DERIVING OPTIMAL KRYLOV SUBSPACE METHODS

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Abstract. We present a unified derivation of several optimal Krylov subspace methods for solving linear systems of equations. Within a single framework, the methods of conjugate gradient, conjugate residual, ORTHOMIN and ORTHODIR are obtained when a particular choice is made with respect to inner products or certain parameters.

Key words. Krylov Subspace Methods, CG, Conjugate Residual, ORTHOMIN, ORTHODIR

AMS subject classifications. 65F10

1. Introduction. Krylov subspace projection methods are efficient and popular iterative methods for solving large sparse linear systems. Methods such as conjugate gradient (CG) are routinely taught in numerical analysis classes and can be found in most texts in numerical analysis/numerical linear algebra. There are several possible ways to derive the CG method. One is based on generalizing the steepest descent method through modifying search directions so as to obtain a globally optimal approximation (as in Golub and Van Loan [2] for example). Another one that is often used is to derive it indirectly from the Lanczos algorithm, which involves quite heavy algebraic manipulations (as in Demmel [1] for example). It is also possible to first present the algorithm and then demonstrate its optimal approximation property (as in Trefethen and Bau [4]). However, all these approaches could be challenging to beginning students in the subject. Furthermore, for students going on to learn other optimal Krylov subspace method such as conjugate residual (CR), ORTHOMIN and ORTHODIR (see Saad [3]), it is probably not easy to make a connection among these algorithmically similar methods that appear to have different origins.

In this article, we present a unified derivation of these methods that uses only the Gram-Schmidt orthogonalization. We shall first define an optimal Krylov subspace method such as CG by its optimal approximation property in a certain inner product and then proceed to construct the best approximation vector. With a particular choice of the inner product or other parameters, the construction leads to one of the CG, CR, ORTHOMIN and ORTHODIR methods. In this way, all these methods share a common recurrence structure and the similarity found in them is easily understood.

We shall present the detailed construction for CG (the best known Krylov subspace method) in Section 2.1. We then show in later subsections that the other methods can be obtained in the same framework of construction.

2. Optimal Krylov Subspace Methods. Consider the linear system $Ax = b$ where A is a nonsingular $n \times n$ matrix and $b \in R^n$. The k-th Krylov subspace is defined as

$$\mathcal{K}_k = \text{span}\{b, Ab, \cdots, A^{k-1}b\}.$$

Throughout, we shall assume $\mathcal{K}_n$ has dimension n.

For an inner product $[\cdot, \cdot]$ on R^n, we define an optimal Krylov subspace method that generates the best approximation x_k from the Krylov subspace $\mathcal{K}_k$ as follows.

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DEFINITION 2.1. AN OPTIMAL KRYLOV SUBSPACE METHOD *in the inner product* $[\cdot, \cdot]$ *is to approximate* $x = A^{-1}b$ *by a sequence* $\{x_k\}$ *such that*

$$x_k \in \mathcal{K}_k \text{ and } \|x_k - x\| = \min_{z \in \mathcal{K}_k} \|z - x\|, \tag{2.1}$$

where $\|\cdot\| = [\cdot, \cdot]^{1/2}$ *is the norm associated with* $[\cdot, \cdot]$.

It is easy to prove that the optimal approximation condition (2.1) is equivalent to the orthogonality (projection) condition

$$x_k - x \perp \mathcal{K}_k, \quad \text{in } [\cdot, \cdot] \tag{2.2}$$

(i.e. $[x_k - x, z] = 0$ for all $z \in \mathcal{K}_k$). This orthogonality property can be used in place of (2.1) to define x_k, and indeed it is this property that will be used in our later derivation.

We discuss in the following subsections algorithms to compute x_k as defined above. With different inner products, different methods are obtained. However, Our main observation is that x_k can be constructed in a single framework that is independent of the inner product used. This framework of construction will be presented in the context of CG in Section 2.1.

Although $[\cdot, \cdot]$ can be any inner product in theory, it should certainly be one that is computable in practice. Furthermore, for the reason that will become clear in our construction of x_k, we shall also require that

$$[\cdot, \cdot] \text{ is such that } [u, A^{-1}v] \text{ is computable} \tag{2.3}$$

for any $u, v \in R^n$.

2.1. Conjugate Gradient Method. First, consider the case that A is symmetric positive definite and we use the inner product

$$[u, v] = u^T A v,$$

(which satisfies (2.3)). In that case, the optimal Krylov subspace method of Definition 2.1 finds $x_k \in \mathcal{K}_k$ to minimize the A-norm of the error $x_k - x$. We now derive a recursive construction of x_k. In the following, $r_k = b - Ax_k$ is the residual of x_k.

