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Fridrich Sloboda

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PARALLEL METHOD OF CONJUGATE DIRECTIONS FOR MINIMIZATION*)

FRIDRICH SLOBODA

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INTRODUCTION

Recently developed minimization methods which generate conjugate directions are of two types: either they require the knowledge of the gradient vector or not. All methods of conjugate directions have the quadratic convergence property, i.e., the minimum of a quadratic function is achieved by a finite number of iterations. Methods requiring the gradient vector have been unified in terms of a general algorithm [1, 2]. The class of these methods includes Davidon-Fletcher-Powell's method [3] and the method of conjugate gradients [4, 5], which is the simplest. The most effective nongradient methods generating conjugate directions are Powell's method [6, 7] and Chazan-Miranker's method [8].

In this paper a method of conjugate directions for minimization not requiring the gradient vector is described. In [15] a projection method for linear algebraic systems is suggested. Let us consider the system

$$(1) \qquad Ax = b$$

where A is a regular n by n matrix and b is an n-vector.

Let $x_0^{(0)}, x_0^{(1)}, \ldots, x_0^{(n)}$ be $n + 1$ linearly independent points of the space E_n. Then the algorithm [15] is described by the recurrent relation

$$x_i^{(k)} = x_{i-1}^{(k)} + \frac{b_i - (a_i, x_{i-1}^{(k)})}{(a_i, v_{i-1}^{(i)})} v_{i-1}^{(i)}$$

where

$$v_{i-1}^{(i)} = x_{i-1}^{(i)} - x_{i-1}^{(i-1)}, \quad i = 1, 2, \ldots, n, \quad k = i, i + 1, \ldots, n$$

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and a_i is the i-th row of the matrix A and b_i is the i-th component of the vector b. Let $x_0^{(0)} = (0, \ldots, 0)^T$ and $x_0^{(k)} = (0, \ldots, t_k, \ldots, 0)^T$ where $t_k = 1$. Let the matrix A be a strictly regular matrix. Then

$$(a_i, v_{i-1}^{(i)}) \neq 0$$

and the matrix of the vectors $v_{i-1}^{(i)}$ is upper triangular with unit elements in the diagonal and the point $x_n^{(n)}$ is the solution of (1). The following lemma is proved [15]:

Lemma 1. *Let A be a strictly regular, q-diagonal band matrix. Let $x_0^{(0)} = (0, \ldots, 0)^T$ and $x_0^{(k)} = (0, \ldots, t_k, \ldots, 0)^T$ where $t_k = 1$. Then*

$$x_i^{(k)} = x_i^{(i)} + x_0^{(k)}$$

for $k > (q-1)/2 + i\,, \quad i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n\,.$

This lemma affects also the structure of the algorithm for minimization. Let us denote for the sake of brevity

$$\alpha_{i-1}^{(k)} = \frac{b_i - (a_i, x_{i-1}^{(k)})}{(a_i, v_{i-1}^{i})}\,, \quad i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n\,.$$

In the next part we show how the algorithm [15] can be modified by a suitable choice of $\alpha_{i-1}^{(k)}$ to become an algorithm for minimization. This will be demonstrated on an example of the well-known equivalence between the solution of a system of linear algebraic equations with a symmetric, positive definite matrix A, and the minimization of the function

$$f(x) = (Ax, x) - 2(b, x) + c\,. \tag{2}$$

MATHEMATICAL DESCRIPTION OF THE ALGORITHM

Definition. Let $x_0^{(0)}, x_0^{(1)}, \ldots, x_0^{(n)}$ be $n + 1$ linearly independent points of the Euclidean space E_n. Then the algorithm for minimization of (2) is defined as follows:

$$x_i^{(k)} = x_{i-1}^{(k)} + \alpha_{i-1}^{(k)} v_{i-1}^{(i)} \tag{3}$$

where

$$v_{i-1}^{(i)} = x_{i-1}^{(i)} - x_{i-1}^{(i-1)}$$

and $\alpha_{i-1}^{(k)}$ are scalar coefficients such that

$$f(x_{i-1}^{(k)} + \alpha v_{i-1}^{(i)}) = \min!$$

$$\alpha = \alpha_{i-1}^{(k)}\,, \quad i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n\,.$$

