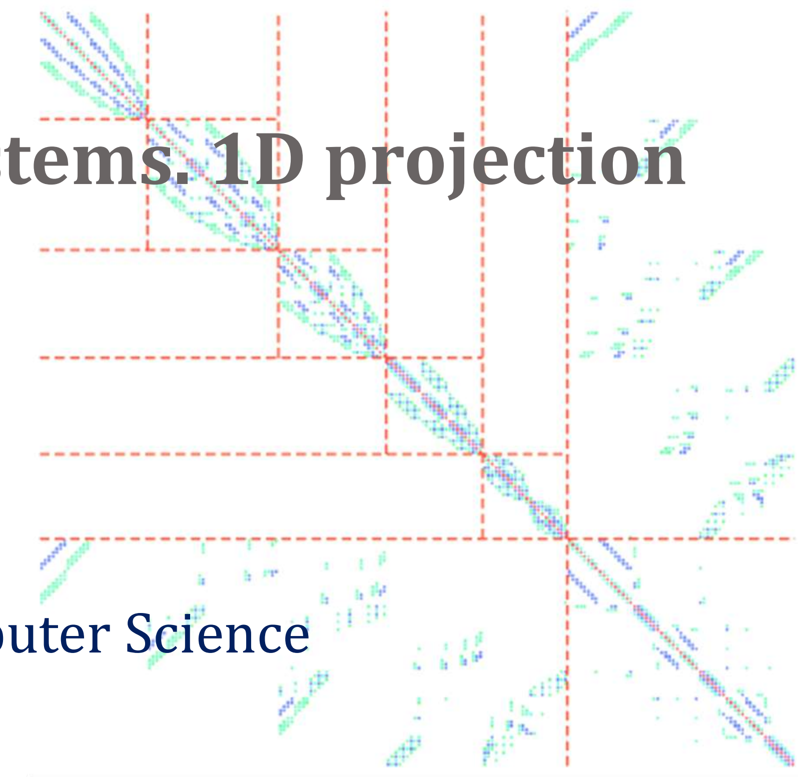
Numerical Methods of Linear Algebra for Sparse Matrices

Lecture 12

Projection methods for linear systems. 1D projection methods



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Projection methods for linear systems

Idea of projection

General formulation of projection method

1D projection methods

Idea of projection method

- Search the solution $\tilde{x}$ of the system $Ax = b, A \in \mathbb{C}^{n \times n}$, $b \in \mathbb{C}^n$ in the search subspace $K \subset \mathbb{C}^n$
- If $\dim(K) = m$ (the basis of K is defined by m vectors), then it is necessary to impose m constraints to extract approximate solution
- These constraints are defined by the subspace of constraints L, which should also have m vectors in the basis: $\dim(L) = m$
- Typical way to impose constraints is to take orthogonality condition, making residual

  $r = b - A\tilde{x}$ orthogonal to the subspace of constraints L: $r \perp L$ (Petrov-Galerkin condition)

General formulation of a projection method

x_0 is initial guess, K is the search subspace, L is the subspace of constraints

Express approximate solution $\tilde{x}$ as $\tilde{x} = x_0 + \delta$, where δ is correction vector $\delta \in K$

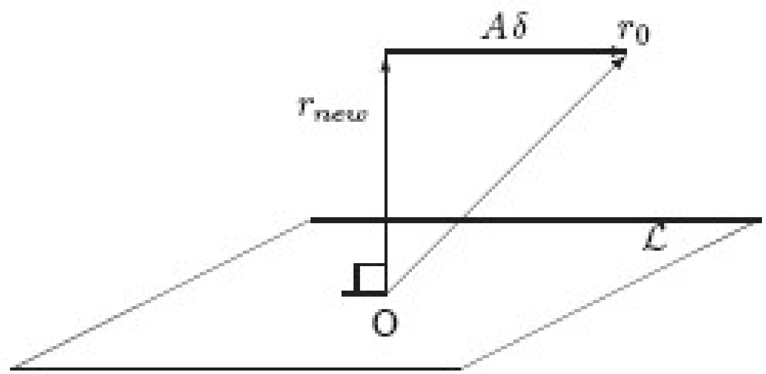
We need to find solution $\tilde{x} \in x_0 + K$, such that residual $r = b - A\tilde{x} \perp L$

