

Lecture 12: Conjugate gradients



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1. The principle of conjugate gradients

- Consider a Hermitian positive definite linear system

$$\mathbf{Ax} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{C}^{m \times m}, \quad \mathbf{b} \in \mathbb{C}^m.$$

For initial guess \mathbf{x}_0 , at step j , the conjugate gradient method finds an approximate solution

$$\mathbf{x}_j \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$$

satisfying

$$\mathbf{r}_j := \mathbf{b} - \mathbf{Ax}_j \perp \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0),$$

where

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0) := \text{span}\{\mathbf{r}_0, \mathbf{Ar}_0, \dots, \mathbf{A}^{j-1}\mathbf{r}_0\}.$$

- Note that the residual of GMRES satisfies

$$\mathbf{r}_j \perp \mathbf{A}\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0).$$

2. Conjugate gradients

Algorithm CG: $\mathbf{Ax} = \mathbf{b}$, $\mathbf{A} \in \mathbb{C}^{m \times m}$ Hermitian positive definite.

Choose arbitrary \mathbf{x}_0 ;

Set $\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0$ and $\mathbf{p}_0 = \mathbf{r}_0$;

for $j = 1, 2, \dots$, **do** until convergence:

$$\alpha_j = \frac{\langle \mathbf{r}_{j-1}, \mathbf{r}_{j-1} \rangle}{\langle \mathbf{Ap}_{j-1}, \mathbf{p}_{j-1} \rangle} = \frac{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{Ap}_{j-1}}; \quad (\text{step length})$$

$$\mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1}; \quad (\text{approximation solution})$$

$$\mathbf{r}_j = \mathbf{r}_{j-1} - \alpha_j \mathbf{Ap}_{j-1}; \quad (\text{residual})$$

$$\beta_j = \frac{\langle \mathbf{r}_j, \mathbf{r}_j \rangle}{\langle \mathbf{r}_{j-1}, \mathbf{r}_{j-1} \rangle} = \frac{\mathbf{r}_j^* \mathbf{r}_j}{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}};$$

$$\mathbf{p}_j = \mathbf{r}_j + \beta_j \mathbf{p}_{j-1}; \quad (\text{search direction})$$

end

- M.R. Hestenes and E. Stiefel

Methods of conjugate gradients for solving linear systems

J. Research Nat. Bur. Standards 49 (1952), 409–436

2.1. The Lanczos process

- Since \mathbf{A} is Hermitian, then $\mathbf{H}_j = \mathbf{Q}_j^* \mathbf{A} \mathbf{Q}_j$ in the Arnoldi process is also Hermitian. Since \mathbf{H}_j is upper Hessenberg, it is tridiagonal:

$$\mathbf{H}_j = \mathbf{Q}_j^* \mathbf{A} \mathbf{Q}_j = \begin{bmatrix} a_1 & b_2 & & & \\ b_2 & a_2 & b_3 & & \\ & b_3 & a_3 & \ddots & \\ & & \ddots & \ddots & b_j \\ & & & b_j & a_j \end{bmatrix} =: \mathbf{T}_j.$$

Note that $\mathbf{T}_j \in \mathbb{R}^{j \times j}$. We have the Lanczos relation

$$\mathbf{A} \mathbf{Q}_j = \mathbf{Q}_{j+1} \tilde{\mathbf{T}}_j, \quad \text{where} \quad \tilde{\mathbf{T}}_j := \mathbf{Q}_{j+1}^* \mathbf{A} \mathbf{Q}_j.$$

- Compared with the Arnoldi process, we have

$$a_j = h_{jj}, \quad b_{j+1} = h_{j+1,j} = h_{j,j+1}.$$

- The tridiagonal structure means that in the inner loop of the Arnoldi process, the limits 1 to j can be replaced by $j - 1$ to j . Therefore, we have the Lanczos process.

Algorithm: Lanczos process generating the orthonormal basis

\mathbf{r} = arbitrary nonzero vector, $b_1 = 0$, $\mathbf{q}_0 = \mathbf{0}$

$\mathbf{q}_1 = \mathbf{r} / \|\mathbf{r}\|_2$

for $j = 1, 2, 3, \dots$,

$\mathbf{v} = \mathbf{A}\mathbf{q}_j$

$\mathbf{v} = \mathbf{v} - b_j\mathbf{q}_{j-1}$

$a_j = \mathbf{q}_j^* \mathbf{v}$

$\mathbf{v} = \mathbf{v} - a_j\mathbf{q}_j$

$b_{j+1} = \|\mathbf{v}\|_2$

$\mathbf{q}_{j+1} = \mathbf{v} / b_{j+1}$

end

- Note that the Lanczos process can be written down easily by using the Lanczos relation.

