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Paper Authors: **Turemuratova Ariuxan**



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SOLUTION OF SYSTEMS OF LINEAR ALGEBRAIC EQUATIONS BY MODIFIED CONJUGATE GRADIENT METHODS

Turemuratova Ariuxan

Tashkent Branch of the Russian Economic University named after G. V. Plekhanov, Tashkent, Uzbekistan

ABSTRACT: Several modifications of the method of conjugate gradients for solving systems of linear algebraic equations are carried out in the article, and the application of some of them is illustrated with the solution of a given system of equations.

Keywords: sparse gradients, norms, scalar product, orthogonal, A-orthogonal, residual vector, search direction, binomial and three-term formulas, symmetric and positive with a definite matrix, nonsingular matrix.

INTRODUCTION

Consider one of the effective methods for solving a system of linear algebraic equations

$$Ax = b$$

with matrix A of order n and vector $b \in R^n$ to the space of n -dimensional real vectors with

$$(x, y) = \sum_{i=1}^n x_i y_i$$

scalar product and norm

$\|x\| = (x, x)^{1/2}$, $x, y \in R^n$, called the conjugate gradient method [1,2,3].

Let us assume that the matrix A of system (1) is symmetric and positive definite. Then the computational formulas of the conjugate gradient method as applied to system (1) in the accepted notation can be represented as [2,3,4]:

$$x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}) \in R^n$$

arbitrary initial approximation,

$$p^{(k)} = \begin{cases} r^{(0)}, & \text{если } k=1, \\ \beta_k r^{(k-1)} + p^{(k-1)}, & \text{иначе} \end{cases}$$

$$\beta_k = \frac{(r^{(k-1)}, p^{(k-1)})_A}{\|p^{(k-1)}\|_A^2}; \quad (1) \quad (2)$$

$$x^{(k)} = x^{(k-1)} - \alpha_k p^{(k)}$$

$$\alpha_k = (r^{(k-1)}, p^{(k)}) / \|p^{(k)}\|_A^2,$$

$$k = 1, 2, \dots, s; \quad s \leq n$$

Here $r^{(k)} = Ax^{(k)} - b$, $k = 0, 1, 2, \dots$, and

$(\cdot, \cdot)_A$ denotes the scalar product generated by the matrix A , i.e. $(x, y)_A = (Ax, y)$ for all $x, y \in R^n$, respectively $\|x\|_A = (Ax, x)^{1/2}$.

The main properties of method (2), the proof of which is carried out by induction, are the following:

$$(p^{(i)}, p^{(j)}) = \delta_{ij} \|p^{(i)}\|_A^2$$

$$(r^{(i)}, p^{(j)}) = 0 \text{ для всех } i, j$$

$$(r^{(i)}, r^{(j)}) = \delta_{ij} \|r^{(i)}\|^2, \quad i, j$$

where δ_{ij} - is the Kronecker symbol. From these properties of the method, it immediately follows that the residual vectors $r^{(0)}, r^{(1)}, \dots$ form an orthogonal system, and the vectors $p^{(0)}, p^{(1)}, \dots$, which determine the search directions, form an A -orthogonal system of vectors.

It follows from the last relation (3) that $r^{(s)} = 0$ for some $s \leq n$. Therefore, in the absence of rounding errors, method (2) converges at most in n iterations. Residual vectors and search directions in the conjugate gradient method are not calculated in advance, but are determined sequentially in the order of $r^{(0)}, p^{(0)}, r^{(1)}, p^{(1)}, \dots$ with increasing number of iterations.

The conjugate gradient method will be correctly defined only after setting the method for calculating the direction vectors $p^{(0)}, p^{(1)}, \dots$. For this, various formulas can be proposed, obtaining a specific method in each case.

In this paper, by transforming the formulas of the iterative parameters α_k and β_k into (2), using relations (3), two-term and three-term computational formulas of the conjugate gradient method are constructed. The application of some of them is illustrated with the solution of a particular system of equations.

