Iterative Methods

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Contents

1 General Projection Methods

Let A $\in \mathbb{R}^{n\times n}$ and $\mathcal{K}\ and\ \mathcal{L}$ be two m-dimensional subspaces of $\mathbb{R}^n$. A projection technique onto the subspace $\mathcal{K}$ and orthogonal to $\mathcal{L}$ with an initial guess x_0 is a process which finds an approximate solution $\tilde{x}$ by imposing the conditions that $\tilde{x}$ belong to $x_0 + \mathcal{K}$ and that the new residual vector be orthogonal to $\mathcal{L}$, i.e,

$$find\quad \tilde{x} \in x_0 + \mathcal{K},\ such\ that\ \ b - A\tilde{x} \perp \mathcal{L}.$$

$$\tilde{x} = x_0 + \delta,\ \delta \in \mathcal{K}$$

$$(r_0 - A\delta, w) = 0,\ \forall\, w \in \mathcal{L},\ where\ r_0 = b - Ax_0.$$

Let $V = [v_1, \cdots, v_m]_{n\times m}\ and\ W = [w_1, \cdots, w_m]_{n\times m}$ whose column-vectors form a basis of $\mathcal{K}$ and $\mathcal{L}$, respectively. Then approximate solution can be written as:

$$\tilde{x} = x_0 + Vy,$$

where y can found from the orthogonality constraint:

$$W^T AVy = W^T r_0.$$

If $W^T AV$ is non-singular, then $\tilde{x} = x_0 + V(W^T AV)^{-1} W^T r_0$.

Algorithm 1 Prototype Projection Method

```
repeat
    Select a pair of subspaces $\mathcal{K}\ and\ \mathcal{L}$
    Choose basis $V$=$[v_1, \cdots, v_m]$, $W$=$[w_1, \cdots, w_m]$ $for\ \mathcal{K}\ and\ \mathcal{L}$
    $r \leftarrow b - Ax$
    $y \leftarrow (W^T AV)^{-1} W^T r$
    $x \leftarrow x + Vy$
until Convergence
```

Non-singularity of A is not sufficient condition for non-singularity of $W^T AV$.

Proposition. *Let A, $\mathcal{L}$ and $\mathcal{K}$ satisfy either one of the two following conditions:*

i. A is SPD and $\mathcal{L} = \mathcal{K}$, or

ii. A is non-singular and $\mathcal{L} = A\mathcal{K}$.

Then $B = W^T AV$ is non-singular for any bases V and W of $\mathcal{K}$ and $\mathcal{L}$.

Proof. Consider case(i). Since $\mathcal{L} = \mathcal{K}$, then $W = VG$, where G is a non-singular $m \times m$ matrix. Then $B = W^T AV = G^T V^T AV$. Since A is SPD, so is $V^T AV$ and since G is non-singular, B is non-singular.
Now, consider case(ii). Since $\mathcal{L} = A\mathcal{K}$, then $W = AVG$, where G is a non-singular $m \times m$ matrix. Then $B = W^T AV = G^T (AV)^T AV$. Since A is non-singular, then $(AV)_{n\times m}$ full rank matrix and so is $(AV)^T AV$ and therefore, B is non-singular. □

Theorem 1. *Assume that A is SPD and $\mathcal{L} = \mathcal{K}$. Then a vector $\tilde{x}$ is the result of an (orthogonal) projection method onto $\mathcal{K}$ with the starting vector x_0 iff it minimizes the A-norm if the error over $x_0 + \mathcal{K}$, i.e, iff*

$$\tilde{x} = \underset{x\in x_0+\mathcal{K}}{\arg\min} \|x_* - x\|_A = \underset{x\in x_0+\mathcal{K}}{\arg\min} (A(x_* - x), x_* - x)^{\frac{1}{2}}$$