2.2. Derivation of conjugate gradients

- Note that the matrix

$$\mathbf{T}_j = \mathbf{Q}_j^* \mathbf{A} \mathbf{Q}_j = \begin{bmatrix} a_1 & b_2 & & & \\ b_2 & a_2 & b_3 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{j-1} & a_{j-1} & b_j \\ & & & b_j & a_j \end{bmatrix}$$

in the Lanczos process is Hermitian positive definite (since \mathbf{A} is HPD). Hence, \mathbf{T}_j can be LU factorized into

$$\mathbf{T}_j = \mathbf{L}_j \mathbf{U}_j = \begin{bmatrix} 1 & & & & \\ c_2 & 1 & & & \\ & \ddots & \ddots & & \\ & & c_{j-1} & 1 & \\ & & & c_j & 1 \end{bmatrix} \begin{bmatrix} d_1 & b_2 & & & \\ d_2 & b_3 & & & \\ & \ddots & \ddots & & \\ & & d_{j-1} & b_j & \\ & & & d_j & \end{bmatrix}$$

with the recurrences for c_j and d_j :

$$c_j = b_j/d_{j-1}, \quad d_j = \begin{cases} a_1 & \text{if } j = 1, \\ a_j - c_j b_j & \text{if } j > 1. \end{cases}$$

- Assume that $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{Q}_j \mathbf{y}_j$. By $\mathbf{r}_j \perp \mathcal{K}_j$, i.e., $\mathbf{Q}_j^* \mathbf{r}_j = \mathbf{0}$, we have

$$\mathbf{T}_j \mathbf{y}_j = \|\mathbf{r}_0\|_2 \mathbf{e}_1.$$

Rewrite $\mathbf{x}_j = \mathbf{x}_0 + \mathbf{Q}_j \mathbf{y}_j$ as

$$\mathbf{x}_j = \mathbf{x}_0 + \mathbf{Q}_j \mathbf{T}_j^{-1} (\|\mathbf{r}_0\|_2 \mathbf{e}_1) = \mathbf{x}_0 + \mathbf{Q}_j \mathbf{U}_j^{-1} \mathbf{L}_j^{-1} (\|\mathbf{r}_0\|_2 \mathbf{e}_1).$$

Let

$$\mathbf{P}_j := \mathbf{Q}_j \mathbf{U}_j^{-1} = [\mathbf{p}_0 \quad \mathbf{p}_1 \quad \cdots \quad \mathbf{p}_{j-1}],$$

$$\mathbf{z}_j := \mathbf{L}_j^{-1} (\|\mathbf{r}_0\|_2 \mathbf{e}_1) = [\zeta_1 \quad \zeta_2 \quad \cdots \quad \zeta_j]^\top,$$

where $\mathbf{p}_0 = \mathbf{q}_1/a_1$, $\zeta_1 = \|\mathbf{r}_0\|_2$ and, for $j \geq 2$,

$$\mathbf{p}_{j-1} = \frac{1}{d_j}(\mathbf{q}_j - b_j \mathbf{p}_{j-2}), \quad \zeta_j = -c_j \zeta_{j-1}.$$

It is now important to observe that (why?)

$$\begin{aligned} \mathbf{P}_j &= [\mathbf{p}_0 \quad \mathbf{p}_1 \quad \cdots \quad \mathbf{p}_{j-1}] = [\mathbf{P}_{j-1} \quad \mathbf{p}_{j-1}], \\ \mathbf{z}_j &= [\zeta_1 \quad \zeta_2 \quad \cdots \quad \zeta_j]^\top = \begin{bmatrix} \mathbf{z}_{j-1} \\ \zeta_j \end{bmatrix}, \end{aligned}$$

With this formulation, we arrive at a simple recurrence for \mathbf{x}_j :

$$\mathbf{x}_j = \mathbf{x}_0 + \mathbf{P}_j \mathbf{z}_j = \mathbf{x}_0 + \mathbf{P}_{j-1} \mathbf{z}_{j-1} + \zeta_j \mathbf{p}_{j-1} = \mathbf{x}_{j-1} + \zeta_j \mathbf{p}_{j-1}.$$

- The residual \mathbf{r}_j is essentially a multiple of \mathbf{q}_{j+1} (see below for a proof), therefore, all residuals are mutually orthogonal.