Remark. For $k = i$, it is also possible to write

$$x_i^{(k)} = x_{i-1}^{(i-1)} + \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}$$

where

$$v_{i-1}^{(i)} = x_{i-1}^{(i)} - x_{i-1}^{(i-1)}$$

and

$$f(x_{i-1}^{(i-1)} + \alpha v_{i-1}^{(i)}) = \min!$$

$$\alpha = \alpha_{i-1}^{(i-1)} .$$

First we prove a theorem about parallel directions.

Theorem 1. *Let $f : E_n \to E_1$ be the quadratic function (2). Let $v \in E_n$ be a non-zero vector. Let $x_0, y_0 \in E_n, x_0 \neq y_0$ be points that*

$$\min_{\alpha \in E_1} f(x_0 + \alpha v) = f(x_0) ,$$

$$\min_{\beta \in E_1} f(y_0 + \beta v) = f(y_0) .$$

Then

$$(Av, x_0 - y_0) = 0 .$$

Proof. Let us consider the function (2). For $x = x_0 + \alpha v$ we obtain

$$f(x_0 + \alpha v) = (A(x_0 + \alpha v) , \quad x_0 + \alpha v) - 2(b, x_0 + \alpha v) + c =$$
$$= \alpha^2 (Av, v) + 2\alpha[(Ax_0, v) - (b, v)] + f(x_0)$$

and

$$\frac{\partial f(x_0 + \alpha v)}{\partial \alpha} = 2\alpha(Av, v) + 2[(Ax_0, v) - (b, v)] .$$

According to the assumption of the theorem we have

$$\alpha(Av, v) + (Ax_0, v) - (b, v) = 0 , \quad \alpha = 0 \tag{4}$$
$$\beta(Av, v) + (Ay_0, v) - (b, v) = 0 , \quad \beta = 0$$

Equations (4), when rearranged, show that

$$(Av, x_0 - y_0) = 0$$

which is the assertion of the theorem.

Theorem 2. *The vectors $v_0^{(1)}, v_1^{(2)}, \ldots, v_{n-1}^{(n)}$ defined by the algorithm (3) are mutually conjugate.*

Proof. Let $x_0^{(0)}, x_0^{(1)}, \ldots, x_0^{(n)}$ be $n + 1$ linearly independent points of the space E_n. Let us denote

$$v_0^{(i)} = x_0^{(i)} - x_0^{(0)}, \quad i = 1, 2, \ldots, n .$$

From (3) we obtain

$$\begin{aligned}
(5) \qquad x_1^{(1)} &= x_0^{(1)} + \alpha_0^{(1)} v_0^{(1)} = x_0^{(0)} + \alpha_0^{(0)} v_0^{(1)} \\
x_1^{(2)} &= x_0^{(2)} + \alpha_0^{(2)} v_0^{(1)} \\
&\ldots\ldots\ldots\ldots\ldots\ldots \\
x_1^{(n)} &= x_0^{(n)} + \alpha_0^{(n)} v_0^{(1)}
\end{aligned}$$

where $\alpha_0^{(k)}$ are real numbers. Let us denote

$$v_1^{(i)} = x_1^{(i)} - x_1^{(i)}, \quad i = 2, 3, \ldots, n .$$

Equations (5), when rearranged, show that

$$\begin{aligned}
(6) \quad v_1^{(2)} &= x_1^{(2)} - x_1^{(1)} = x_0^{(2)} - x_0^{(0)} + \left(\alpha_0^{(2)} - \alpha_0^{(0)}\right) v_0^{(1)} = v_0^{(2)} + \left(\alpha_0^{(2)} - \alpha_0^{(0)}\right) v_0^{(1)} , \\
v_1^{(3)} &= v_0^{(3)} + \left(\alpha_0^{(3)} - \alpha_0^{(0)}\right) v_0^{(1)} , \\
&\ldots\ldots\ldots\ldots\ldots\ldots \\
v_1^{(n)} &= v_0^{(n)} + \left(\alpha_0^{(n)} - \alpha_0^{(0)}\right) v_0^{(1)} .
\end{aligned}$$