Proof. First we prove that if $\tilde{x}$ minimizes A-norm of the error, then it is the result of orthogonal projection method with x_0 onto $\mathcal{K}$. Assume columns of V to be basis vectors of $\mathcal{K}$, then the objective function can be written as:

$$\begin{aligned}
E(x) &= (A(x_* - x), x_* - x)^{\frac{1}{2}}, \qquad (x \in x_0 + \mathcal{K}) \\
\implies E(y) &= (A(x_* - x_0 - Vy), x_* - x_0 - Vy)^{\frac{1}{2}}, \quad (y \in \mathbb{R}^m) \\
\implies E^2(y) &= (A(x_* - x_0 - Vy), x_* - x_0 - Vy), \\
&= (x_* - x_0 - Vy)^T A(x_* - x_0 - Vy), \\
&= c + 2y^T V^T (Ax_0 - Ax_*) + y^T V^T AVy, \\
&= c - 2y^T V^T (b - Ax_0) + y^T V^T AVy = f(y), \\
\frac{\partial f(y)}{\partial y} = 0 &\implies V^T(b - A(x_0 + Vy)) = 0 \\
&\implies V^T(b - A\tilde{x}) = 0 \\
&\implies b - A\tilde{x} \perp \mathcal{K}.
\end{aligned}$$

Therefore the residue of vector which minimizes A-norm of error over $x_0 + \mathcal{K}$ is orthogonal to $\mathcal{K}$, therefore it is the result of orthogonal projection method onto $\mathcal{K}$ starting with x_0. Now we prove the converse, i.e, the result of orthogonal projection method onto $\mathcal{K}$ starting with x_0 minimizes A-norm of error over $x_0 + \mathcal{K}$. We know $V^T(b - A\tilde{x}) = 0$, i.e, $(x_* - \tilde{x}, v)_A = 0 \; \forall \; v \in \mathcal{K}$.

$$\begin{aligned}
\implies \|x_* - x\|_A &= \|x_* - \tilde{x} + \tilde{x} - x\|_A, \qquad (\tilde{x}, x \in x_0 + \mathcal{K}) \\
&= \|x_* - \tilde{x}\|_A + \|\tilde{x} - x\|_A, \text{ (since } x_* - \tilde{x} \text{ is A-orthogonal to } \mathcal{K}) \\
\implies \|x_* - \tilde{x}\|_A &\leq \|x_* - x\|_A, \; \forall \; x \in x_0 + \mathcal{K}.
\end{aligned}$$

Therefore $\tilde{x}$ minimizes the A-norm of the error. □

Corollary 1.1. *Let A be an arbitrary square matrix and assume that $\mathcal{L} = A\mathcal{K}$. Then a vector $\tilde{x}$ is the result of an (oblique) projection method onto $\mathcal{K}$ orthogonally to $\mathcal{L}$ with the starting vector x_0 iff it minimizes the 2-norm of the residual vector $b - Ax$ over $x \in x_0 + \mathcal{K}$, i.e, iff*

$$\tilde{x} = \underset{x \in x_0 + \mathcal{K}}{\arg\min} \|b - Ax\|_2$$

Proposition. *Let $\tilde{x}$ be the approximate solution obtained from a projection process onto $\mathcal{K}$ orthogonally to $\mathcal{L} = A\mathcal{K}$, and let $\tilde{r} = b - A\tilde{x}$. Then,*

$$\tilde{r} = (I - P)r_0,$$

where P denotes the orthogonal projector onto $\mathcal{K}$.

Proof. Let $r_0 = b - Ax_0$, then

$$\begin{aligned}
\tilde{r} &= b - A\tilde{x} \\
&= b - A(x_0 + \delta), \qquad (\delta \in \mathcal{K}) \\
&= r_0 - A\delta.
\end{aligned}$$

By orthogonality condition we have $\tilde{r} \perp A\mathcal{K}$, i.e, $A\delta$ is the projection of r_0 onto $A\mathcal{K}$. Therefore, if P is the orthogonal projector onto $A\mathcal{K}$, then

$$Pr_0 = A\delta \implies \tilde{r} = (I - P)r_0$$

It follows from the above that $\|\tilde{r}\|_2 \leq \|r_0\|_2$. Therefore, this class of methods can be termed as **Residual Projection Methods**. $\square$

Proposition. *Let $\tilde{x}$ be the approximate solution obtained from an orthogonal projection process onto $\mathcal{K}$, and let $\tilde{d} = x_* - \tilde{x}$. Then,*

$$\tilde{d} = (I - P_A)d_0,$$

where P_A denotes the projector onto $\mathcal{K}$, which is orthogonal with respect to A-inner product.