1. Let us derive some formulas for the conjugate gradient method, having previously transformed the expressions for the parameters α_k and β_k into (2). So

$$r^{(k-1)} = r^{(k-2)} - \alpha_{k-1} A p^{(k-1)}, \quad A p^{(k-1)} = \frac{1}{\alpha_{k-1}} (r^{(k-2)} - r^{(k-1)})$$

then

$$(r^{(k-1)}, A p^{(k-1)}) = \frac{1}{\alpha_{k-1}} (r^{(k-1)}, r^{(k-2)} - r^{(k-1)}) = -\frac{1}{\alpha_{k-1}}$$

$$(p^{(k-1)}, A p^{(k-1)}) = \frac{1}{\alpha_{k-1}} (p^{(k-1)}, r^{(k-2)} - r^{(k-1)}) = \frac{1}{\alpha_{k-1}}$$

Hence we have

$$\alpha_k = \frac{(r^{(k-1)}, p^{(k)})}{(p^{(k)}, A p^{(k)})} = \frac{(r^{(k-1)}, r^{(k-1)} - \beta_k p^{(k-1)})}{(p^{(k)}, A p^{(k)})} = \frac{\|r^{(k-1)}\|^2}{\|p^{(k)}\|^2} \quad (4)$$

$$\beta_k = \frac{(r^{(k-1)}, A p^{(k-1)})}{(p^{(k-1)}, A p^{(k-1)})} = -\frac{\|r^{(k-1)}\|^2}{\|r^{(k-2)}\|^2} \quad (5)$$

Based on formulas (4) and (5), we can write the following two-term formulas for the conjugate gradient method;

$$x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}) \in R^n \text{ - arbitrary initial approximation,}$$

$$p^{(k)} = \begin{cases} r^{(0)}, & \text{если } k=1, \\ \dots \end{cases}$$

$$\beta_k = -\frac{\|r^{(k-1)}\|^2}{\|r^{(k-2)}\|^2}, \quad (6)$$

$$x^{(k)} = x^{(k-1)} - \alpha_k p^{(k)}$$

$$\alpha_k = \|r^{(k-1)}\|^2 / \|p^{(k)}\|_A^2, \quad k=1, 2, \dots, s,$$

where s is the maximum integer for which $\alpha_s > 0, \beta_s < 0, \alpha_1 > 0$.

Note that method (6) uses the norms of pre-computed vectors $r^{(k-1)}$ and $r^{(k-2)}$ to calculate the parameters α_k and β_k , which creates convenience in applying these formulas

and significantly reduces the amount of calculations compared to methods (2).

2. Using the obtained formulas (4) and (5) for the parameters α_k and β_k , we can construct the so-called three-term formulas of the conjugate gradient method.

Substituting expressions

$$p^{(k)} = \frac{1}{\alpha_k} (x^{(k-1)} - x^{(k)}), \quad p^{(k-1)} = \frac{1}{\alpha_{k-1}} (x^{(k-2)} - x^{(k-1)})$$

into the formula

$$p^{(k)} = r^{(k-1)} - \beta_k p^{(k-1)}$$

we get

$$x^{(k)} = x^{(k-1)} - \alpha_k \left[r^{(k-1)} - \left(\frac{\beta_k}{\alpha_{k-1}} \right) (x^{(k-2)} - x^{(k-1)}) \right] \quad A'Ax = A'b, \quad (7)$$

We introduce the notation

$$d_k = 1/\alpha_k, \quad l_{k-1} = -\beta_k/\alpha_{k-1} \quad (8)$$

Then, after performing simple transformations, we obtain

$$d_k = \|p^{(k)}\|_A^2 / \|r^{(k-1)}\|^2 = \|r^{(k-1)}\|_A^2 / \|r^{(k-1)}\|^2 - l_{k-1} \\ l_k = -\beta_{k+1}/\alpha_k = -d_k \beta_{k+1} = d_k \|r^{(k)}\|^2 / \|r^{(k-1)}\|^2 \quad (9)$$

Note that when deriving the formula for α_k , we used, in particular, the representation $A p^{(k)} = (r^{(k-1)} - r^{(k)})/\alpha_k$.

Thus, we finally arrive at the following three-term formulas of the conjugate gradient method:

$$x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}) \in R^n \text{ - arbitrary initial approximation,} \\ x^{(k)} = x^{(k-1)} - \left[r^{(k-1)} - l_{k-1} (x^{(k-1)} - x^{(k-2)}) \right] / d_k$$

$$l_{k-1} = \begin{cases} 0, & \text{если } k=1, \\ \dots \end{cases} \quad (10)$$

$$d_k = \|r^{(k-1)}\|_A^2 / \|r^{(k-1)}\|^2 - l_{k-1}, \\ k=1, 2, \dots, s, \quad s \leq n$$

3. The conjugate gradient method can also be used to solve systems of linear equations with an arbitrary non-singular matrix A . To do this, one can pass from such a system of equations to an equivalent system of equations with a symmetric and positive definite matrix of the form [1,2,5].