From (2.2) and $\mathcal{K}_{k-1} \subset \mathcal{K}_k$, we have for $k \geq 2$,

$$x_k - x_{k-1} = (x_k - x) - (x_{k-1} - x) \perp \mathcal{K}_{k-1}, \tag{2.4}$$

Since we also have $x_k - x_{k-1} \in \mathcal{K}_k$, the direction of $x_k - x_{k-1}$ is uniquely determined by (2.4). Namely, if $p_k \neq 0$ is any vector such that

$$p_k \in \mathcal{K}_k \quad \text{and} \quad p_k \perp \mathcal{K}_{k-1}, \tag{2.5}$$

$x_k - x_{k-1}$ and p_k must be linearly dependent and there is some α_k such that $x_k - x_{k-1} = \alpha_k p_k$, i.e.

$$x_k = x_{k-1} + \alpha_k p_k. \tag{2.6}$$

From the orthogonality (2.2), we have $x_k - x = x_{k-1} - x + \alpha_k p_k \perp p_k \in \mathcal{K}_k$, which implies

$$\alpha_k = -\frac{[p_k, x_{k-1} - x]}{[p_k, p_k]} = \frac{[p_k, A^{-1}r_{k-1}]}{[p_k, p_k]}. \tag{2.7}$$

We conclude that x_k can be constructed from x_{k-1} by (2.6), provided we have p_k. Note that this is derived for $k \geq 2$; but for $k = 1$, (2.6) and (2.7) are still valid if we take $p_1 \in \mathcal{K}_1$ (i.e. $p_1 = b$) and set $x_0 = 0$.

We now proceed to construct p_k. We first observe that, if $p_1, p_2, \cdots, p_{k-1}$ are the vectors defined in the same way as p_k for the previous steps, i.e. $p_i \in \mathcal{K}_i$ and $p_i \perp \mathcal{K}_{i-1}$, then $\{p_1, p_2, \cdots, p_i\}$ forms an orthogonal basis for $\mathcal{K}_i$ (for $1 \leq i \leq k$). Such a sequence can be constructed by the Gram-Schmidt method. Specifically, if $p_1, p_2, \cdots, p_{k-1}$ have been constructed, p_k can be obtained by picking a vector w with

$$w \in \mathcal{K}_k \text{ and } w \notin \mathcal{K}_{k-1} \tag{2.8}$$

and orthogonalizing it against the previous p_i's, i.e.,

$$p_k = w + \sum_{i=1}^{k-1} \gamma_i p_i \quad \text{with} \quad \gamma_i = -\frac{[p_i, w]}{[p_i, p_i]}. \tag{2.9}$$

Now, $w = Ap_{k-1}$ and $w = b - Ax_{k-1}$ are two easily available choices for the vector w; but there are others as well, e.g., $w = Ar_{k-2}$.

Up to this point, we have not used the particular inner product $[u, v] = u^T Av$ and the fact that A is symmetric positive definite, which we shall exploit now. It turns out that if we choose $w = r_{k-1} = b - Ax_{k-1}$, the Gram-Schmidt process (2.9) will be significantly simplified. Indeed, for $i \leq k - 2$, we have $Ap_i \in \mathcal{K}_{k-1}$ and hence

$$[p_i, r_{k-1}] = [p_i, A(x - x_{k-1})] = [Ap_i, x - x_{k-1}] = 0, \tag{2.10}$$

where we have used $[u, Av] = u^T A^2 v = [Au, v]$ and (2.2). Thus, (2.9) reduces to

$$p_k = r_{k-1} + \gamma_{k-1} p_{k-1}. \tag{2.11}$$

This completes the construction of x_k from x_{k-1}. The algorithm defined by the recurrences (2.6) and (2.11) is called the conjugate gradient (CG) method. We omit a detailed statement of the algorithm.

Remark 1. Since we have used the particular inner product $[u, v] = u^T Av$ as well as the symmetry of A only in (2.10) and subsequently (2.11), it is clear that the constructions of x_k by (2.6) and p_k by (2.9) are valid for any other inner product and for a general A.

Remark 2. Choosing a different w for (2.9) would lead to a different algorithm for constructing the same x_k. For example, $w = Ap_{k-1}$ can be used (see section 2.2); but $w = r_{k-1}$ appears to be the most efficient choice.

Remark 3. The constraint on the inner product (2.3) is to allow computation of α_k by (2.7).

Remark 4. If A is symmetric but indefinite, $u^T Av$ is no longer an inner product. In this case, if we apply the CG recurrence and no breakdown (i.e. $[p_i, p_i] = 0$) occurs, the above constructs x_k that satisfies the orthogonality (2.2).

2.2. Conjugate Residual and Symmetric ORTHODIR Methods. If A is symmetric only, we can consider the inner product

$$[u, v] = u^T A^2 v$$

which satisfies (2.3). To construct p_k by (2.9), we first choose $w = r_{k-1}$ again. Then, in this inner product, (2.10) is still valid as $[u, Av] = [Au, v]$ holds. Thus, we have (2.11). So, the exactly same recurrences as in CG (with the coefficients α_k, γ_{k-1} computed in the new inner product $[u, v] = u^T A^2 v$) computes the minimizer of $[z - x, z - x] = \|Az - b\|_2^2$ over $\mathcal{K}_k$, i.e., $x_k \in \mathcal{K}_k$ that satisfies

$$\|Ax_k - b\|_2 = \min_{z \in \mathcal{K}_k} \|Az - b\|_2.$$

This is called conjugate residual algorithm [3, p.183], which is theoretically equivalent to MINRES.