Proof. Let $d_0 = x_* - x_0$ be the initial error, and let $\tilde{d} = x_* - \tilde{x}$, where $\tilde{x} = x_0 + \delta$ is the approximate solution resulting from the projection step. We know that residual of the approximate solution is orthogonal to $\mathcal{K}$, i.e, $\tilde{r} = A\tilde{d} = A(d_0 - \delta)$, $\tilde{r} \perp \mathcal{K}$.

$$\begin{aligned} &\implies (A(d_0 - \delta), w) = 0 \; \forall \; w \in \mathcal{K} \\ &\implies (d_0 - \delta, w)_A = 0 \; \forall \; w \in \mathcal{K} \end{aligned}$$

Therefore, if P_A is the projector onto $A\mathcal{K}$, which is orthogonal with respect to A-inner product, then δ is the A-orthogonal projection of d_0, i.e,

$$P_A d_0 = \delta \implies \tilde{d} = (I - P_A)d_0.$$

It follows from the above that $\|\tilde{d}\|_A \leq \|d_0\|_A$. Therefore, this class of methods can be termed as **Error Projection Methods**. $\square$

Define $\mathcal{P}_\mathcal{K}$ to be the orthogonal projector onto $\mathcal{K}$ and let $\mathcal{Q}_\mathcal{K}^\mathcal{L}$ be the (oblique) projector onto $\mathcal{K}$ and orthogonally to $\mathcal{L}$. Then

$$\mathcal{P}_\mathcal{K} x \in \mathcal{K} \; and \; x - \mathcal{P}_\mathcal{K} x \perp \mathcal{K},$$

$$\mathcal{Q}_\mathcal{K}^\mathcal{L} x \in \mathcal{K} \; and \; x - \mathcal{Q}_\mathcal{K}^\mathcal{L} x \perp \mathcal{L}$$

Theorem 2. *Assume that $\mathcal{K}$ is invariant under A and the initial residue, i.e, $r_0 = b - Ax_0$ belongs to $\mathcal{K}$. Then the approximate solution obtained from any (oblique or orthogonal) projectioon method onto $\mathcal{K}$ is exact.*

Proof. An approximate solution $\tilde{x}$ is defined by

$$\begin{aligned} &\mathcal{Q}_\mathcal{K}^\mathcal{L}(b - A\tilde{x}) = 0, \; where \; \tilde{x} = x_0 + \delta, \; \delta \in \mathcal{K}. \\ &\implies \mathcal{Q}_\mathcal{K}^\mathcal{L}(b - Ax_0 - A\delta) = 0 \\ &\implies \mathcal{Q}_\mathcal{K}^\mathcal{L} r_0 = \mathcal{Q}_\mathcal{K}^\mathcal{L} A\delta \\ &\text{But } \mathcal{K} \text{ is invariant under A, then } A\delta \in \mathcal{K}. \\ &\implies r_0 = A\delta, \; \text{(since } r_0 \in \mathcal{K} \text{ and } \mathcal{Q}_\mathcal{K}^\mathcal{L} A\delta = A\delta) \\ &\implies A\tilde{x} = b \end{aligned}$$

$\square$

Theorem 3 (**General Error Bound**). *Let $\gamma = \|\mathcal{Q}_\mathcal{K}^\mathcal{L} A(I - \mathcal{P}_\mathcal{K})\|_2$ and assume that b is a member of $\mathcal{K}$ and $x_0 = 0$. Then the exact solution x_* of the problem is such that*

$$\|b - \mathcal{Q}_\mathcal{K}^\mathcal{L} A \mathcal{P}_\mathcal{K} x_*\|_2 \leq \gamma \|(I - \mathcal{P}_\mathcal{K})x_*\|_2.$$