It is shown in [15] that $v_1^{(k)}$ for $k = 2, 3, \ldots, n$ are linearly independent vectors. By means of Theorem 1 we have

$$\left(Av_0^{(1)}, v_1^{(i)}\right) = 0 , \quad i = 2, 3, \ldots, n .$$

Let us denote

$$v_2^{(i)} = x_2^{(i)} - x_2^{(2)} , \quad i = 3, 4, \ldots, n .$$

Further, we show that

$$\left(Av_{i-1}^{(i)}, v_2^{(k)}\right) = 0 , \quad i = 1, 2, \quad k = 3, 4, \ldots, n .$$

By means of Theorem 1 we have

$$\left(Av_1^{(2)}, v_2^{(k)}\right) = 0 , \quad k = 3, 4, \ldots, n$$

and therefore it is sufficient to prove that also

$$\left(Av_0^{(1)}, v_2^{(k)}\right) = 0 , \quad k = 3, 4, \ldots, n .$$

According to the algorithm (3) and the relations analogous (6) we may express

$$v_2^{(k)} = x_2^{(k)} - x_2^{(2)} = v_1^k + \beta_k v_1^{(2)} , \quad k = 3, 4, \ldots, n$$

where β_k are real numbers. Vectors $v_2^{(k)}$ are linearly independent and by virtue of Theorem 1 we obtain

$$\left(Av_0^{(1)}, v_2^{(k)}\right) = \left(Av_0^{(1)}, v_1^{(k)} + \beta_k v_1^{(2)}\right) = \left(Av_0^{(1)}, v_1^{(k)}\right) + \beta_k\left(Av_0^{(1)}, v_1^{(2)}\right) = 0\,,$$

$$k = 3, 4, \ldots, n\,.$$

Let us denote

$$v_k^{(i)} = x_k^{(i)} - x_k^{(k)}\,, \quad i = k + 1, \ldots, n\,.$$

Let

(7) $\left(Av_i^{(i+1)}, v_j^{(r)}\right) = 0\,, \quad j = 1, 2, \ldots, k\,, \quad i = 0, 1, \ldots, j - 1\,, \quad r = j + 1, \ldots, n\,.$

According to Theorem 1,

$$\left(Av_k^{(k+1)}, v_{k+1}^{(r)}\right) = 0\,, \quad r = k + 2, \ldots, n\,. \tag{8}$$

Since

$$v_{k+1}^{(r)} = v_k^{(r)} + \gamma_r v_k^{(k+1)}\,, \quad r = k + 2, \ldots, n$$

where γ_r are real numbers and vectors $v_{k+1}^{(r)}$ are linearly independent, we obtain from (7)

$$\left(Av_i^{(i+1)}, v_{k+1}^{(r)}\right) = \left(Av_i^{(i+1)}, v_k^{(r)} + \gamma_r v_k^{(k+1)}\right) =$$

$$= \left(Av_i^{(i+1)}, v_k^{(r)}\right) + \gamma_r\left(Av_i^{(i+1)}, v_k^{(k+1)}\right) = 0\,, \quad i = 0, 1, \ldots, k - 1\,,$$

$$r = k + 2, \ldots, n\,.$$

Theorem 3. *At the point $x_n^{(n)}$ defined by the algorithm (3), the function (2) achieves its minimum.*

Proof. The point $x_n^{(n)}$ at which the function (2) achieves its minimum may be expressed in the form

$$x_n^{(n)} = x_0^{(0)} + \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}$$

where $v_{i-1}^{(i)}$ are conjugate vectors and $\alpha_{i-1}^{(i-1)}$ are real coefficients defined by the algorithm (3). Then we have [6]

$$f(x_n^{(n)}) = \left(A\left(x_0^{(0)} + \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right),\ x_0^{(0)} + \sum_{i-1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right) -$$

$$- 2\left(b, x_0^{(0)} + \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right) + c = \left(A \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)},\ \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right) +$$