Calculate initial residual $r_0 = b - Ax_0$, then

$r = b - A\tilde{x} = b - A(x_0 + \delta) = b - Ax_0 - A\delta = r_0 - A\delta$

$r = r_0 - A\delta \perp L$

$(r_0 - A\delta, w) = 0, \ \forall w \in L$



Matrix representation of a projection method

Consider a linear system $Ax = b,\ A \in \mathbb{C}^{n\times n}$

Size n of the system is large

Take a search subspace $K \subset \mathbb{C}^n,\ \dim(K) = m << n$

$\{v_1, v_2, ..., v_m\}$ is the basis in K

Form a matrix with basis vectors as columns:

$$V = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_m \\ | & | & & | \end{pmatrix},\ V \in \mathbb{C}^{n\times m},\ v_i \in \mathbb{C}^n,\ i = \overline{1,m}$$

Take a subspace of constraints $L \subset \mathbb{C}^n,\ \dim(L) = m << n$

$\{w_1, w_2, ..., w_m\}$ is the basis in L

Form a matrix with basis vectors as columns:

$$W = \begin{pmatrix} | & | & & | \\ w_1 & w_2 & \dots & w_m \\ | & | & & | \end{pmatrix},\ W \in \mathbb{C}^{n\times m},\ w_i \in \mathbb{C}^n,\ i = \overline{1,m}$$

Matrix representation of a projection method

Approximate solution $\tilde{x}$ is given by $\tilde{x} = x_0 + \delta,\ \delta \in K \subset \mathbb{C}^n$

Let's represent correction vector δ as a linear combination of basis vectors of K: $\delta = y_1 v_1 + y_2 v_2 + \ldots + y_m v_m = Vy$, where

$y = (y_1, y_2, \ldots, y_m)^T$ is the vector of the coefficients of linear combination

V is the matrix of the basis vectors: $V = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \ldots & v_m \\ | & | & & | \end{pmatrix},\ V \in \mathbb{C}^{n \times m},$

$v_i \in \mathbb{C}^n,\ y_i \in \mathbb{C},\ i = \overline{1,m} \ \Rightarrow \ \tilde{x} = x_0 + \delta = x_0 + Vy$

Orthogonality condition $(r_0 - A\delta, w) = 0\ \forall w \in L$ is equivalent to the condition for the basis vectors of L:

$(r_0 - A\delta, w_i) = 0;\ \{w_1, w_2, \ldots, w_m\}$ is the basis in L

$(r_0 - AVy, w_i) = 0$

Matrix representation of a projection method

$(r_0 - AVy, w_i) = 0,\ w_i \in \mathbb{C}^n,\ i = \overline{1, m}$

Recall that an inner product can be written as matrix product: $(a, b) = b^H a$

Matrix of basis vectors in L: $W = \begin{pmatrix} | & | & & | \\ w_1 & w_2 & \dots & w_m \\ | & | & & | \end{pmatrix},\ W \in \mathbb{C}^{n\times m}$

Hence inner product $(r_0 - AVy, w_i) = 0$ in matrix form is:

$W^H (r_0 - AVy) = 0$

$W^H r_0 - W^H AVy = 0$

$W^H AVy = W^H r_0$

1) We can find y by solving the system $(W^H AV)y = W^H r_0$

Formally $y = (W^H AV)^{-1} W^H r_0$, matrix $W^H AV$ must be nonsingular

2) After finding y we can find the solution x of initial system $Ax = b$ as

$x = x_0 + Vy = x_0 + V(W^H AV)^{-1} W^H r_0$

General projection method: matrix representation and algorithm

- x_0 is initial guess
- $\tilde{x}$ is approximate solution

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

$\tilde{x} = x_0 + Vy$

- V is the matrix of the basis vectors in K
- y is the vector of the coefficients to be found
- W is the matrix of the basis vectors in L

