EUCLIDEAN CONJUGATE GRADIENT: AN ITERATIVE ALGORITHM FOR LARGE UNSYMMETRIC MATRICES*

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Abstract. A Conjugate Gradient method (ECG) which minimizes the error with respect to the Euclidean norm, is here proposed for the solution of large unsymmetric systems of linear equations. The method is here derived starting from first principles. Then, it is tested, comparing its performance with ORTHOMIN(m) and GCR(m). The preliminary results here presented indicate that the method is promising, specially for matrices whose condition number is not too close to 1, and deserves further study.

1. Introduction. A class of very effective procedures for solving large sparse symmetric and unsymmetric linear systems of equations is derived from the conjugate gradient method (CG) and its variants, such as ORTHOMIN(m) [13], GCR(m) [5] and GMRES(m) [12], combined with some preconditioning technique.

The main idea of CG associated procedures is to generate a search space conveniently and then to chose the approximate solution of the system, as the vector of such space that minimizes the residual with respect to a suitable norm.

The CG method, as originally formulated by Hestenes and Stiefel [10] (see also [11], [9] and [4]), applies to symmetric positive definite matrices (A) and possesses the following features:

i) The search space is generated by applying the matrix A and its powers to the residual of the system;
ii) At every iteration the residual is minimized with respect to the norm induced by A^{-1} [3].

In general the minimization of the error leads to an orthogonalization process. The main advantage of CG, in its original formulation is that such orthogonalization has to be carried out with respect to the last search direction, only. However, for non symmetric matrices this advantage is lost and in order to save computational effort and memory requirements, modifications in which at each iteration the orthogonalization is not completed, have been introduced.

Recently, the authors have proposed [8], [7] a modification of CG, here called Euclidean Conjugate Gradient (ECG), applicable to non-symmetric systems with the following features:

i) The search space is generated by applying the matrix A^*A and its powers to the residual of the system;
ii) At every iteration the error (exact solution minus approximate one) is minimized with respect to the Euclidean norm. The name ECG was chosen, because this is the main distinguishing feature of the method here proposed.

The main advantages of our procedure when applied to non-symmetric matrices are:

a) The orthogonalization has to be carried out with respect to the last search direction only, as in CG. This is a feature that none of the procedures most extensively used for non-symmetric matrices, possesses.

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b) The minimization of the error is achieved in the Euclidean norm and not in the norm induced by A^*A, as it is done in many other approaches that are being used for non-symmetric matrices. Actually, in standard presentations of such methods [12] the Euclidean norm of the residual is minimized, but this is equivalent to minimize the A^*A-norm of the error as defined above.

However, the main disadvantage is that the search space is generated using the matrix A^*A, which is generally thought to be inconvenient [1]. Since, on the other hand, the Euclidean norm is used, it is natural to inquire to what extent this fact might compensate the above mentioned shortcoming. These considerations lead the authors to carry out preliminary computations oriented to compare the efficiency of ECG with other well established methods. Preliminary results obtained during the Thesis work of one the authors exhibitted certain number of cases in which the new approach have better performance than GCR(m) and ORTHOMIN(m). These results motivated initiating a project of research, now under way, in which the new procedures are being compared systematically with well established methods including GMRES(m) and Tchebycheff, in addition to ORTHOMIN(m) and GCR(m).

This paper is devoted to present such modification of the Conjugate Gradient Method, as well as some of the numerical results obtained thus far.

2. Formulation of the Conjugate Gradient method. In this Section we revise the formulation of CG, in order to motivate the modification here proposed. In what follows P is a non-singular matrix, generally non-symmetric, while the notation A is reserved for the case when such matrix is symmetric and positive definite.

Consider the equation

$$Au = c \tag{1}$$

Let $\mathbf{u}_s$ be the exact solution of (1). Choose $\mathbf{u}^0$ as any vector and define the error $\mathbf{e}^0$ by

$$\mathbf{e}^0 = \mathbf{u}_s - \mathbf{u}^0.$$

For every $m = 1, \dots, N$ the Krylov space K_m is

$$K_m = \text{span}\,\{A\mathbf{e}^0, \dots, A^m\mathbf{e}^0\} = \text{span}\,\{\mathbf{r}^0, A\mathbf{r}^0, \quad , A^{m-1}\mathbf{r}^0\}$$

where $\mathbf{r}^0 = A\mathbf{e}^0 = \mathbf{c} - A\mathbf{u}^0$. It is easy to see that $\dim K_m = m$. Define

$$\mathbf{e}^k = \mathbf{u}_s - \mathbf{u}^k, \qquad k = 1, \dots, N$$

where $\mathbf{u}^k$ is the projection of $\mathbf{u}_s$ on K_k It is well known that when A is positive definite [7]