In fact, we have $\mathbf{r}_0 = \|\mathbf{r}_0\|_2 \mathbf{q}_1$ and, for $j \geq 1$,

$$\begin{aligned}\mathbf{r}_j &= \mathbf{b} - \mathbf{A}\mathbf{x}_j = \mathbf{b} - \mathbf{A}(\mathbf{x}_0 + \mathbf{Q}_j\mathbf{y}_j) \\ &= \mathbf{r}_0 - \mathbf{A}\mathbf{Q}_j\mathbf{y}_j = \mathbf{r}_0 - \mathbf{Q}_{j+1}\tilde{\mathbf{T}}_j\mathbf{y}_j \\ &= \mathbf{r}_0 - \mathbf{Q}_j\mathbf{T}_j\mathbf{y}_j - b_{j+1}(\mathbf{e}_j^*\mathbf{y}_j)\mathbf{q}_{j+1} \\ &= \|\mathbf{r}_0\|_2\mathbf{q}_1 - \mathbf{Q}_j(\|\mathbf{r}_0\|_2\mathbf{e}_1) - b_{j+1}(\mathbf{e}_j^*\mathbf{y}_j)\mathbf{q}_{j+1} \\ &= -b_{j+1}(\mathbf{e}_j^*\mathbf{y}_j)\mathbf{q}_{j+1}.\end{aligned}$$

- If we allow \mathbf{p}_{j-1} to scale and compensate for the scaling in the scalars, we potentially can have simpler recurrences of the form:
 $\mathbf{p}_0 = \mathbf{r}_0$ and for $j \geq 1$,

$$\begin{aligned}\mathbf{x}_j &= \mathbf{x}_{j-1} + \alpha_j\mathbf{p}_{j-1}, \\ \mathbf{r}_j &= \mathbf{r}_{j-1} - \alpha_j\mathbf{A}\mathbf{p}_{j-1}, \\ \mathbf{p}_j &= \mathbf{r}_j + \beta_j\mathbf{p}_{j-1}.\end{aligned}$$

- Note that at present we have

$$\mathbf{P}_{j+1} = [\mathbf{p}_0 \quad \mathbf{p}_1 \quad \cdots \quad \mathbf{p}_j] = \mathbf{Q}_{j+1} \mathbf{U}_{j+1}^{-1} \mathbf{D}_{j+1},$$

where \mathbf{D}_{j+1} is a diagonal matrix with scaling parameters as diagonal entries. We now derive the \mathbf{A} -conjugacy of \mathbf{p}_j , i.e., for each $0 \leq i < j$,

$$\mathbf{p}_i^* \mathbf{A} \mathbf{p}_j = 0.$$

It suffices to show that $\mathbf{P}_{j+1}^* \mathbf{A} \mathbf{P}_{j+1}$ is diagonal. Since

$$\begin{aligned} \mathbf{P}_{j+1}^* \mathbf{A} \mathbf{P}_{j+1} &= \mathbf{D}_{j+1}^* \mathbf{U}_{j+1}^{-*} \mathbf{Q}_{j+1}^* \mathbf{A} \mathbf{Q}_{j+1} \mathbf{U}_{j+1}^{-1} \mathbf{D}_{j+1} \\ &= \mathbf{D}_{j+1}^* \mathbf{U}_{j+1}^{-*} \mathbf{T}_{j+1} \mathbf{U}_{j+1}^{-1} \mathbf{D}_{j+1} \\ &= \mathbf{D}_{j+1}^* \mathbf{U}_{j+1}^{-*} \mathbf{L}_{j+1} \mathbf{D}_{j+1} \end{aligned}$$

is Hermitian and lower triangular simultaneously, then $\mathbf{P}_{j+1}^* \mathbf{A} \mathbf{P}_{j+1}$ must be diagonal.