$W^H AVy = W^H r_0$

$\tilde{x} = x_0 + V(W^H AV)^{-1} W^H r_0$

Algorithm of general projection method

Take initial guess x_0, calculate initial residual

$r_0 = b - Ax_0$

Until convergence do:

1) Select subspaces K and L, take bases

$$V = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_m \\ | & | & & | \end{pmatrix} \text{ in } K$$

$$W = \begin{pmatrix} | & | & & | \\ w_1 & w_2 & \dots & w_m \\ | & | & & | \end{pmatrix} \text{ in } L$$

2) Calculate residual $r = b - Ax$, estimate residual norm: $\|r\|_2 < \varepsilon$

3) Find y from solving the system $W^H AVy = W^H r$:

$y = (W^H AV)^{-1} W^H r$

3) Calculate x as $x = x + Vy$

End do

Theorems on general projection method

Matrix $W^H AV$ can be singular, even when A is nonsingular.

Example. Take a block matrix consisting of zero and identity matrices:

$A = \begin{pmatrix} 0 & I \\ I & I \end{pmatrix}$, $0 \in \mathbb{R}^{m \times m}$ is zero matrix, is $I \in \mathbb{R}^{m \times m}$ identity matrix

A is nonsingular. However, if we take the basis with unit orts: $V = W = \{e_1, ..., e_m\}$,

then $W^H AV$ will be singular

Theorem 1. $W^H AV$ is nonsingular $\Leftrightarrow$ there is no $v \in AK$, such that $v \perp L$

Theorem 2. If matrix A is positive definite and $L = K$ or

matrix A is nonsingular and $L = AK$, then $W^H AV$ is nonsingular for any bases W in L, V in K.

Theorem 3. If matrix A is Hermitian (symmetric) positive definite, then $W^H AV$ is Hermitian (symmetric) positive definite.

One-dimensional projection methods

$\dim(K) = \dim(L) = 1$

Then $K = span\{v\}$, vector v is the basis in K

$L = span\{w\}$, vector w is the basis in L

Orthogonality condition: $r_{new} \perp w$ or $(r_{new}, w) = 0$

$r_{new} = r - A\delta$, where δ is correction vector

We had $x_{new} = x + \delta$, $\delta = Vy \Rightarrow x_{new} = x + Vy$

Now $V = v \Rightarrow \delta = \alpha v$, where α is unknown coefficient

$(r_{new}, w) = 0$

$(r - A\delta, w) = 0$

$(r - A\alpha v, w) = 0$

$(r, w) - \alpha(Av, w) = 0$

Hence $\alpha = \dfrac{(r, w)}{(Av, w)}$

General algorithm of 1D projection method

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$

Until convergence (residual becomes small) do:

1. Select v and w as bases for K and L

2. Take approximate solution x, calculate residual $r = b - Ax$,

compute and estimate residual norm: $\|r\|_2 < \varepsilon$

3. Compute coefficient $\alpha = \dfrac{(r, w)}{(Av, w)}$

4. Recompute approximate solution $x = x + \alpha v$

End Do

Examples of 1D projection methods

- Steepest Descent Method
- Minimal Residual Iteration Method
- Residual Norm Steepest Descent Method

Steepest Descent method (SDM)

Matrix $A \in \mathbb{R}^{n\times n}$ is symmetric positive definite

Take $L = K$, $v = w = r$ as the basis in $K = L$

Algorithm of SDM

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$

Until convergence (residual becomes small) do:

1. Calculate residual at current iteration $r_k = b - Ax_k$,

compute and estimate residual norm: $\|r_k\|_2 < \varepsilon$

2. Compute coefficient $\alpha = \dfrac{(r,w)}{(Av,w)} \Rightarrow \alpha_k = \dfrac{(r_k, r_k)}{(Ar_k, r_k)}$

3. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$

End Do

Here $(Ar_k, r_k) > 0$, because A is symmetric positive definite

Two different matrix-by-vector products are computed in this loop:

Ax_k and Ar_k

Modification of SDM algorithm

Algorithm of SDM with one matrix-by-vector product in a loop:

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$, calculate $p_0 = Ar_0$

Until convergence (residual becomes small) do:

1. Compute coefficient $\alpha_k = \dfrac{(r_k, r_k)}{(p_k, r_k)}$

2. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$,

3. Compute new residual $r_{k+1} = r_k - \alpha_k p_k$, estimate residual norm: $\|r_{k+1}\|_2 < \varepsilon$

4. Compute new $p_{k+1} = Ar_{k+1}$

End Do

Here only one matrix-by-vector product is computed in the loop: Ar_{k+1}

Theorems on Steepest Descent method

Theorem 1. The functional $f(x) = \|x - x_*\|_A^2$ is minimized at every iteration in the direction of $-\nabla f(x) \uparrow\uparrow r$ and coefficient $\alpha = \dfrac{(r,r)}{(Ar,r)}$ gives minimum to the functional $f(x) = \|x - x_*\|_A^2$, where is x_* exact solution, r is the residual, $\|x\|_A^2$ is defined as $\|x\|_A^2 = (x,x)_A = (Ax,x)$

Convergence of SDM is guaranted when matrix A is symmetric positive definite.

Theorem 2. If matrix A is symmetric positive definite, then

1) $\left\|x_* - x^{(k+1)}\right\|_A \le \dfrac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \left\|x_* - x^{(k)}\right\|_A$, where $\lambda_{\max}$ and $\lambda_{\min}$ are maximal and minimal eigenvalues of A, x_* is the exact solution of the system $Ax = b$

2) SDM converges for any initial guess

Proof of Theorem 1.1

Theorem 1. The functional $f(x) = \|x - x_*\|_A^2$ is minimized at every iteration in the direction of $-\nabla f(x) \uparrow\uparrow r$ and coefficient $\alpha = \dfrac{(r,r)}{(Ar,r)}$ gives minimum to the functional

$\vartriangle$ Proove that 1) $-\nabla f(x) \uparrow\uparrow r$

Recall that $(x,y)_A = (Ax,y) = y^H Ax$ ($y^T Ax$ in real space $\mathbb{R}^n$, also $(x,y) = (y,x)$ in $\mathbb{R}^n$)

$f(x) = \|x - x_*\|_A^2 = (x - x_*, x - x_*)_A = (A(x - x_*), x - x_*) =$

$= (Ax, x) - (Ax, x_*) - (Ax_*, x_*) - (Ax_*, x) =$

$= (Ax, x) - (Ax, x_*) - (b, x_*) - (b, x) = x^T Ax - x_*^T Ax - b^T x_* - b^T x$

As A is symmetric: $A = A^T$, then $x_*^T Ax = x_*^T A^T x = (Ax_*)^T x = b^T x$

$x^T Ax - x_*^T Ax - b^T x_* - b^T x = x^T Ax - b^T x - b^T x_* - b^T x = x^T Ax - 2b^T x - b^T x_*$

Hence $f(x) = x^T Ax - 2b^T x - b^T x_* = x^T Ax - 2b^T x - const$

$\nabla f(x)$ is the gradient of the functional, we differentiate by x:

$\nabla f(x) = 2Ax - 2b = 2(Ax - b) = -2r$, where $r = b - Ax$ is the residual

Hence $-\nabla f(x) = 2r \;\Rightarrow\; -\nabla f(x) \uparrow\uparrow r$ $\square$