$$A'Ax = A'b, \quad (11)$$

where A' is the matrix transposed with respect to the matrix A . Application of the conjugate gradient method to system (11) will lead to the following calculation formulas of the method:

$$x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}) \in R^n \text{ - arbitrary initial approximation,}$$

$$\bar{p}^{(k)} = \begin{cases} A'r^{(0)}, & \text{если } k=1 \\ \dots \end{cases} \\ \beta_k = - \frac{\|A'r^{(k-1)}\|^2}{\|A'r^{(k-2)}\|^2}, \quad (12)$$

$$x^{(k)} = x^{(k-1)} - \bar{\alpha}_k \bar{p}^{(k)}, \quad \bar{\alpha}_k = \frac{\|A'r^{(k-1)}\|^2}{\|A\bar{p}^{(k)}\|}, \\ k=1, 2, \dots,$$

where $r^{(k)}$ is the discrepancy of the original system. The method is controlled by the fulfillment of orthogonality conditions:

$$(A'r^{(k)}, A'r^{(s)}) = 0, \quad k \neq s.$$

4. Let A be an arbitrary non-singular matrix. Application of the conjugate gradient method to an auxiliary system of equations

$$AA'y = b, \quad (13)$$

obtained from the original system (1) is carried out according to the formulas:

$$y^{(0)} = (y_1^{(0)}, y_2^{(0)}, \dots, y_n^{(0)}) \in R^n \text{ - arbitrary initial approximation,}$$

$$p^{(k)} = \begin{cases} r^{(0)}, & \text{если } k=1 \\ -\frac{\|r^{(k-1)}\|^2}{\|r^{(k-2)}\|^2} r^{(k-1)}, & \text{если } k=2, \dots \end{cases} \quad (14)$$

$$y^{(k)} = y^{(k-1)} - \alpha_k p^{(k)}, \quad \alpha_k = \frac{\|r^{(k-1)}\|^2}{\|A' p^{(k)}\|^2}, \quad k=1, 2, \dots$$

where $r^{(k)}$ are the residuals of the transformed system (13), which coincide with the residuals of the original system (1).

We will denote $A' p^{(k)} = q^{(k)}$. Then, since $x = A' y$, after performing simple transformations in formulas (14), we obtain the following method formulas for the original system:

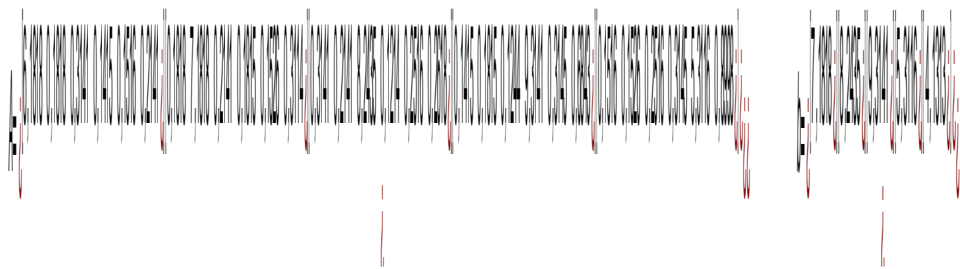
$$x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)}) \in R^n \text{ - arbitrary initial approximation,}$$

$$q^{(k)} = \begin{cases} A' r^{(0)}, & \text{если } k=1 \\ -\frac{\|r^{(k-1)}\|^2}{\|r^{(k-2)}\|^2} A' r^{(k-1)}, & \text{если } k=2, \dots \end{cases} \quad (15)$$

$$x^{(k)} = x^{(k-1)} - \alpha_k q^{(k)}, \quad \alpha_k = \frac{\|r^{(k-1)}\|^2}{\|q^{(k)}\|^2}, \quad k=1, 2, \dots$$

Obviously, $(r^{(k)}, r^{(s)}) = 0$ for $k \neq s$.

Let us illustrate the application of methods (2), (6) and (10) by the example of solving the system of equations (1) for



To compare the convergence of these methods, the same initial approximation $x^{(0)} = (0, 0, 0, 0, 0, 0)$ to the solution of system (16) was taken. Iterative processes were stopped on the sign

$$\max_{1 \leq i \leq 6} |r_i^{(k)}| = \max_{1 \leq i \leq 6} |a_{i1} x_1^{(k)} + a_{i2} x_2^{(k)} + \dots + a_{i6} x_6^{(k)} - b_i|$$

The calculation results are shown in tables No. 1, No. 2, No. 3.