Proof. Since $b \in \mathcal{K}$,

$$\begin{aligned}
b - \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A \mathcal{P}_{\mathcal{K}} x_* &= \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} b - \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A \mathcal{P}_{\mathcal{K}} x_* \\
&= \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} (b - A \mathcal{P}_{\mathcal{K}} x_*) \\
&= \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A (I - \mathcal{P}_{\mathcal{K}}) x_* \\
&= \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A (I - \mathcal{P}_{\mathcal{K}})(I - \mathcal{P}_{\mathcal{K}}) x_* \\
\implies \|b - \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A \mathcal{P}_{\mathcal{K}} x_*\|_2 &= \|\mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A (I - \mathcal{P}_{\mathcal{K}})(I - \mathcal{P}_{\mathcal{K}}) x_*\|_2 \\
&\leq \|\mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A (I - \mathcal{P}_{\mathcal{K}})\|_2 \|(I - \mathcal{P}_{\mathcal{K}}) x_*\|_2 \\
\implies \|b - \mathcal{Q}_{\mathcal{K}}^{\mathcal{L}} A \mathcal{P}_{\mathcal{K}} x_*\|_2 &\leq \gamma \|(I - \mathcal{P}_{\mathcal{K}}) x_*\|_2
\end{aligned}$$

□

2 One-Dimensional Projection Methods

One-dimensional projection processes are defined when $\mathcal{K} = span\{v\}$ *and* $\mathcal{L} = span\{w\}$. In this case, the new approximation takes the form $x \leftarrow x + \alpha v$, where the orthogonality condition $r - A\delta \perp w$ yields,

$$\alpha = \frac{(r, w)}{(Av, w)}, \; where \; r = b - Ax_0.$$

2.1 Steepest Descent

The steepest descent algorithm is defined when A is SPD and $v = w = r$.

Lemma 4 (**Kantorovich inequality**). *Let B be any real SPD matrix and* λ_1, λ_n *its largest and smallest eigenvalues. Then,*

$$\frac{(Bx, x)(B^{-1}x, x)}{(x, x)} \leq \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n}, \; \forall \, x \neq 0$$

Proof. It is equvivalent to prove the statement for any unit vector x. Since B is SPD, it can be diagonalized by similarity transformation with an orthogonal matrix Q, $B = Q^T DQ$.

$$(Bx, x)(B^{-1}x, x) = (Q^T DQx, x)(Q^T D^{-1}Qx, x) = (DQx, Qx)(D^{-1}Qx, Qx).$$

Define $y = Qx = (y_1, y_2, \cdots, y_n)^T, \; and \; \beta_i = {y_i}^2$. Then,

$$\lambda \equiv (Dy, y) = \sum_{i=1}^{n} \beta_i \lambda_i, \; \sum_{i=1}^{n} \beta_i = 1$$

$$\psi(y) = (D^{-1}y, y) = \sum_{i=1}^{n} \beta_i \frac{1}{\lambda_i}.$$

Note that λ is a convex combinations of eigenvalues of B. Then,

$$(Bx, x)(B^{-1}x, x) = \lambda \psi(y).$$

Noting that $f(\lambda) = 1/\lambda$ is a convex function for $x \in \mathbb{R}_{++}$, $\psi(y)$ containis all the convex combinations of $1/\lambda_i$s which is bounded above by line passing through $(\lambda_1, 1/\lambda_1)$ *and* $(\lambda_n, 1/\lambda_n)$, i.e,

$$\psi(y) \leq \frac{1}{\lambda_1} + \frac{1}{\lambda_n} - \frac{\lambda}{\lambda_1 \lambda_n}.$$

$$\implies (Bx, x)(B^{-1}x, x) = \lambda\psi(y) \leq \lambda\Big(\frac{1}{\lambda_1} + \frac{1}{\lambda_n} - \frac{\lambda}{\lambda_1 \lambda_n}\Big).$$

The right-hand side is maximum when $\lambda = \frac{\lambda_1 + \lambda_n}{2}$ yielding,

$$(Bx, x)(B^{-1}x, x) \leq \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n}$$

□

Algorithm 2 Steepest Descent Algorithm

```
Compute $r = b - Ax$ and $p = Ar$
repeat
    $\alpha \leftarrow (r, r)/(p, r)$
    $x \leftarrow x + \alpha r$
    $r \leftarrow r - \alpha p$
    Compute $p = Ar$
until Convergence
```

Theorem 5. *Let A be a SPD. Then, A-norms of the error vectors $d_k = x_* - x_k$ generated by the above algorithm satsify the following relation:*

$$\|d_{k+1}\|_A \leq \Big(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\Big)\|d_k\|_A,$$

and the algorithm converges for any initial guess x_0.

