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CONJUGATE RESIDUAL METHODS FOR LEAST SQUARES PROBLEM

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Abstract
A wide class of iterative algorithm based on the conjugate directions is proposed for solving large-scale linear least squares problems. The linear convergence of the process is proved.

§1. Introduction

Recently several versions of methods have been proposed for solving large sets of linear equations

$$A\,x = b \qquad (1)$$

with nonsymmetric coefficient matrix[1,2,3]. They are based upon minimizing the Euclidean norm of the residual $\| b - Ax \|^2$ over the space x_i + SPAN$\{p_i, p_{i-1}, \ldots, p_{i-k}\}$, where x_i is the i-th approximation.

In the present paper we extend this method to a linear least squares problem which minimizes $\| b - Ax \|^2$, where A is a large sparse m×n rectangular matrix. We assume that the coefficient matrix is so large that the amount of work and the storage required in the direct methods such as QR or singluar value

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decompositions is nearly prohibitive. A common technique for solving such least squares problem is to apply the conjugate gradient method[4] to the normal equation

$$A^T A x = A^T b. \tag{2}$$

On the i-th iteration, the conjugate gradient method computes an approximate solution over a Krylov subspace $x_i + \mathrm{SPAN}\{A^T r, (A^T A) A^T r, \ldots, (A^T A)^{i-1} A^T r\}$. Since the condition number of $A^T A$ is the square of that of A, this dependence on $A^T A$ tends to make the convergence slow.

The method we present depends on a Krylov subspace based on BA rather than $A^T A$, where B is an appropriately chosen n×m matrix, which we call a mapping matrix. They require that the symmetric part of AB be positive semi-definite. If B is close to a generalized inverse of A, the convergence would be fast. The mapping matrix B plays a role similar to the preconditioner in solving large sparse linear equation by conjugate residual method. For the case with m=n, a different algorithm based on a similar Krylov space was presented in [5], where B is given in the form of C^{-1}. We note that the sum of squares itself has a definite statistical meaning and should not be changed by a preconditioning as, say, $\|B(b-Ax)\|^2$.

In the next section we present CR-LS(k) algorithm for the least squares problem. In §3 we show the convergence conditions and the rate of decrease of the residuals. In §4 we discuss the choice of B. §5 is the conclusion.

§2. Conjugate residual methods

A linear least squares problem is to find $\hat{x} \in R^n$ which minimizes

$$S(x) = \| b - A x \|^2 \tag{3}$$

where A is an m×n matrix and b is a vector of dimension m.

The conjugate residual methods is based on minimizing S(x) along a line $S(x_i+\alpha p_i)$ where p_i is a vector of dimension n and is called a correction vector. In case A is a square matrix, p_i is chosen to be r_i plus a linear conbination of former correction vectors, p_{i-1}, p_{i-2}, ... In our case, however, r_i is an m-vector while p_i is an n-vector, so that we need a mapping matrix B, which maps an m-vector to an n-vector.

Adding the mapping matrix to Orthomin(k)[2], we have the following algorithm

$$
\begin{aligned}
& r_0 = b - Ax_0, \quad p_0 = B\,r_0 \\
& \text{for } i = 0 \text{ to max\_i until convergence do} \\
& \quad \alpha_i = (r_i, Ap_i) \,/\, (Ap_i, Ap_i) \\
& \quad x_{i+1} = x_i + \alpha_i p_i \\
& \quad r_{i+1} = r_i - \alpha_i Ap_i \\
& \quad \text{for } j=0 \text{ to } \min(k-1, i) \text{ do} \\
& \qquad \beta_{i,i-j} = -(ABr_i, Ap_{i-j}) \,/\, (Ap_i, Ap_i) \\
& \quad p_{i+1} = Br_i + \beta_{i,i} p_i + \beta_{i,i-1} p_{i-1} + \cdots + \beta_{i,i-k+1} p_{i-k+1}
\end{aligned}
\tag{4}
$$

Here α_i is so chosen as to minimize the new residual $\| r_i - \alpha_i Ap_i \|$ as a function of α_i along the direction p_i. We will call this algorithm CR-LS(k) method. The number k may be 0, 1, 2, ... , depending on the characteristic of the problem. The work vector necessary to implement CR-LS(k) is x, r, ABr and k sets of p and Ap. In order to minimize the multiplication by A, Ap_i is also updated by

$$
Ap_{i+1} = ABr_i + \beta_{i,i}Ap_i + \beta_{i,i-1}Ap_{i-1} + \cdots + \beta_{i,i-k+1}Ap_{i-k+1} \tag{5}
$$

The residual and correction vectors obey the following relations due to the construction of p's.