- Now we can derive the scalar factors α_j and β_j by solely imposing the orthogonality of \mathbf{r}_j and \mathbf{A} -conjugacy of \mathbf{p}_j . Due to the orthogonality of \mathbf{r}_j , it is necessary that

$$\mathbf{r}_{j-1}^* \mathbf{r}_j = \mathbf{r}_{j-1}^* (\mathbf{r}_{j-1} - \alpha_j \mathbf{A} \mathbf{p}_{j-1}) = 0.$$

As a result,

$$\alpha_j = \frac{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}}{\mathbf{r}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}} = \frac{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}}{(\mathbf{p}_{j-1} - \beta_{j-1} \mathbf{p}_{j-2})^* \mathbf{A} \mathbf{p}_{j-1}} = \frac{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}}.$$

Similarly, due to the \mathbf{A} -conjugacy of \mathbf{p}_j , it is necessary that

$$\mathbf{p}_j^* \mathbf{A} \mathbf{p}_{j-1} = (\mathbf{r}_j + \beta_j \mathbf{p}_{j-1})^* \mathbf{A} \mathbf{p}_{j-1} = 0.$$

As a result,

$$\beta_j = -\frac{\mathbf{r}_j^* \mathbf{A} \mathbf{p}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}} = -\frac{\mathbf{r}_j^* (\mathbf{r}_{j-1} - \mathbf{r}_j)}{\alpha_j \mathbf{p}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}} = \frac{\mathbf{r}_j^* \mathbf{r}_j}{\mathbf{r}_{j-1}^* \mathbf{r}_{j-1}}.$$

2.3. Convergence of conjugate gradients

Theorem 1

Assume CG does not converge at step l (i.e., $\mathbf{r}_j \neq \mathbf{0}$, $0 \leq j \leq l$). Then $\forall 1 \leq j \leq l$:

- (1) The j th residual \mathbf{r}_j satisfies $\mathbf{r}_i^* \mathbf{r}_j = 0$ for $0 \leq i < j$. (*orthogonal*)
- (2) The j th search direction \mathbf{p}_j is nonzero ($\mathbf{p}_j \neq \mathbf{0}$) and satisfies $\mathbf{p}_i^* \mathbf{A} \mathbf{p}_j = 0$ for $0 \leq i < j$. (*A-conjugate or $\langle \cdot, \cdot \rangle_{\mathbf{A}}$ -orthogonal*)
- (3) The Krylov subspace

$$\begin{aligned}\mathcal{K}_{j+1}(\mathbf{A}, \mathbf{r}_0) &:= \text{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^j \mathbf{r}_0\} \\ &= \text{span}\{\mathbf{x}_1 - \mathbf{x}_0, \mathbf{x}_2 - \mathbf{x}_0, \dots, \mathbf{x}_{j+1} - \mathbf{x}_0\} \\ &= \text{span}\{\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_j\} \\ &= \text{span}\{\mathbf{r}_0, \mathbf{r}_1, \dots, \mathbf{r}_j\}.\end{aligned}$$

- A direct result of Theorem 1: There exists $k \leq m$ such that

$$\mathbf{r}_j \neq \mathbf{0}, \quad \mathbf{r}_j \perp \mathcal{K}_j, \quad j = 1, \dots, k-1, \quad \text{and} \quad \mathbf{r}_k = \mathbf{0},$$

i.e., CG finds the exact solution at step k .

- Since \mathbf{A} is Hermitian positive definite, the function $\|\cdot\|_{\mathbf{A}}$ defined by $\|\mathbf{x}\|_{\mathbf{A}} = \sqrt{\mathbf{x}^* \mathbf{A} \mathbf{x}}$ is a norm, called \mathbf{A} -norm.

Theorem 2 (Optimality of CG)

Let \mathbf{x}_\star denote the exact solution $\mathbf{A}^{-1}\mathbf{b}$. We consider the \mathbf{A} -norm of the vector $\boldsymbol{\varepsilon}_j = \mathbf{x}_\star - \mathbf{x}_j$, the error at step j . If $\mathbf{r}_{j-1} \neq \mathbf{0}$, then \mathbf{x}_j is the unique vector in $\mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$ such that

$$\|\boldsymbol{\varepsilon}_j\|_{\mathbf{A}} = \|\mathbf{x}_\star - \mathbf{x}_j\|_{\mathbf{A}} = \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)} \|\mathbf{x}_\star - \mathbf{x}\|_{\mathbf{A}}.$$

- A direct result of Theorem 2 and $\mathbf{r}_j = \mathbf{A}\boldsymbol{\varepsilon}_j$: There exists $k \leq m$ such that

$$\|\boldsymbol{\varepsilon}_0\|_{\mathbf{A}} \geq \|\boldsymbol{\varepsilon}_1\|_{\mathbf{A}} \geq \cdots \geq \|\boldsymbol{\varepsilon}_{k-1}\|_{\mathbf{A}} > \|\boldsymbol{\varepsilon}_k\|_{\mathbf{A}} = 0.$$

That is to say CG converges monotonically and finds the exact solution at step k .