$$K_{m+1} = K_m + A\mathbf{e}^m$$

unless

$$\mathbf{e}^m = 0; \quad i.e. \quad \mathbf{u}^m = \mathbf{u}_s.$$

Also

$$A\mathbf{e}^k \perp K_m; \qquad m \leq k -$$

Due to this facts, if $\mathbf{p}^1$ is defined by

$$\mathbf{p}^1 = A\mathbf{e}^0 = \mathbf{c} - A\mathbf{u}^0, \tag{2}$$

then $\mathbf{u}^k$ can be constructed recursively using the formulas

$$\begin{aligned} \mathbf{p}^{k+1} &= A\mathbf{e}^k - \beta^{k+1}\mathbf{p}^k = \mathbf{r}^k - \beta^{k+1}\mathbf{p}^k && (3)\\ \mathbf{u}^{k+1} &= \mathbf{u}^k + \alpha^{k+1}\mathbf{p}^{k+1} && (4) \end{aligned}$$

where $\mathbf{r}^k = A\mathbf{e}^k$

$$\beta^{k+1} = \frac{(\mathbf{r}^k, \mathbf{p}^k)}{(\mathbf{p}^k, \mathbf{p}^k)}, \tag{5}$$

and

$$\begin{aligned} \alpha^{k+1} &= \frac{(\mathbf{e}^k, \mathbf{p}^{k+1})}{(\mathbf{p}^{k+1}, \mathbf{p}^{k+1})} \\ &= \frac{(\mathbf{e}^k, A\mathbf{e}^k)}{(\mathbf{p}^{k+1}, \mathbf{p}^{k+1})} && (6) \end{aligned}$$

The results presented up to now are valid irrespectively of which inner product (,) is considered. Unfortunately, α^{k+1} as given by (6), can not be evaluated in general. This is because $\mathbf{e}^k = \mathbf{u}_s - \mathbf{u}^k$ is not known since so is $\mathbf{u}_s$. However, Eq. (6) is computable for some special choices of the inner product (,).

If the inner product is defined by

$$(\mathbf{u}, \mathbf{v}) = A\mathbf{u} * \mathbf{v}$$

where the star stands for the Euclidean inner product, then

$$\alpha^{k+1} = \frac{\mathbf{r}^k * \mathbf{r}^k}{\mathbf{p}^{k+1} * A\mathbf{p}^{k+1}}$$

3. Formulation of the Euclidean Conjugate Gradient method. Consider the equation

$$P\mathbf{u} = \mathbf{b}.$$

Its associated "normal" equation is

$$P^* P\mathbf{u} = P^*\mathbf{b}. \tag{7}$$

The developments of Section 2 up to Eq. (6) can be applied with $A = P^*P$. Then the Krylov spaces corresponding to Eq. (7) are

$$K_m = \operatorname{span}\{P^*P\mathbf{e}^0, \ldots, (P^*P)^m\mathbf{e}^0\}$$

and the construction of $\mathbf{u}^k$ can be carried out applying formulas (2) to (6), using the Euclidean inner product, *i.e.*,

$$(\mathbf{u}, \mathbf{v}) = \mathbf{u} * \mathbf{v}.$$

In particular,

$$(\mathbf{e}^k, A\mathbf{e}^k) = (\mathbf{e}^k, P^* P\mathbf{e}^k) = (P\mathbf{e}^k, P\mathbf{e}^k) = \mathbf{s}^k * \mathbf{s}^k,$$

where

$$\mathbf{s}^k = P(\mathbf{u}_s - \mathbf{u}^k) = \mathbf{b} - P\mathbf{u}^k$$

Then Eqs. (2) to (6) yield the following

ALGORITHM:

1. *Start*: Choose $\mathbf{u}^0$ and compute $\mathbf{s}^1 = \mathbf{b} - P\mathbf{u}^0$. Set $\mathbf{p}^1 = 0$.

2. *Iterate*: For $k = 0$ until convergence do:

$$\mathbf{p}^{k+1} = P^*\mathbf{s}^k - \beta^{k+1}\mathbf{p}^k$$
$$\mathbf{u}^{k+1} = \mathbf{u}^k + \alpha^{k+1}\mathbf{p}^{k+1}$$
$$\mathbf{s}^{k+1} = \mathbf{b} - P\mathbf{u}^{k+1}$$

with

$$\beta^{k+1} = P^*\mathbf{s}^k * \mathbf{p}^k / \mathbf{p}^k * \mathbf{p}^k$$

and

$$\alpha^{k+1} = \mathbf{s}^k * \mathbf{s}^k / \mathbf{p}^{k+1} * \mathbf{p}^{k+1}$$

