(j)} P^{(i)}) w^{(j)} = 0 \quad \begin{matrix} i \neq j & i = 1, \dots, n \\ & j = 1, \dots, n. \end{matrix}$$

DEFINITION The set of vectors $(w^{(1)}, \dots, w^{(n)})$ are mutually duals if for any pair $(w^{(i)}, w^{(j)})$ we can find a product, $(P^{(j)} P^{(i)})$, of positive diagonal matrices such that $w^{(i)T} (P^{(j)} P^{(i)}) w^{(j)} = 0$.

There are many ways to generate dual vectors. We form the dual vector by the following procedure.

- (I) Choose a nonzero vector $v^{(1)} \in \mathbb{R}^n$.
- (ii) Find n-linearly independent orthogonal vectors using the Gram-Schmidt orthogonalization procedure. i.e. if $\Omega = \{v^{(1)}, \dots, v^{(n)}\}$ then $\langle v^{(i)}, v^{(j)} \rangle = 0 \quad i \neq j$, where \langle , \rangle stands for the scalar product.
- (III) Set $w^{(i)} = P^{(i)-\frac{1}{2}} v^{(i)} \quad i = 1, \dots, n$ where $P^{(i)}$ is a $n \times n$ positive diagonal matrix, and $v^{(i)} \in \Omega$.

PROPOSITION 1 The set of vectors $w^{(1)} \dots w^{(n)}$ defined by $w^{(i)} = P^{(i)-\frac{1}{2}} v^{(i)}$ form a set of mutually duals.

PROOF Let $w^{(i)} \neq w^{(j)}$. Then for any i and any j

$$\begin{aligned} w^{(i)T} (P^{(j)} P^{(i)}) w^{(j)} &= w^{(i)T} P^{(i)^{\frac{1}{2}} P^{(j)^{\frac{1}{2}}} w^{(j)} \\ &= (P^{(i)-\frac{1}{2}} v^{(i)})^T P^{(i)^{\frac{1}{2}} P^{(j)^{\frac{1}{2}}} (P^{(i)-\frac{1}{2}} v^{(i)}) \\ &= v^{(i)T} P^{(i)-\frac{1}{2}} P^{(i)^{\frac{1}{2}} P^{(j)^{\frac{1}{2}}} P^{(j)^{-\frac{1}{2}}} v^{(j)} \\ &= v^{(i)T} v^{(j)} \\ &= 0. \end{aligned}$$

THE QUADRATIC CASE

If $F(x)$ is a quadratic function:

$$F(x) = a + b^T x + x^T Q x.$$

$x, b \in \mathbb{R}^n$, Q is positive definite. Then minimizing F using line searches in the direction of mutually dual vectors will give us an indication of the improvement from one iteration to another.

Let $w^{(i)} = P_i^{-1/2} v^{(i)}$. Then the sequence of iterates generated by the algorithm is

$$x^{(n+1)} = x^{(n)} + \lambda^{(n)} w^{(n)} \quad n = 0, 1, 2, \dots$$

or

$$x^{(n+1)} = x^{(0)} + \sum_{i=0}^n \lambda^{(i)} w^{(i)} \quad n = 0, 1, 2, \dots$$

where $\lambda^{(n)}$ satisfy the inequality

$$F[x^{(i+1)}] \leq F[x^{(i)}] \quad i = 0, 1, 2 \dots n.$$

The restriction of F on the line $x^{(k)} + \lambda^{(k)} w^{(k)}$ is given by

$$F[x^{(k)} + \lambda^{(k)} w^{(k)}] = F[x^{(k)}] + 2\lambda^{(k)} w^{(k)} [Qx^{(k)} + b] + (\lambda^{(k)})^2 [w^{(k)}]^T Q w^{(k)}$$

and the minimum is given by $\frac{\partial F}{\partial \lambda^{(k)}} = 0$. That is

$$\frac{1 \partial F}{2 \partial \lambda^{(k)}} = w^{(k)} [Qx^{(k)} + b] + \lambda^{(k)} (w^{(k)})^T Q w^{(k)}$$

which imply that

$$\lambda^{(k)} = - \frac{w^{(k)} [Qx^{(k)} + b]}{(w^{(k)})^T Q w^{(k)}}.$$

The minimum F value in the k^{th} direction is given by

$$F = F[x^{(k)}] - \frac{2w^{(k)} [Qx^{(k)} + b]}{[w^{(k)}]^T Q w^{(k)}} w^{(k)} [Qx^{(k)} + b] +$$