Proof. We know that $d_{k+1} = x_* - x_{k+1}$, but $x_{k+1} = x_k + \alpha_k r_k$.

$$\implies d_{k+1} = x_* - (x_k + \alpha_k r_k) = d_k - \alpha_k r_k.$$

Now consider,

$$\begin{aligned}
\|d_{k+1}\|_A^2 &= (d_{k+1}, d_k - \alpha_k r_k)_A \\
&= (d_{k+1}, d_k)_A - (d_{k+1}, \alpha_k r_k)_A \\
(d_{k+1}, \alpha_k r_k)_A &= (Ad_{k+1}, \alpha_k r_k) = (r_{k+1}, \alpha_k r_k), \\
&= (r_k - \alpha_k A r_k, r_k), \text{ where } \alpha_k = \frac{(r_k, r_k)}{(Ar_k, r_k)}, \\
&= (r_k, r_k) - \frac{(r_k, r_k)}{(Ar_k, r_k)}(Ar_k, r_k) = 0 = (r_{k+1}, r_k). \\
\implies (d_{k+1}, \alpha_k r_k)_A &= 0, \\
\implies \|d_{k+1}\|_A^2 &= (d_{k+1}, d_k)_A \\
&= (d_{k+1}, Ad_k) \qquad \text{(since A is SPD)}, \\
&= (d_k - \alpha_k r_k, r_k) \\
&= (A^{-1} r_k, r_k) - \alpha_k (r_k, r_k) \\
\text{But, } \|d_k\|_A^2 = (Ad_k, d_k) &= (r_k, d_k) = (A^{-1} r_k, r_k), \\
\implies \|d_{k+1}\|_A^2 &= (A^{-1} r_k, r_k)\Big(1 - \frac{(r_k, r_k)^2}{(Ar_k, r_k)(A^{-1} r_k, r_k)}\Big),
\end{aligned}$$

From Kantorovich inequality,

$$\begin{aligned}
&\le \|d_k\|_A^2 \Big(1 - \frac{4\lambda_1 \lambda_n}{(\lambda_1 + \lambda_n)^2}\Big), \\
\implies \|d_{k+1}\|_A &\le \Big(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\Big) \|d_k\|_A.
\end{aligned}$$

□

3 Krylov Subspace Methods

We define Krylov Subspace to be

$$\mathcal{K}_m(A, v) = span\{v, Av, A^2 v, \cdots, A^{m-1} v\}.$$

Then, $x = p(A)v, \ \forall \ x \in \mathcal{K}_m$, where $deg(p) < m$.

Definition 1 (Minimal Polynomial of a vector)**.** *Monic polynomial of least degree such that $p(A)v = 0$ is called minimal polynomial of v and degree of such polynomial is called grade(μ).*

Theorem 6. *Let μ be the grade of v. Then $\mathcal{K}_\mu$ is invariant under A and $\mathcal{K}_\mu = \mathcal{K}_m \ \forall \ m \ge \mu$.*

Proof. Since, grade of v is μ there exists a polynomial p of degree μ, such that $p(A)v = 0, \ where \ p(A) = p_0 I + p_1 A + \cdots + p_{\mu-1} A^{\mu-1} + A^\mu$.

$$\implies A^\mu v = -(p_0 I + p_1 A + \cdots + p_{\mu-1} A^{\mu-1}) v \qquad (1)$$

But, $\forall\ x \in \mathcal{K}_\mu,\ x = q(A)v,\ deg(q) < \mu$, i.e,

$$\begin{aligned} x &= q_0 v + q_1 Av + \cdots + q_{\mu-1}A^{\mu-1}v,\ \forall\ x \in \mathcal{K}_\mu, \\ \implies Ax &= q_0 Av + q_1 A^2 v + \cdots + q_{\mu-1}A^{\mu}v, \\ &\text{Case 1: } q_{\mu-1} = 0,\ then\ Ax \in \mathcal{K}_\mu. \\ &\text{Case 2: } q_{\mu-1} \neq 0,\ \text{then replace } A^\mu v\ by\ (1),\ Ax \in \mathcal{K}_\mu. \end{aligned}$$

Therefore, $\mathcal{K}_\mu$ is invariant under A. Similarily it can be seen that $\mathcal{K}_\mu = \mathcal{K}_m$ $\forall\ m \geq \mu$. □

Corollary 6.1. *$dim(\mathcal{K}_m) = min\{m, grade(v)\}$.*

4 Arnoldi's Method for Linear Systems (FOM)

Arnoldi's procedure is an algorithm for building an orthogonal basis of the Krylov subspace $\mathcal{K}_m$.