<u>Theorem 1</u>

a) $(Ap_i, Ap_j) = 0$	$\lvert i-j \rvert \le k,\ i \ne j$	(6a)
b) $(r_i, Ap_j) = 0$	$0 < i-j < k$	(6b)
c) $(r_i, Ap_i) = (r_i, ABr_i)$		(6c)
d) $(r_i, ABr_j) = 0$	$0 < i-j < k$	(6d)
e) $(r_i, Ap_j) = (r_{i-k}, Ap_j)$	$0 \le i-j \le k$	(6e)

§3. Convergence properties

In the previous section we did not specify the mapping matrix B. The most trivial choice would be $B = A^-$, where A^- is a generalized inverse of A, i.e. $AA^-A = A$ and $(AA^-)^T = (AA^-)$. In this case the first step in (4) would proceed as

$$p_0 = Br_0 = A^-(b - Ax_0)$$
$$(r_0, Ap_0) = (b-Ax_0, AA^-b-Ax_0) = (Ap_0, Ap_0)$$
$$\alpha = 1$$
$$x_1 = x_0 + A^-b - A^-Ax = A^-b - (I-A^-A)x_0,$$

so that x_1 gives one of the least squares solutions. This choice is unrealistic, since if we knew A^- we would simply compute A^-b without applying any iterative methods.

There is a certain trade-off between the number of iterations and the complexity to compute Br. The more the B resembles A^-, the faster the method will converge. On the other hand, the cost to compute Br at each iteration will become large if B is made close to A^-. We will discuss the rate of convergence of the method and the requirement for the mapping matrix B.

We first define the projector P onto Im(A), which is written as AA^- using a generalized inverse. The matrix P obeys the relation $P = P^T = P^2$. We can also write $P = QQ^T$, using the QR decomposition of A, where Q is an $m \times \rho$ matrix (ρ=rank A) with orthonormal column vectors.

We first prove the following lemma.

<u>Lemma 2</u>

$$(Ap_i, Ap_i) \le (ABr_i, ABr_i). \tag{9}$$

<u>Proof</u>

If k=0, eq.(9) is an identity. For k>0, the correction vector p_i is given by (4) in the form

$$p_i = Br_i + \sum \beta_{ij} p_j.$$

From properties (6) we have

$$(Ap_i, Ap_i) = (ABr_i, ABr_i) + 2 \sum \beta_{ij}(ABr_i, Ap_j) + \sum \beta^2_{jj}(ABr_j, ABr_j)$$

$$= (ABr_i, ABr_i) - \sum (ABr_i, Ap_j)^2/(Ap_j, Ap_j)$$
$$\leq (ABr_i, ABr_i). \qquad \text{QED.}$$

Now we will present the main theorem.

Theorem 3

Let $\{r_i\}$ be a sequence of residuals in algorithm (4), then the following inequality holds:

$$\frac{\|r_{i+1} - \hat{r}\|^2}{\|r_i - \hat{r}\|^2} \leq 1 - \frac{\lambda_{min}(M)^2}{\lambda_{max}(M)\lambda_{min}(M) + \rho(R)^2}, \qquad (10)$$

provided

(a) $B P = B$ and

(b) $M \equiv Q^T(AB + B^TA^T) Q / 2$ is positive definite,

where $\hat{r} = b - A\hat{x}$, $R = Q^T (AB - B^TA^T) Q / 2$, λ_{min} and λ_{max} are the maximum and minimum eigenvalues and $\rho(R)$ is the spectral radius of R.