$$+ \left(\frac{w^{(k)} [Qx^{(k)} + b]}{[w^{(k)}]^T Q w^{(k)}} \right)^2 [w^{(k)}]^T Q w^{(k)}$$

$$\rightarrow F = F[x^{(k)}] - \frac{(w^{(k)} [Qx^{(k)} + b])^2}{[w^{(k)}]^T Q w^{(k)}}$$

$$\rightarrow F_{\min} = F[x^{(k)}] - [\lambda^{(k)}]^2 ([w^{(k)}]^T Q w^{(k)})$$

$$\rightarrow [\lambda^{(k)}]^2 = \frac{F[x^{(k)}] - F[x^{(k)} + \lambda^{(k)} w^{(k)}]}{[w^{(k)}]^T Q w^{(k)}}$$

$$\rightarrow \lambda_{\min}^{(k)} = \sqrt{\frac{F[x^{(k)}] - F[x^{(k+1)}]}{[w^{(k)}]^T Q w^{(k)}}}$$

MEASURE OF IMPROVEMENT

The ratio $F[x^{(i+1)}] / F[x^{(i)}]$ is defined as the improvement factor for direction $w^{(k)}$, [1]. This ratio gives an estimate of rate of convergence of the algorithm.

Denote by θ_i the improvement factor for the $w^{(i)}$ direction,

i.e. $\theta_i = \frac{F[x^{(i)}]}{F[x^{(i-1)}]}$. Then a measure of the rate of improvement

after k iterations is given by $\hat{\theta}_k = \frac{F[x^{(k)}]}{F[x^{(k-1)}]}$.

PROPOSITION 2. The minimum of F is equal to

$$F_{\min} = F[x^{(0)}] \prod_{i=1}^k \theta_i.$$

PROOF. If $\theta_1 = \frac{F[x^{(1)}]}{F[x^{(0)}]}$... $\theta_k = \frac{F[x^{(k)}]}{F[x^{(k-1)}]} = \frac{F_{\min}}{F[x^{(k-1)}]}$.

Then $\prod_{i=1}^k \theta_i = \frac{F[x^{(1)}]}{F[x^{(0)}]} \dots \frac{F[x^{(k-1)}]}{F[x^{(1)}]} \frac{F[x^{(k)}]}{F[x^{(k-1)}]}$

$$= \frac{F[x^{(k)}]}{F[x^{(0)}]} = \frac{F_{\min}}{F[x^{(0)}]}$$

$$F_{\min} = F[x^{(0)}] \prod_{i=1}^k \theta_i.$$

The ratio $F_{\min}/F[x^{(0)}]$ is a measure of the maximum improvement factor.

PROPOSITION 2. If $F[x] > 0 \quad \forall x \in \mathbb{R}^n$ then

$$\text{Log } F_{\min} = \frac{\sum_{i=1}^k \text{Log } \theta_i}{\text{Log } F[x^{(0)}]}$$

THE INTERPOLATION STEP

We use two interpolation schemes: (A) Five points Lagrangian interpolation, (B) Cubic spline interpolation with variable nodes. The Lagrangian step is extremely efficient in the search for the minimum in the early stages while the spline converges faster when in the proximity of the minimum.

Let $h = \max \|x^{(i+1)} - x^{(i)}\|$ be the maximum step size between the interpolated points and denote by $E[x] = F(x) - S(x)$ the error between the cubic spline approximation and $F(x)$. $S(x)$ is the cubic spline. The $E[x]$ and its derivative $E'[x]$ are bounded by

$$|E[x]| \leq h^{3/2} \left(\int_a^b [F''(t)]^2 dt \right)^{1/2} \quad \forall x \in [a, b]$$

([a,b] is the interval of approximation)

and

$$|E'[x]| \leq h^{1/2} \left(\int_a^b [F''(t)]^2 dt \right)^{1/2} \quad \forall x \in [a, b].$$

Thus $E[x]$ and $E'[x]$ are bounded by an expression proportional to $h^{3/2}$ and $h^{1/2}$ respectively [7].

In the k^{th} iteration the choice of h in our method is given by

$$h = \min(1, \sqrt{F[x^{(k)}]})$$

Therefore for $F \leq 1$ the interval of the cubic approximation over

n points is of length $(n-1) \sqrt{F[x^{(k)}]}$. If n increases and $h \rightarrow 0$ then $S(x)$ and $S'(x)$ converge uniformly to $F(x)$ and $F'(x)$ respectively [7].