Algorithm 3 Arnoldi-Modified Gram-Schmidt

```
1: Choose a vector $v_1$ of norm 1
2: for $j = 1, 2, \cdots, m$ do
3:     Compute $w_j = Av_j$
4:     for $i = 1, 2, \cdots, j$ do
5:         $h_{ij} = (w_j, v_i)$
6:         $w_j = w_j - h_{ij}v_i$
7:     EndDo
8:     $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ Stop
9:     $v_{j+1} = w_j / h_{j+1,j}$
10: EndDo
```

Proposition. *Denote by $V_m = [v_1, v_2, \cdots, v_m]_{n\times m}$ and $\bar{H}_m$, the $(m+1)\times m$ Hessenberg matrix whose non-zero entries h_{ij} are defined by the above algorithm and by H_m the matrix obtained from $\bar{H}_m$ by removing the last row. Then,*

$$AV_m = V_m H_m + w_m e_m^T = V_{m+1}\bar{H}_m,$$

$$V_m^T A V_m = H_m.$$

Proof. From lines 6,8 we have, $w_j = Av_j - h_{ij}v_i$ and $w_j = v_{j+1}h_{j+1,j}$.

$$\implies Av_j = \sum_{i=1}^{j+1} h_{ij}v_i \implies AV_m = V_m H_m + w_m e_m^T = V_{m+1}\bar{H}_m.$$

Since V_m^T is orthogonal, we get $V_m^T A V_m = H_m$.

□

Given an initial guess x_0 to the original linear system $Ax = b$, we now consider an orthogonal projection method which takes $\mathcal{L} = \mathcal{K} = \mathcal{K}_m(A, r_0)$, with

$$\mathcal{K}_m(A, r_0) = span\{r_0, Ar_0, A^2 r_0, \cdots, A^{m-1}r_0\},$$

in which $r_0 = b - Ax_0$. This method seeks an approximate solution x_m from the affine subspace $x_0 + \mathcal{K}_m$ of dimension m by imposing the following orthogonality constraint:

$$b - Ax_m \perp \mathcal{K}_m.$$

If $v_1 = r_0/\|r_0\|_2$ in Arnoldi's method, and we set $\beta = \|r_0\|_2$, then

$$V_m^T A V_m = H_m,$$

$$V_m^T r_0 = V_m^T(\beta v_1) = \beta e_1.$$

As a result, the approximate solution using the above m-dimensional subspaces is given by:

$$x_m = x_0 + V_m y_m,$$

where y_m can be found by imposing orthogonality constraint that

$$V_m^T(b - Ax_m) = 0 \implies y_m = H_m^{-1}(\beta e_1).$$

Algorithm 4 Full Orthogonalization Method (FOM)

```
Compute $r_0 = b - Ax_0,\ \beta = \|r_0\|_2,\ and\ v_1 = r_0/\beta$
Define the $m \times m$ matrix $H_m = \{h_{ij}\}_{i,j=1,2,\cdots,m}; Set\ H_m = 0$
for $j = 1, 2, \cdots, m$ do
    Compute $w_j = Av_j$
    for $i = 1, 2, \cdots, j$ do
        $h_{ij} = (w_j, v_i)$
        $w_j = w_j - h_{ij} v_i$
    EndDo
    $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ Stop
    $v_{j+1} = w_j / h_{j+1,j}$
EndDo
Compute $y_m = H_m^{-1} \beta e_1$ and $x_m = x_0 + V_m y_m$
```

Proposition. *The residual vector of the approximate solution x_m computed by the FOM Algorithm is such that*

$$b - Ax_m = -h_{m+1,m} e_m^T y_m v_{m+1}$$

and, therefore,

$$\|b - Ax_m\|_2 = h_{m+1,m} |e_m^T y_m|.$$

Proof.

$$\begin{aligned} b - Ax_m &= b - Ax_0 - AV_m y_m \\ &= r_0 - (V_m H_m + w_m e_m^T) y_m \\ &= r_0 - V_m H_m (H_m^{-1} \beta e_1) - w_m e_m^T y_m \\ &= r_0 - V_m V_m^T r_0 - h_{m+1,m} e_m^T y_m v_{m+1} \\ \implies b - Ax_m &= -h_{m+1,m} e_m^T y_m v_{m+1}. \end{aligned}$$