4. Numerical results. The numerical experiments were performed in a 386 IBM PC compatible machine (MS DOS 3.3 and MS FORTRAN compiler) using double precision. The test problems were the linear systems of equations derived applying the cell method to the $3D$ differential equation governing the steady-state of advective-diffusive transport:

$$\mathbf{v} \cdot \nabla c - \nabla \cdot (K \nabla c) = 0.$$

This problem was solved in a cubic region, for the case when $\mathbf{v}$ is a constant velocity field pointing in a diagonal direction of the cube. The velocity was varied, so that the Peclet number changed from 10^2 to 10^5. The diffusion coefficient was set to be one (*i.e.*, $K \equiv 1$). A partition of the cube was introduced dividing each side into ten elements, so that the dimension of the resulting matrices was 512. The boudary conditions were

$$\begin{aligned} c &= 1 \quad \text{for } x = 0 \text{ or } y = 0 \text{ or } z = 0, \\ c &= 0 \quad \text{for } x = 1 \text{ or } y = 1 \text{ or } z = 1. \end{aligned}$$

Such linear systems of equations were solved applying successively ORTHOMIN(m) and GCR(m), with $m = 1, 2, 3$, in addition to ECG. The stopping criterium was

$$\|\mathbf{r}^k\|_2 \leq 10^{-4}.$$

For the purpose of comparison the results of such numerical experiments are presented in Tables 1 and 2. In this Tables the formulas given in Table 3 were used. For ORTHOMIN(m) and GCR(m) they were taken from Ref. [5], while for ECG were derived by the authors on the basis of well established methods [2].

It may be observed in Table 1 that ECG becomes more competitive as Pe increases. This can be correlated with an increase in condition number. In particular,

Table 1
Iterations and operations (×10⁵) for different Peclet numbers. Matrix dimension $N = 512$

Pe	ORTHOMIN						GCR					
	(1)		(2)		(3)		(1)		(2)		(3)	
	It	Op	It	Op	It	Op	It	Op	It	Op	It	O
10^2	27	1.94	30	2.61	27	2.76	48	3.07	36	2.58	27	2
10^3	45	3.23	43	3.74	43	4.4	66	4.22	56	4.01	44	3
10^4	275	19.71	305	26.55	316	32.36	592	37.89	490	35.12	408	32
10^5	600	43.01	1556	135.43	752	77	> 1990	> 127.4	> 2132	> 152.82	> 2978	> 23

See below for the complete results. (Editor's note)

Table 2
Work per loop and storage requirements.

	ORTHOMIN			GCR			ECG
	(1)	(2)	(3)	(1)	(2)	(3)	
Work/iteration	7168	8704	10240	6400	7168	7936	9728
Storage	2560	3584	4608	2560	3584	4608	2048

for $Pe = 10^4$ it is better than any other of the options considered, requiring only less that one-half of the best alternative (ORTHOMIN(1)). For $Pe = 10^5$, the difference is even greater, since ECG requires about one-fourth the work required by the best of the other procedures compared.

5. Conclusions. On the basis of the numerical results presented in Table 1 and additional numerical work to be published, in which preconditioners are incorporated, our preliminary conclusions are:

i) ECG is competitive when the condition number is not very close to one;
ii) The Euclidean Conjugate Gradient method (ECG), deserves further study.

In particular, it is important to include in the comparisons GMRES and Tcheby-cheff, and the use of preconditioners.

Work along the lines of ii) is being performed by the authors, including applications to test problems derived from oil reservoir simulation [6].

Table 3
Work per loop and storage requirements formulas. mv = matrix-vector product.

	ORTHOMIN(m)	GCR(m)	Proposed method
Work/iteration	$(3m+4)N + 1$ mv	$((3/2)m+4)N + 1$ mv	$5N + 2$ mv
Storage	$(2m+3)N$	$(2m+3)N$	$4N$

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Table 1

Iterations and operations ($\times 10^5$) for different Peclet numbers. Matrix dimension $N = 512$.

Pe	ORTHOMIN						GCR						ECG	
	(1)		(2)		(3)		(1)		(2)		(3)			
	It	Op	It	Op	It	Op	It	Op	It	Op	It	Op	It	Op
10^2	27	1.94	30	2.61	27	2.76	48	3.07	36	2.58	27	2.14	56	5.45
10^3	45	3.23	43	3.74	43	4.4	66	4.22	56	4.01	44	3.49	40	3.89
10^4	275	19.71	305	26.55	316	32.36	592	37.89	490	35.12	408	32.38	98	9.53
10^5	600	43.01	1556	135.43	752	77	> 1990	> 127.4	> 2132	> 152.82	> 2978	> 236.33	121	11.77