ALGORITHM 1. CONJUGATE RESIDUAL (CR):
Initialize: $x_0 = 0$, $r_0 = b$, $p_1 = r_0$.
For $k = 1, 2, \cdots$
$\alpha_k = \frac{[p_k, A^{-1} r_{k-1}]}{[p_k, p_k]} = \frac{p_k^T A r_{k-1}}{p_k^T A^2 p_k}$
$x_k = x_{k-1} + \alpha_k p_k$
$r_k = r_{k-1} - \alpha_k A p_k$
$\gamma_k = -\frac{[p_k, r_k]}{[p_k, p_k]} = -\frac{p_k^T A^2 r_k}{p_k^T A^2 p_k}$
$p_{k+1} = r_k + \gamma_k p_k$

Remark 5. In this process, we have assumed that r_{k-1} satisfies (2.8) (i.e. $r_{k-1} \notin \mathcal{K}_{k-1}$). It is easy to see form the recurrence that this is the case if $\alpha_i \neq 0$ for all $i \leq k - 1$. If $\alpha_{k-1} = 0$, however, then

$$r_{k-1} = r_{k-2} - \alpha_{k-1} A p_{k-1} = r_{k-2} \in \mathcal{K}_{k-1}.$$

So, r_{k-1} can not be used to construct p_k and the process breaks down.

Remark 6. A more practical version of the conjugate residual algorithm is to compute Ap_k rather than p_k by $Ap_{k+1} = Ar_k + \gamma_k Ap_k$. The resulting algorithm requires one multiplication by A at each iteration.

The possibility that the choice of $w = r_{k-1}$ may fail leads us to consider choosing $w = Ap_{k-1}$, which always satisfies (2.8). The resulting recurrence will be a bit more complicated but does not have the problem of breakdown.

Let $w = Ap_{k-1}$ in the Gram-Schmidt process (2.9). We have, for $i \leq k - 3$,

$$[p_i, Ap_{k-1}] = [Ap_i, p_{k-1}] = 0. \tag{2.12}$$

where we note that $Ap_i \in \mathcal{K}_{k-2}$. Thus, (2.9) reduces to

$$p_k = Ap_{k-1} + \gamma_{k-2} p_{k-2} + \gamma_{k-1} p_{k-1}. \tag{2.13}$$

This construction is the symmetric case of ORTHODIR algorithm.

ALGORITHM 2. SYMMETRIC ORTHODIR:
Initialize: $x_0 = 0$, $r_0 = b$, $p_1 = r_0$.
For $k = 1, 2, \cdots$
$\alpha_k = \frac{[p_k, A^{-1} r_{k-1}]}{[p_k, p_k]} = \frac{p_k^T A r_{k-1}}{p_k^T A^2 p_k}$
$x_k = x_{k-1} + \alpha_k p_k$
$r_k = r_{k-1} - \alpha_k A p_k$
$\gamma_{k-1} = -\frac{[p_{k-1}, Ap_k]}{[p_{k-1}, p_{k-1}]} = -\frac{p_{k-1}^T A^3 p_k}{p_{k-1}^T A^2 p_{k-1}}$,
$\gamma_k = -\frac{[p_k, Ap_k]}{[p_k, p_k]} = -\frac{p_k^T A^3 p_k}{p_k^T p_k}$,
$p_{k+1} = Ap_k + \gamma_{k-1} p_{k-1} + \gamma_k p_k$

2.3. ORTHOMIN and ORTHODIR. If A is nonsymmetric, we can consider the inner product

$$[u, v] = u^T A^T A v$$

which satisfies (2.3). In this case, the derivation of Section 2.1 up to (2.9) is still valid and the computed x_k minimizes $[z - x, z - x] = \|Az - b\|_2$ over $\mathcal{K}_k$. Then, the recurrence using (2.6) and (2.9) with $w = r_{k-1}$ is called the ORTHOMIN (or GCR) algorithm while the one using (2.6) and (2.9) with $w = Ap_{k-1}$ is called the ORTHODIR algorithm (see Saad [3, p.183]). Unfortunately, with either choice of w, the long recurrence can not be reduced to a short one in general as orthogonality like (2.10) or (2.12) no longer holds. This is due to the fact that A is not self-adjoint in the inner product $[u, v]$. If A is nonsymmetric but there is an inner product $[u, v]$ such that A is self-adjoint in it, then a short recurrence will be obtained. A preconditioned CG algorithm, for example, can be derived in this way.

3. Conclusion. We conclude that optimal approximations x_k from Krylov subspaces in a general inner product can be obtained by a recursive update of x_k and a simultaneous construction of an orthogonal basis by the Gram-Schmidt method. If A is self-adjoint in the inner product, the Gram-Schmidt orthogonalization reduces to a short recurrence. For the inner products that we discuss in Section 2, this coincides with the fact that A is symmetric.

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