□

4.1 Variation 1: Restarted FOM

Algorithm 5 Restarted FOM (FOM(m))

```
1: Compute $r_0 = b - Ax_0,\ \beta = \|r_0\|_2,\ and\ v_1 = r_0/\beta$
2: Generate $V_m\ and\ H_m$ using Arnoldi algorithm starting with $v_1$.
3: Compute $y_m = H_m^{-1}\beta e_1$ and $x_m = x_0 + V_m y_m$. If satisfied then Stop.
4: Set $x_0 = x_m$ and go to 1.
```

4.2 Variation 1: IOM and DIOM

Algorithm 6 Incomplete Orthogonalization Method (IOM)

```
Compute $r_0 = b - Ax_0,\ \beta = \|r_0\|_2,\ and\ v_1 = r_0/\beta$
Define the $m \times m$ matrix $H_m = \{h_{ij}\}_{i,j=1,2,\cdots,m}; Set\ H_m = 0$
for $j = 1, 2, \cdots, m$ do
    Compute $w_j = Av_j$
    for $i = max\{1, j - (k-1)\}, 2, \cdots, j$ do
        $h_{ij} = (w_j, v_i)$
        $w_j = w_j - h_{ij} v_i$
    EndDo
    $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$ Stop
    $v_{j+1} = w_j / h_{j+1,j}$
EndDo
Compute $y_m = H_m^{-1}\beta e_1$ and $x_m = x_0 + V_m y_m$
```

A formula can be developed whereby the current approximate solution x_m can be computed from the previous approximation x_{m-1} and a small number vectors are updated at each step. This progressive formulation of the solution leads to an algorithm termed as Direct IOM (DIOM).
The Hessenberg matrix obtained from IOM has a band structure with bandwidth $k + 1$, i.e,

$$H_m = \begin{pmatrix} h_{11} & h_{12} & h_{13} & & \\ h_{21} & h_{22} & h_{23} & h_{24} & \\ & h_{32} & h_{33} & h_{34} & h_{35} \\ & & h_{43} & h_{44} & h_{45} \\ & & & h_{54} & h_{55} \end{pmatrix} = L_m U_m$$

$$= \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ & l_{32} & 1 & & \\ & & l_{43} & 1 & \\ & & & l_{54} & 1 \end{pmatrix} \times \begin{pmatrix} u_{11} & u_{12} & u_{13} & & \\ & u_{22} & u_{23} & u_{24} & \\ & & u_{33} & u_{34} & u_{35} \\ & & & u_{44} & u_{45} \\ & & & & u_{55} \end{pmatrix}$$

The approximate solution then is given by

$$x_m = x_0 + V_m U_m^{-1} L_m^{-1} (\beta e_1).$$

Define $P_m \equiv V_m U_m^{-1}$ *and* $z_m = L_m^{-1}(\beta e_1)$, we have $x_m = x_0 + P_m z_m$. Because of the structure of U_m, P_m can be updated easily. Indeed, equating the last columns of the matrix relation $P_m U_m = V_m$ yields,

$$\sum_{i=m-k+1}^{m} u_{im} p_i = v_m \implies p_m = \frac{1}{u_{mm}} \left(v_m - \sum_{i=m-k+1}^{m-1} u_{im} p_i \right).$$

Therefore, p_m can be computed using previous $p_i's$ and v_m. In addition, due to the structure of L_m, we have compute z_m by,

$$z_m = \begin{bmatrix} z_{m-1} \\ \zeta_m \end{bmatrix}, \text{ where } \zeta_m = -l_{m,m-1}\zeta_{m-1}.$$

Now, the approximate solution is,

$$x_m = x_0 + \begin{bmatrix} P_{m-1} & p_m \end{bmatrix} \begin{bmatrix} z_{m-1} \\ \zeta_m \end{bmatrix} = x_0 + P_{m-1} z_{m-1} + p_m \zeta_m.$$

Noting that $x_{m-1} = P_{m-1} z_{m-1}$, x_m can be updated as follows:

$$x_m = x_{m-1} + \zeta_m p_m.$$

This gives the following algorithm, called **Incomplete Orthogonalization Method**(DIOM).