$$+ 2\left(Ax_0^{(0)}, \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right) - 2\left(b, \sum_{i=1}^{n} \alpha_{i-1}^{(i-1)} v_{i-1}^{(i)}\right) +$$

$$+ \left(Ax_0^{(0)}, x_0^{(0)}\right) - 2\left(b, x_0^{(0)}\right) + c\,.$$

According to Theorem 2,

$$\left(Av_{i-1}^{(i)}, v_{j-1}^{(j)}\right) = 0\,, \quad i \neq j\,.$$

Thus we get

$$f(x_n^{(n)}) = f(x_0^{(0)}) + \sum_{i=1}^{n} (\alpha_{i-1}^{(i-1)2}(Av_{i-1}^{(i)}, v_{i-1}^{(i)}) + $$

$$+ 2\alpha_{i-1}^{(i-1)}[(Ax_0^{(0)}, v_{i-1}^{(i)}) - (b, v_{i-1}^{(i)})]),$$

i.e., the minimum of the function (2) is achieved by succesive minimizations in linearly independent directions $v_0^{(1)}, v_1^{(2)}, \ldots, v_{n-1}^{(n)}$.

Theorem 4. *Let* $x_0^{(0)} = (0, \ldots, 0)^T$ *and*

(9) $$x_0^{(k)} = (0, \ldots, 0, t_k, 0, \ldots, 0)^T$$

where $t_k = 1$. *Then* $\alpha_{i-1}^{(k)}$ *defined by the algorithm* (3) *satisfies*

$$\alpha_{i-1}^{(k)} = \frac{b_i - (a_i, x_{i-1}^{(k)})}{(a_i, v_{i-1}^{(i)})}, \quad i = 1, 2, \ldots, n, \quad k = i, i+1, \ldots, n$$

where a_i *is the i-th row of the matrix* A *and* b_i *is the i-th component of the vector* b.

Proof. For the function (2) we obtain

$$\frac{\partial f(x)}{\partial y} = 2(Ax - b, y)$$

where y is a direction vector. It is shown in [15] that the algorithm (3) for

$$\alpha_{i-1}^{(k)} = \frac{b_i - (a_i, x_{i-1}^{(k)})}{(a_i, v_{i-1}^{(i)})}$$

solves the linear system

$$Ax = b$$

whereby

(10) $$(a_j, x_i^{(k)}) = b_j, \quad i = 1, 2, \ldots, n, \quad j = 1, 2, \ldots, i, \quad k = i, i+1, \ldots, n$$

and if $x_0^{(k)}$ are in the form (9), then the vectors $v_0^{(1)}, v_1^{(2)}, \ldots, v_{n-1}^{(n)}$ are mutually conjugate and $v_i^{(i+1)}, x_i^{(i)}, x_i^{(k)}$ are in the form

(11) $$v_i^{(i+1)} = \begin{pmatrix} + \\ \cdot \\ + \\ 1 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad x_i^{(i)} = \begin{pmatrix} + \\ \cdot \\ + \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad x_i^{(k)} = \begin{pmatrix} + \\ \cdot \\ + \\ 0 \\ \cdot \\ 1 \\ \cdot \\ 0 \end{pmatrix}$$

$$i = 0, 1, \ldots, n, \quad k = i+1, \ldots, n$$

where the lower index indicates that the first i components are in general non-zero while the upper index indicates that the k-th component of the corresponding vector is one. It is sufficient to show that

$$(12) \qquad (Ax_i^{(k)} - b, v_{i-1}^{(i)}) = 0\,, \quad i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n\,.$$

From (10), (11) we obtain

$$[(a_i, x_i^{(k)}) - b_i] + \sum_{j=1}^{i-1} \oplus [(a_j, x_i^{(k)}) - b_j] = 0\,,$$
$$i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n$$

where $\oplus$ is in general a non-zero component.
Let A be a sparse matrix. Then reduced algorithms can be derived for the minimization of the quadratic function (2).