Proof of Theorem 1.2

$\triangle$ Proove that 2) coefficient $\alpha = \dfrac{(r,r)}{(Ar,r)}$ gives minimum to the functional $f(x) = \|x - x_*\|_A^2$:

$$f(x) = \|x - x_*\|_A^2 = x^T Ax - 2b^T x - const$$

Approximate solution x is recomputed in the algrorithm of SDM as $x + \alpha r$

$$f(x + \alpha r) = (x + \alpha r)^T A(x + \alpha r) - 2b^T (x + \alpha r) - const =$$

$$= \underline{\underline{x^T Ax}} + \underline{\alpha x^T Ar} + \alpha^2 r^T Ar + \underline{\alpha r^T Ax} - \underline{\underline{2b^T x}} - 2\alpha b^T r + const =$$

$$= (x^T Ax - b^T x) - b^T x + \underline{\alpha x^T Ar} + \underline{\alpha r^T Ax} - 2\alpha b^T r + \alpha^2 r^T Ar + const$$

$$\underline{\alpha r^T Ax} = \alpha(Ax, r) = \alpha(x, A^T r) = \alpha(x, Ar) = \alpha(A^T x, r) = \alpha(Ax, r) = \underline{\alpha x^T Ar}$$

Hence $f(x + \alpha r) = (x^T Ax - b^T x) - b^T x + 2\alpha x^T Ar - 2\alpha b^T r + \alpha^2 r^T Ar + const$

$$x^T Ax - b^T x = (Ax)^T x - b^T x = ((Ax)^T - b^T)x = (Ax - b)^T x = -r^T x$$

$$2\alpha x^T Ar - 2\alpha b^T r = 2\alpha(x^T Ar - b^T r) = 2\alpha((Ax)^T r - b^T r) = 2\alpha(Ax - b)^T r = -2\alpha r^T r$$

Hence $f(x + \alpha r) = -r^T x - b^T x - 2\alpha r^T r + \alpha^2 r^T Ar + const = \varphi(\alpha)$

$\dfrac{d\varphi(\alpha)}{d\alpha} = -2r^T r + 2\alpha r^T Ar$. In the algorithm of SDM $\alpha = \dfrac{(r,r)}{(Ar,r)} \Rightarrow$

$$\frac{d\varphi(\alpha)}{d\alpha} = -2r^T r + 2\frac{(r,r)}{(Ar,r)} r^T Ar = -2r^T r + 2\frac{r^T r}{r^T Ar} r^T Ar = -2r^T r + 2r^T r = 0$$

Hence $\alpha = \dfrac{(r,r)}{(Ar,r)}$ gives minimum to the functional $\square$

Minimal Residual Iteration method (MRIM)

Matrix $A \in \mathbb{R}^{n\times n}$ is positive definite

Take $L = AK$, $v = r$ is the basis in K, $w = Av = Ar$ is the basis in L

Algorithm of MRIM

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$

Until convergence (residual becomes small) do:

1. Calculate residual at current iteration $r_k = b - Ax_k$,

compute and estimate residual norm: $\|r_k\|_2 < \varepsilon$

2. Compute coefficient $\alpha = \dfrac{(r, w)}{(Av, w)} \Rightarrow \alpha_k = \dfrac{(Ar_k, r_k)}{(Ar_k, Ar_k)}$

3. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$

End Do

Here $(Ar_k, Ar_k) > 0$, because A is positive definite:

$(Ar_k, Ar_k) = (r_k, A^T Ar_k) = (A^T Ar_k, r_k) > 0$, as $A^T A$ is symmetric positive definite.

Two different matrix-by-vector products are computed in this loop:

Ax_k and Ar_k

Modification of MRIM algorithm

Algorithm of MRIM with one matrix-by-vector product in a loop:

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$, calculate $p_0 = Ar_0$

Until convergence (residual becomes small) do:

1. Compute coefficient $\alpha_k = \dfrac{(p_k, r_k)}{(p_k, p_k)}$

2. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$,

3. Compute new residual $r_{k+1} = r_k - \alpha_k p_k$, estimate residual norm: $\|r_{k+1}\|_2 < \varepsilon$

4. Compute new $p_{k+1} = Ar_{k+1}$

End Do

Here only one matrix-by-vector product is computed in the loop: Ar_{k+1}

Theorems on Minimal Residual Iteration method

Theorem 1. The functional $f(x) = \|b - Ax\|_2^2 = \|r\|_2^2$ is minimized at every iteration in the direction of r, where r is the residual.