Algorithm 7 Direct Incomplete Orthogonalization Method (DIOM)

```
Choose $x_0$ and compute $r_0 = b - Ax_0,\ \beta = \|r_0\|_2,\ and\ v_1 = r_0/\beta$
for $m = 1, 2, \cdots,$ until convergence do
    Compute $w_m = Av_m$
    for $i = max\{1, m-k+1\}, 2, \cdots, m$ do
        $h_{im} = (w_m, v_i)$
        $w_m = w_m - h_{im} v_i$
    $h_{m+1,m} = \|w_m\|_2$. If $h_{m+1,m} = 0$ Stop
    $v_{m+1} = w_m / h_{m+1,m}$
    Update the LU factorization of $H_m$, i.e, obtain the last column
        $U_m$ using the previous k pivots. If $u_{mm} = 0$ Stop.
    $\zeta_m = \beta$ if $m = 1$ else $-l_{m,m-1}\zeta_{m-1}$
    $p_m = u_{mm}^{-1}\left(v_m - \sum_{i=m-k+1}^{m-1} u_{im} p_i\right)$(for $i \leq 0$ set $u_{im} p_i \equiv 0$)
    $x_m = x_{m-1} + \zeta_m p_m$
EndDo
```

Remark. *Observe that $V_m^T A V_m = H_m$ is still valid because the orthogonality properties were not used to derive this relation. As a consequence the following result is also valid,*

$$\begin{aligned} b - Ax_m &= -h_{m+1,m} e_m^T y_m v_{m+1} \\ \implies \|b - Ax_m\|_2 &= h_{m+1,m} |e_m^T y_m| \\ \textit{But, } y_m = H_m^{-1}(\beta e_1) &= U_m^{-1} z_m \implies e_m^T y_m = \zeta_m / u_{mm} \\ \implies \|b - Ax_m\|_2 &= h_{m+1,m} \left| \frac{\zeta_m}{u_{mm}} \right| \end{aligned}$$

Since the residual vectors is a scalar multiple of v_{m+1} and since the v_i's are no longer orthogonal, IOM and DIOM are not orthogonal projection techniques. They can however be viewed as oblique projection techniques onto $\mathcal{K}_m$ orthogonally to an artificially constructed subspace.

Proposition. *IOM and DIOM are mathematically equivalent to projection process onto $\mathcal{K}_m$ and orthogonally to*

$$\mathcal{L}_m = span\{z_1, z_2, \cdots, z_m\},$$

$$where\ z_i = v_i - (v_i, v_{m+1})v_{m+1},\ i = 1, 2, \cdots, m.$$

Proof. From the construction of $\mathcal{L}_m,\ v_{m+1}$ is orthogonal to $\mathcal{L}_m$ and we know the final residue r_m is a scalar multiple of v_{m+1}, hence the approximate solution $x_m \in \mathcal{K}_m$ and residue vector $r_m \perp \mathcal{L}_m$. □

5 Symmetric Lanczos Algorithm

The symmetric lanczos algorithm can be viewed as a simplification of Arnoldi's method for the particular case of symmetric matrix. When A is symmetric, then the Hessenberg matrix H_m will become symmetric tridiagonal. The standard notation used to descsribe the Lanczos algorithm is obtained by setting

$$\alpha_j = h_{jj},\ \beta_j = h_{j-1,j},$$

and if T_m denotes the resulting H_m matrix, it is of the form,

$$T_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & . & . & . & \\ & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & \beta_m & \alpha_m \end{pmatrix}.$$

This leads to the following form of Modified Gram-Schmidt variant of Arnoldi's method:

Algorithm 8 Lanczos Algorithm

```
Choose an initial vector $v_1$ with 2-norm unity. Set $\beta_1 \equiv 0,\ v_0 \equiv 0$
for $j = 1, 2, \cdots, m$ do
    $w_j = Av_j - \beta_j v_{j-1}$
    $\alpha_j = (w_j, v_j)$
    $w_j = w_j - \alpha_j v_j$
    $\beta_{j+1} = \|w_j\|_2$. If $\beta_{j+1} = 0$ then Stop
    $v_{j+1} = w_j / \beta_{j+1}$
EndDo
```