Theorem 5. *Let A be a positive definite, symmetric, q-diagonal band matrix. Let $x_0^{(0)} = (0, \ldots, 0)^T$ and*

$$x_0^{(k)} = (0, \ldots, 0, t_k, 0, \ldots, 0)^T$$

where $t_k = 1$. Then the algorithm (3) for the minimization of the quadratic function (2) assumes the form

$$x_i^{(k)} = x_{i-1}^{(k)} + \alpha_{i-1}^{(k)} v_{i-1}^{(i)}\,, \quad v_{i-1}^{(i)} = x_{i-1}^{(i)} - x_{i-1}^{(i-1)}\,,$$
$$i = 1, 2, \ldots, n\,, \quad k = i, i+1, \ldots, n$$

where $\alpha_{i-1}^{(k)}$ are scalar coefficients such that

$$f(x_{i-1}^{(k)} + \alpha v_{i-1}^{(i)}) = \min!\,,$$
$$\alpha = \alpha_{i-1}^{(k)}$$

and

$$x_i^{(k)} = x_i^{(i)} + x_0^{(k)}\,, \quad k > (q-1)/2 + i\,.$$

Proof follows directly from Theorem 4 and Lemma 1.

LINEAR MINIMIZATION

Let us consider the quadratic function (2). Linear minimization consists in determining the scalar coefficient λ such that $f(x + \lambda v)$ for given x and v achieves its minimum. In the case of quadratic function, the minimum is defined by three function values $f(x + \lambda_1 v) = f_1$, $f(x + \lambda_2 v) = f_2$, $f(x + \lambda_3 v) = f_3$. For λ we obtain

$$\lambda = -\frac{1}{2}\frac{(\lambda_3^2 - \lambda_2^2) f_1 + (\lambda_1^2 - \lambda_3^2) f_2 + (\lambda_2^2 - \lambda_1^2) f_3}{(\lambda_2 - \lambda_3) f_1 + (\lambda_3 - \lambda_1) f_2 + (\lambda_1 - \lambda_2) f_3}\,.$$

Let us denote

$$(13) \qquad u = \frac{(\lambda_2 - \lambda_3) f_1 + (\lambda_3 - \lambda_1) f_2 + (\lambda_1 - \lambda_2) f_3}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3)} .$$

Since the second derivative on parallel directions is constant, the minimum on these directions is defined by two function values. Let us denote $f(x + tv) = f_1$, $f(x) = f_0$. Then the minimum on parallel directions is defined by

$$\lambda = (\tfrac{1}{2})t - \frac{f_1 - f_0}{2ut}$$

where u is defined by (13) and t is a scalar coefficient. This property enables us to reduce the number of values of the function $f(x)$ to be calculated.

The above described method requires $n/2(n + 1)$ linear minimizations, calling for $n^2 + 2n$ function values for a quadratic function. If the quadratic function corresponds to a sparse matrix, reduced algorithm can be used, which require substantially less function values. When explicit gradients are not available, then the gradient vector

$$\nabla f(x) = (\partial f/\partial x_1, \partial f/\partial x_2, \ldots, \partial f/\partial x_n)^T$$

is approximated by the difference formulas

$$\partial f/\partial x_j \sim \frac{f(x + \delta e_j) - f(x)}{\delta}$$

where e_j is the vector with the j-th component equal to one and the other components zero. This approximation requires $n + 1$ function values. The trouble with this approach consists in choosing δ. The exact determination of the gradient vector of a quadratic function, not considering rounding errors, is given by the formulas

$$\partial f/\partial x_j = \frac{f(x + \delta e_j) - f(x - \delta e_j)}{2\delta}$$

which require $2n$ function values. The effectiveness of conjugate gradients schemes depends on the ability to generate mutually conjugate directions, and the use of approximate gradients may cut it down. The structure of the matrix has no influence on the total number of function values required for minimization. For illustration, the number of the function values requires by the above described method and the method of conjugate gradients is compared below:

	PPM	Conjugate gradient
general matrix	$n^2 + 2n$	$2n^2 + 3n$
5-diagonal matrix	$7n - 6$	$2n^2 + 3n$
3-diagonal matrix	$5n - 2$	$2n^2 + 3n$

The algorithm (3) can be viewed also as an iterative algorithm in the sense that the point $x_n^{(n)}$ is considered the new initial point $x_0^{(0)}$ for the new computation given by the relation (3). It can be proved that such an algorithm converges for strictly convex functions. This will be investigated in a separated paper. Nongradient methods [6, 8] require n^2 linear minimizations per iteration.