Proof

The proof goes parallel with ref.[3]. The displacement from the minimum residual $\hat{r}$ is the projection of r to Im(A) as,

$$r_i - \hat{r} = A\hat{x} - Ax_i = Pb - PAx_i = Pr_i.$$

The ratio is bounded from above if the assumption (b) holds,

$$\frac{\|r_{i+1} - \hat{r}\|^2}{\|r_i - \hat{r}\|^2} = \frac{\|Pr_{i+1}\|^2}{\|Pr_i\|^2} = 1 - \frac{(r_i, Ap_i)^2}{(Ap_i, Ap_i)(r_i, Pr_i)}$$

$$\leq 1 - \frac{(r_i, ABr_i)}{(ABr_i, ABr_i)}\cdot\frac{(r_i, ABr_i)}{(r_i, Pr_i)} < 1. \qquad (11)$$

Here Lemma 2 has been used.

We now estimate the first factor in the second term of the RHS of eq.(11). The assumption (a), $BP = BQQ^T=B$, enables us to estimate the quantities in the subspace Im(A). We suppress the suffices i.

$$(r, ABr)/(ABr, ABr) = (Pr, ABPr)/(ABPr, ABPr)$$

$$= (QQ^T r,\ ABQQ^T r)/(ABQQ^T r,\ ABQQ^T r),$$
$$= (C^{-1}y,\ y)\ /\ (y,\ y) \geq \lambda_{min}((C^{-1}+C^{-T})/2) \qquad (12)$$

with

$$C = Q^T\ A\ B\ Q,\ y = Q^T ABQ\ Q^T r.$$

Using the relation $X^{-1}+Y^{-1}=(X(X+Y)^{-1}Y)^{-1}$, we have

$$\lambda_{min}((C^{-1}+C^{-T})/2) = \lambda_{max}(M+R^T M^{-1}R)^{-1}$$
$$\geq (\lambda_{max}(M) + \lambda_{min}(M)^{-1}\rho(R)^2)^{-1} \qquad (13)$$

On the other hand the second factor can be transformed

$$(r,\ ABr)/(r,\ Pr) = (Pr,\ ABPr)/(Pr,\ Pr)$$
$$= (V^T r,\ V^T ABV\ V^T r)/(V^T r,\ V^T r)$$
$$\geq \lambda_{min}(M) \qquad (14)$$

Combining eqs.(12), (13) and (14), we have eq. (10). This completes the proof. QED.

This theorem shows that the CR-LS(k) method is at least linearly convergent.

§4. Choise of B

CR-LS(k) algorithm covers a wide class of methods. They differ in the choice of the mapping matrix B and the parameter k. The particular choice of B critically depends on the application and cannot be discussed in general. We will give here a few general comments.

The simplest choice of B which automatically satisfies the two conditions (a) and (b) in Theorem 3 is $B = A^T$. In this case C is symmetric and the convergence rate is controled by $1 - \lambda_{min}(C)/\lambda_{max}(C)$. As is easily expected, this case is equivalent to the conjugate gradient method for the normal equation (2) and CR-LS(k) ($k \geq 1$) is equivalent to CR-LS(1).

We next consider a family of mapping matrices in the form

$$B = D\ A^T, \qquad (15)$$

where D is an appropriate n×n matrix. In practical cases A is a large sparse matrix, so that multiplying A^T from left will not be too time consuming. The matrix D should not have too complex structure. In this choice, the condition (a) is automatically satisfied. If the symmetric part of D is positive definite, the condition (b) is also safisfied, since

$$2 M = Q^T(ADA^T + AD^TA^T) Q = Q^TA (D + D^T) A^TQ. \qquad (16)$$

We have to make the condition number of M as small as possible. The extreme choice would be to set D equal to $(A^TA)^-$. In this case, B is a generalized inverse of A. If the columns of A are approximately orthogonal, we may take D as the inverse of the diagonal part of (A^TA). Incomplete Cholesky decomposition[6] of (A^TA) will also be applicable.

§5. Conclusion

We have shown that the conjugate residual method can be extended to the linear least squares problem and pointed out the computational advantages with using a mapping matrix B. We have also presented a proof for the rate of convergence of this mathod. One disadvatage may be that we cannot obtain the variance matrix $(A^TA)^{-1}$ in this algorithm. Extention to the weighted least squares problem with nondiagonal weight is straightforward.

Several numerical tests have been performed on the data smoothing problem by discrete splines, which will be discussed elsewhere.

Finally we would like to remark that the method of the type presented in this paper are efficiently performed on vector supercomputers, since the dominant computation is the innner product of long vectors and the linked triad operation $(x + \alpha y)$.

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SUPPLEMENTARY NOTES

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