When $S'[\alpha]$ approximates $F'[\alpha]$ for $\alpha \in [a,b]$, we can calculate $S'(x)$ and apply a Newton-Raphson step using $S'(x)$ instead of $F'(x)$ (which is unknown). That is

$$x^{(n+1)} = x^{(n)} - \frac{F[x^{(n)}]}{S'[x^{(n)}]} \quad \text{for } n = 1, \dots, s$$

The errors for the Lagrangian interpolation are extensively analyzed in [7] [1].

RESULTS.

We have solved standard test problems with our algorithm.

These functions were

- (1) Rosenbroock; Parabolic Valley [8]

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

- (2) Powell's singular of 4 variables [14]

$$f(x) = (x_1 + 10 \cdot x_2)^2 + 5(x_3 - x_4)^2 + (x_2 - 2x_3)^4 + 10(x_1 - x_4)^4$$

- (3) Rosenbroock Parabolic Valley - 50 Dimensional [13]

$$\begin{aligned} F[x] = & \sum_{i=1}^{19} \left(x^{(i)} + \left(\frac{i-10.4}{2} \right)^{(-1)^{(i)}} x^{(i+1)} \right)^2 + 2 \sum_{i=20}^{24} (x^{(i)} - x^{(i+1)})^2 \\ & + \sum_{i=25}^{29} (x^{(i)} - 0.5 x^{(i+1)})^2 \\ & + 3 \sum_{i=30}^{49} \left(x^{(i)} - \left(\frac{i-40.5}{3} \right)^{(-1)^{(i)}} x^{(i+1)} \right)^2 + 2 \sum_{i=1}^{20} (x^{(i)} - x^{(51-i)})^4 \\ & + \sum (x^i - x^{(51-i)})^4 \end{aligned}$$

(4) Zangwill (1967)

$$F[x] = \left(\frac{1}{15}\right) [16x_1^2 + 16x_2^2 - 8x_1x_2 - 56x_1 - 256x_2 + 991]$$

In addition to these functions the method was tested on nonlinear systems defined by ordinary differential equations, among them; a model of gluconeogenesis described by twenty differential equations having 31 unknown parameters [12], an inducible system model having 14 differential equations having 12 unknown parameters [10], and an ecological model with 8 unknown parameters [11]. In all of the dynamical systems the optimization was performed to find least square minimum of a function with noise in the data [11]. The following table gives a summary of the numerical results*.

Function	# of Variables	# of Function Evaluations**	# of Spline Iteration
(1) Rosenbroock	2	1310	25
(2) Zangwill	2	64	5
(3) Powell Singular	4	302	7
(4) Rosenbroock	50	571	6
(5) Gluconeogenesis Model	31	1176	39
†(6) Gluconeogenesis Model	12	885	28
(7) Inducible System	12	1300	40
(8) Ecological Model	8	370	16

* The computations were done on a PDP-11 computer and the termination criteria for the functions 1-4, was $\epsilon = 10^{-12}$, and for systems 5-8 the minimum of F was: (# of noisy data points) * (Relative value of data point + assumed level of noise).

** Includes all function evaluations of F; spline interpolation, Lagrangian, and pseudo Newton.

†This is a linear model described by 6 differential equations having 12 unknown parameters.

CONCLUSIONS

In this article we have presented a method for unconstrained optimization which is based on interpolation schemes and random weighted direction. The algorithm is the result of the author's extensive experience with Bremermann's methods based on Lagrangian interpolation. No one method can be optimum in the sense of being best for all functions (or even for a given function), moreover, it is unlikely to find a method which works well in all regions, far from the minimum as well as near. In this article we confronted this problem precisely by using the Lagrangian while far away from the minimum and the spline while in its vicinity. The direction of search is always weighted by the best present vector value, and because of the randomness the algorithm is insensitive to the change in the local geometry of the problem. The method is well suited to optimize functions for which their derivatives are unknown and cannot be computed accurately. From the numerical results we can see the effectiveness of the method on problem with many variables, and it is clear that the higher the dimension the more effective is the algorithm.

Additional applications of this algorithm in the field of nonlinear chemical kinetics, and in determining multiple equilibrium states of dynamical systems will be reported soon.

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