NUMERICAL EXAMPLE

Let us consider the minimization problem of a quadratic function

$$f(x) = (Ax, x) - 2(b, x) .$$

Let $n = 10$,

$$A = \begin{pmatrix} 2 & 1 & . & . & . & 1 \\ 1 & 2 & 1 & . & . & 1 \\ . & . & . & . & . & . \\ . & & & & & \\ . & & & & & . \\ 1 & . & . & . & . & 2 \end{pmatrix}$$

and $b = (21, 23, 21, 23, 21, 23, 21, 23, 21, 23)^T$. The exact solution is $x = (1, 3, 1, 3, 1, 3, 1, 3, 1, 3)^T$. The starting point was chosen to be $x_0^{(0)} = (0, \ldots, 0)^T$. The results obtained by the above described method and by the conjugate gradients method with exact difference formulas are as follows:

PPM	Conjugate gradient
0·9999861	0·9924156
2·9999863	3·0061550
1·0000472	0·9924156
3·0000011	3·0061571
1·0000022	0·9924087
2·9999975	3·0061560
1·0000046	0·9924136
2·9999960	3·0061477
0·9999981	0·9924098
2·9999956	3·0061556

APPLICATIONS

The above described method can be applied

a) to the solution of ill-conditioned linear systems minimizing a quadratic form [10],

b) in optimal control theory, where in many cases explicit gradients are not available at all or only at excessive costs [11, 12, 13]; the structure of the corresponding matrix is in many cases sparse [14],

c) to functions of quadratic forms for which the algorithm (3) terminates after a finite number of iterations, e.g. $y = \exp[f(x)]$.

According to Theorem 4 the total storage requirements are less then $n^2 + n + 2$. For a q-diagonal band matrix it is necessary to store $(q - 1)/2 + 1$ vectors. The above described method is suitable for implementation on a parallel computer, because the minimizations on parallel directions are independent from the computational point of view. The storage requirements are in a suitable disseminated form, i.e., each processor of a multiprocessor system has to store only one vector.

In the next paper we shall consider the convergence of iterative methods of the general form

Step(i): For given $x_0^{(0)}$, $x_0^{(k)} = x_0^{(0)} + v_0^{(k)}$ do the calculation by the recurrent relation

$$x_i^{(k)} = x_{i-1}^{(k)} + \alpha_{i-1}^{(k)} v_{i-1}^{(i)},$$

where

$$v_{i-1}^{(i)} = x_{i-1}^{(i)} - x_{i-1}^{(i-1)}, \quad i = 1, 2, \ldots, n, \quad k = i, i + 1, \ldots, n.$$

Step(ii): Replace $x_0^{(0)}$ by $x_n^{(n)}$ and go to Step(i);
for finding the minimizer of a given continuously differentiable strictly convex function $f : E_n \to E_1$. Here $\alpha_{i-1}^{(k)}$ is the basic steplength and $v_0^{(k)} = (0, \ldots, t_k, \ldots, 0)^T$ where $t_k = \lambda$, $0 < \lambda \leqq 1$.

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Súhrn

PARALELNÁ METÓDA KONJUGOVANÝCH SMEROV PRE MINIMALIZÁCIU

FRIDRICH SLOBODA

V článku je popísaná metóda konjugovaných smerov pre minimalizáciu ktorá nevyžaduje znalosť gradientu. Metóda má vlastnosť kvadratickej konvergencie a úzko súvisí s metódou pre riešenie systému lineárnych algebraických rovníc čo umožňuje definovať redukované algoritmy ak odpovedajúca matica je riedka.

Author's address: Dr. *Fridrich Sloboda,* Ústav technickej kybernetiky SAV, Dúbravská cesta 1, 809 31 Bratislava.