Theorem 3

Let \mathbb{P}_j denote the set of polynomials p of degree $\leq j$. If $\mathbf{r}_{j-1} \neq \mathbf{0}$, then we have

$$\frac{\|\boldsymbol{\varepsilon}_j\|_{\mathbf{A}}}{\|\boldsymbol{\varepsilon}_0\|_{\mathbf{A}}} = \min_{p \in \mathbb{P}_j, p(0)=1} \frac{\|p(\mathbf{A})\boldsymbol{\varepsilon}_0\|_{\mathbf{A}}}{\|\boldsymbol{\varepsilon}_0\|_{\mathbf{A}}} \leq \min_{p \in \mathbb{P}_j, p(0)=1} \max_{\lambda \in \Lambda(\mathbf{A})} |p(\lambda)|,$$

where $\Lambda(\mathbf{A})$ denotes the spectrum of \mathbf{A} .

Exercise: Prove that if $\mathbf{r}_{j-1} \neq \mathbf{0}$, then the j th error $\boldsymbol{\varepsilon}_j$ of CG can be uniquely expressed as $\boldsymbol{\varepsilon}_j = p_j(\mathbf{A})\boldsymbol{\varepsilon}_0$ with $\deg(p_j) = j$ and $p_j(0) = 1$. What is the unique polynomial?

Theorem 4

If \mathbf{A} has only n distinct eigenvalues, then the CG iteration converges in at most n steps.

Hint: construct a special polynomial of degree n and prove that $\boldsymbol{\varepsilon}_n = \mathbf{0}$.

Theorem 5 (rate of convergence)

Let \mathbf{A} have the 2-norm condition number $\kappa = \lambda_{\max}(\mathbf{A})/\lambda_{\min}(\mathbf{A})$. Then the \mathbf{A} -norms of the errors satisfy

$$\frac{\|\varepsilon_j\|_{\mathbf{A}}}{\|\varepsilon_0\|_{\mathbf{A}}} \leq 2 / \left[\left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^j + \left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^{-j} \right] \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^j.$$

Proof. Consider the scaled and shifted Chebyshev polynomial

$$p(x) = T_j \left(\gamma - \frac{2x}{\lambda_{\max} - \lambda_{\min}} \right) / T_j(\gamma),$$

where $T_j(x)$ is the Chebyshev polynomial of degree j (for $|x| \leq 1$, $T_j(x) = \cos(j \arccos(x))$, and for $|x| \geq 1$, $T_j(x) = \cosh(j \operatorname{arccosh}(x))$), and

$$\gamma = \frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} = \frac{\kappa + 1}{\kappa - 1}.$$

For all $x \in [\lambda_{\min}, \lambda_{\max}]$, it follows from $\gamma - \frac{2x}{\lambda_{\max} - \lambda_{\min}} \in [-1, 1]$ that

$$\left| T_j \left(\gamma - \frac{2x}{\lambda_{\max} - \lambda_{\min}} \right) \right| \leq 1, \text{ which implies } \max_{x \in [\lambda_{\min}, \lambda_{\max}]} |p(x)| \leq \frac{1}{|T_j(\gamma)|}.$$

Note that

$$T_j(x) = \frac{(x + \sqrt{x^2 - 1})^j + (x - \sqrt{x^2 - 1})^j}{2}, \quad \forall |x| \geq 1.$$

By the change of variables $x = \frac{1}{2}(z + z^{-1})$, we have

$$T_j(x) = \frac{1}{2}(z^j + z^{-j}), \quad \forall |x| \geq 1.$$

which is standard in the study of Chebyshev polynomials. Note that

$$x = \frac{\kappa + 1}{\kappa - 1} \Rightarrow z = \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \text{ or } \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}.$$