Convergence of MRIM is guaranted when matrix A is real positive definite.

Theorem 2. If matrix A is real positive definite, then

1) $\|r_{k+1}\|_2 \leq \sqrt{1 - \frac{\mu^2}{\sigma^2}} \|r_k\|_2$, where $\mu = \frac{1}{2}\lambda_{\min}$ $\lambda_{\min}$ is the minimal eigenvalue of $A + A^T$, and $\sigma = \|A\|_2$

2) MRIM converges for any initial guess

Residual Norm Steepest Descent method (RNSD)

Matrix $A \in \mathbb{R}^{n\times n}$ is nonsingular

Take $L = AK$, $v = A^T r$ is the basis in K, $w = Av$ is the basis in L

In general $\alpha = \dfrac{(r,w)}{(Av,w)} \Rightarrow$ here $\alpha_k = \dfrac{(r_k, AA^T r_k)}{(Av_k, Av_k)} = \dfrac{(A^T r_k, A^T r_k)}{(Av_k, Av_k)} = \dfrac{(v_k, v_k)}{(Av_k, Av_k)} = \dfrac{\|v_k\|_2^2}{\|Av_k\|_2^2}$

Algorithm of RNSD

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$

Until convergence (residual becomes small) do:

1. Calculate residual at current iteration $r_k = b - Ax_k$,

compute and estimate residual norm: $\|r_k\|_2 < \varepsilon$

2. Compute $v_k = A^T r_k$

2. Compute coefficient $\alpha = \dfrac{(r,w)}{(Av,w)} \Rightarrow \alpha_k = \dfrac{\|v_k\|_2^2}{\|Av_k\|_2^2}$

3. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$

End Do

Three different matrix-by-vector products are computed in this loop: Ax_k, $A^T r_k$, Av_k

Modification of RNSD algorithm

Algorithm of MRIM with two matrix-by-vector products in a loop:

Take initial guess x_0, calculate initial residual $r_0 = b - Ax_0$

Until convergence (residual becomes small) do:

1. Compute $v_k = A^T r_k$, $p_k = Ar_k$

2. Compute coefficient $\alpha_k = \dfrac{\|v_k\|_2^2}{\|Av_k\|_2^2}$

3. Compute new approximate solution $x_{k+1} = x_k + \alpha_k r_k$,

4. Compute new residual $r_{k+1} = r_k - \alpha_k p_k$, estimate residual norm: $\|r_{k+1}\|_2 < \varepsilon$

End Do

Here only two matrix-by-vector products are computed in the loop: $A^T r_k$ and Ar_k

Theorems on Residual Norm Steepest Descent method

Theorem 1. The functional $f(x) = \|b - Ax\|_2^2 = \|r\|_2^2$ is minimized at every iteration in the direction of $-\nabla f(x)$, where r is the residual.

Convergence of RNSD is guaranted when matrix A is nonsingular.

Theorem 2. If matrix A is nonsingular, then RNSD converges for any initial guess

RNSD method is SDM applied to the system $A^T Ax = A^T b$

Theorems on orthogonal and oblique projection methods

- Orthogonal projection method: $L = K$
- Oblique projection method: $L \neq K$

Theorem 1. If matrix A is symmetric positive definite and $L = K$, then the vector of approximate solution $\tilde{x}$ is the result of orthogonal projection method on K $\Leftrightarrow$ $\tilde{x}$ minimizes the functional $f(x) = \|x - x_*\|_A^2$ on K

Theorem 2. If matrix A is nonsingular and $L = AK$, then, then the vector of approximate solution $\tilde{x}$ is the result of oblique projection method on K $\Leftrightarrow$ $\tilde{x}$ minimizes the functional $f(x) = \|b - Ax\|_2^2 = \|r\|_2^2$ on K