Table No. 1

Solution of system (16) by method (2)

k	x1	x2	x3	x4	x5	x6
r(k)						
0	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
	0.0000000	16.1768150				
1	0.8567904	0.9834514	1.1111743	0.6336752	0.4928651	
	0.3795656	2.0278592				
2	1.0184010	1.0636835	1.0479020	0.4542418	0.5559367	
	0.3803313	0.3145463				
3	1.0407138	1.0532564	1.0235623	0.4741263	0.5729511	
	0.3770219	0.0528413				
4	1.0417463	1.0489094	1.0271981	0.4732816	0.5782731	
	0.3700736	0.0174365				
5	1.0408565	1.0506769	1.0265906	0.4737102	0.5791112	
	0.3674352	0.0009840				
6	1.0409385	1.0506747	1.0266086	0.4737404	0.5789850	
	0.3673531	0.0000406				
7	1.0409383	1.0506740	1.0266072	0.4737366	0.5789841	
	0.3673521	0.0000013				
8	1.0409384	1.0506741	1.0266072	0.4737366	0.5789842	
	0.3673521	0.0000012				
9	1.0409384	1.0506741	1.0266070	0.4737366	0.5789843	
	0.3673521	0.0000005				
10	1.0409384	1.0506741	1.0266070	0.4737366	0.5789843	
	0.3673521	0.0000000				

Answer: $x_1=1.0409384$; $x_2=1.0506741$; $x_3=1.0266070$; $x_4=0.4737366$; $x_5=0.5789843$; $x_6=0.3673521$;

Table No. 2

Solution of system (16) by method (6)

k	x1	x2	x3	x4	x5	x6
r(k)						



|| 0 || 0.000000 || 0.000000 || 0.000000 || 0.000000 || 0.000000 ||
0.000000 || 16.1768150 ||
|| 1 || 0.8567903 || 0.9834513 || 1.1111742 || 0.6336750 || 0.4928650 ||
0.3795656 || 2.0278578 ||
|| 2 || 1.0184009 || 1.0636834 || 1.0479020 || 0.4542417 || 0.5559366 ||
0.3803312 || 0.3145466 ||
|| 3 || 1.0407163 || 1.0532577 || 1.0235614 || 0.4741234 || 0.5729521 ||
0.3770219 || 0.0528413 ||
|| 4 || 1.0417467 || 1.0489085 || 1.0271974 || 0.4732845 || 0.5782740 ||
0.3700736 || 0.0174372 ||
|| 5 || 1.0408561 || 1.0506769 || 1.0265907 || 0.4737087 || 0.5791112 ||
0.3674347 || 0.0009856 ||
|| 6 || 1.0409385 || 1.0506748 || 1.0266085 || 0.4737414 || 0.5789855 ||
0.3673532 || 0.0000500 ||
|| 7 || 1.0409383 || 1.0506741 || 1.0266070 || 0.4737366 || 0.5789843 ||
0.3673520 || 0.0000011 ||
|| 8 || 1.0409384 || 1.0506741 || 1.0266072 || 0.4737366 || 0.5789843 ||
0.3673520 || 0.0000005 ||
|| 9 || 1.0409384 || 1.0506741 || 1.0266072 || 0.4737366 || 0.5789843 ||
0.3673520 || 0.0000000 ||

**Answer: $x_1=1.0409384$; $x_2=1.0506741$; $x_3=1.0266072$; $x_4=0.4737366$;
 $x_5=0.5789843$; $x_6=0.3673520$;**

Table No. 3

Solution of system (16) by method (10)

k	x1	x2	x3	x4	x5	x6
0	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1	0.8567903	0.9834513	1.1111742	0.6336750	0.4928650	0.3795656
2	1.0184033	1.0636847	1.0479010	0.4542390	0.5559375	0.3803312
3	1.0407176	1.0532576	1.0235606	0.4741246	0.5729530	0.3770218
4	1.0417466	1.0489085	1.0271976	0.4732836	0.5782740	0.3700731
5	1.0408561	1.0506769	1.0265908	0.4737092	0.5791112	0.3674347
6	1.0409385	1.0506748	1.0266083	0.4737410	0.5789853	0.3673531
7	1.0409383	1.0506741	1.0266070	0.4737366	0.5789843	0.3673520
8	1.0409383	1.0506741	1.0266072	0.4737366	0.5789843	0.3673521
9	1.0409384	1.0506741	1.0266072	0.4737366	0.5789843	0.3673521

Answer: $x_1=1.0409384$; $x_2=1.0506741$; $x_3=1.0266072$; $x_4=0.4737366$; $x_5=0.5789843$; $x_6= 0.3673521$;

From a comparison of the results obtained in the tables, we note that the convergence of the iterative process in all three versions of the conjugate gradient method is almost the same: the 9th approximation in this example gives a result that is correct up to the seventh decimal place.

In conclusion, we note that the conjugate gradient method, like other orthogonalization methods, is widely used to accelerate the convergence of stationary iterative methods for solving systems of linear algebraic equations [2,3,4].

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