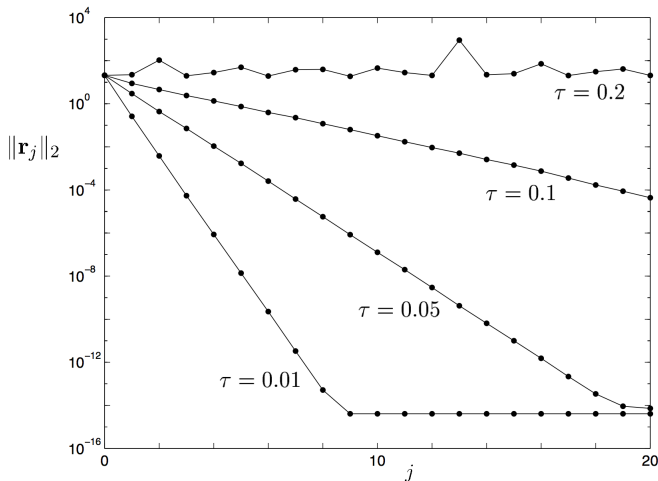
Thus

$$T_j(\gamma) = T_j \left(\frac{\kappa + 1}{\kappa - 1} \right) = \frac{1}{2} \left[\left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^j + \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{-j} \right].$$

The second inequality in Theorem 5 is obvious. □

2.4. A numerical example

- Consider a 500×500 matrix \mathbf{A} constructed as follows. (i) $a_{ii} = 1$, $a_{ij} = a_{ji} = \text{rand}(1)$ for $i \neq j$. (ii) Set off-diagonal entry $a_{ij} = 0$ ($i \neq j$) if $|a_{ij}| > \tau$, where τ is a parameter. \mathbf{b} is random, $\mathbf{x}_0 = \mathbf{0}$.
- For τ close to zero, \mathbf{A} is well-conditioned positive definite.



3. CG as an optimization algorithm

- Consider minimizing the nonlinear function $\varphi(\mathbf{x})$ of $\mathbf{x} \in \mathbb{R}^m$:

$$\varphi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} - \mathbf{x}^\top \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{m \times m} \text{ (SPD)}, \quad \mathbf{b} \in \mathbb{R}^m.$$

A standard algorithm (line search): At step j , the j th iterate

$$\mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1}$$

is computed. The optimal step length α_j is given by

$$\alpha_j = \frac{\mathbf{p}_{j-1}^\top (\mathbf{b} - \mathbf{A}\mathbf{x}_{j-1})}{\mathbf{p}_{j-1}^\top \mathbf{A}\mathbf{p}_{j-1}} = \arg \min_{\alpha} \varphi(\mathbf{x}_{j-1} + \alpha \mathbf{p}_{j-1}),$$

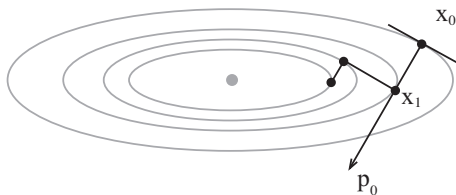
which ensures that

$$\mathbf{x}_j = \arg \min_{\mathbf{x} \in \mathbf{x}_{j-1} + \text{span}\{\mathbf{p}_{j-1}\}} \varphi(\mathbf{x}).$$

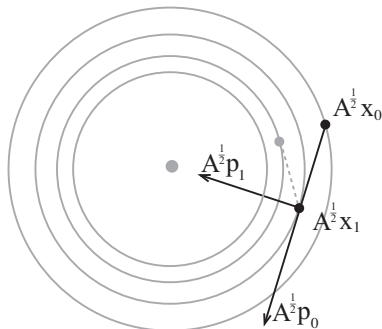
- The steepest descent iteration uses the negative gradient direction:

$$\mathbf{p}_{j-1} = -\nabla \varphi(\mathbf{x}_{j-1}) = \mathbf{b} - \mathbf{A}\mathbf{x}_{j-1}.$$

Example: $\mathbf{A} = \text{diag}\{\lambda_1, \lambda_2\}$
 $\mathbf{b} = \begin{bmatrix} 0 & 0 \end{bmatrix}^\top$



Steepest descent



Conjugate gradients

- CG uses the \mathbf{A} -conjugate direction

$$\mathbf{p}_{j-1} = \mathbf{r}_{j-1} + \beta_{j-1}\mathbf{p}_{j-2},$$

which has the **special property**

$$\mathbf{x}_j = \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \text{span}\{\mathbf{p}_0, \dots, \mathbf{p}_{j-1}\}} \varphi(\mathbf{x}) = \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \text{span}\{\mathbf{p}_0, \mathbf{p}_1, \dots, \mathbf{p}_{j-1}\}} \varphi(\mathbf{x}).$$

4. Preconditioning and PCG

- A good preconditioner \mathbf{M} , which accelerates the convergence, needs to be cheap to perform $\mathbf{M}^{-1}\mathbf{z}$. Moreover, the preconditioned matrix should have eigenvalues clustering behavior.
- For CG, we will assume that \mathbf{M} is also Hermitian positive definite. However, we can not apply CG straightaway for the explicitly preconditioned systems

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}, \quad \text{or} \quad \mathbf{A}\mathbf{M}^{-1}\mathbf{z} = \mathbf{b}, \quad (\mathbf{x} = \mathbf{M}^{-1}\mathbf{z})$$

because $\mathbf{M}^{-1}\mathbf{A}$ and $\mathbf{A}\mathbf{M}^{-1}$ are most likely not Hermitian.

- One way out is to apply the two-sided preconditioning strategy:

$$\mathbf{M} = \mathbf{L}\mathbf{L}^*, \quad (\mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-*})\mathbf{L}^*\mathbf{x} = \mathbf{L}^{-1}\mathbf{b}.$$

The matrix $\mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-*}$ is HPD, so that CG is applicable. We emphasize that this is a formalism; in practice, the only thing needed is to be able to perform $\mathbf{M}^{-1}\mathbf{z}$, and \mathbf{L} is not required.

Exercise: Derive PCG by using CG and variable substitutions.

Algorithm PCG: $\mathbf{A}\mathbf{M}^{-1}\mathbf{z} = \mathbf{b}$, $\mathbf{x} = \mathbf{M}^{-1}\mathbf{z}$

Choose $\mathbf{x} = \mathbf{x}_0$; set $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ and $\mathbf{p}_0 = \mathbf{M}^{-1}\mathbf{r}_0$;

for $j = 1, 2, \dots$, **do** until convergence:

$$\mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1};$$

$$\mathbf{r}_j = \mathbf{r}_{j-1} - \alpha_j \mathbf{A}\mathbf{p}_{j-1};$$

$$\mathbf{p}_j = \mathbf{M}^{-1}\mathbf{r}_j + \beta_j \mathbf{p}_{j-1};$$

where

$$\alpha_j = \frac{\mathbf{r}_{j-1}^* \mathbf{M}^{-1} \mathbf{r}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}}; \quad \beta_j = \frac{\mathbf{r}_j^* \mathbf{M}^{-1} \mathbf{r}_j}{\mathbf{r}_{j-1}^* \mathbf{M}^{-1} \mathbf{r}_{j-1}}.$$

- PCG can also be derived using the same method for CG.

For the left and right preconditioned matrices $\mathbf{M}^{-1}\mathbf{A}$ and $\mathbf{A}\mathbf{M}^{-1}$, replace the standard inner product $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{y}^* \mathbf{x}$ by

$$\langle \mathbf{x}, \mathbf{y} \rangle_L = \langle \mathbf{M}\mathbf{x}, \mathbf{y} \rangle \quad \text{and} \quad \langle \mathbf{x}, \mathbf{y} \rangle_R = \langle \mathbf{M}^{-1}\mathbf{x}, \mathbf{y} \rangle,$$

respectively.

It is easy to verify that $\mathbf{M}^{-1}\mathbf{A}$ and $\mathbf{A}\mathbf{M}^{-1}$ are *self-adjoint* and *positive definite* with respect to the inner products $\langle \cdot, \cdot \rangle_{\mathbf{L}}$ and $\langle \cdot, \cdot \rangle_{\mathbf{R}}$, respectively. For example,

$$\begin{aligned}\langle \mathbf{A}\mathbf{M}^{-1}\mathbf{x}, \mathbf{y} \rangle_{\mathbf{R}} &= \langle \mathbf{M}^{-1}\mathbf{A}\mathbf{M}^{-1}\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{M}^{-1}\mathbf{x}, \mathbf{A}\mathbf{M}^{-1}\mathbf{y} \rangle \\ &= \langle \mathbf{x}, \mathbf{A}\mathbf{M}^{-1}\mathbf{y} \rangle_{\mathbf{R}}.\end{aligned}$$

- *Optimality of PCG.* By $\mathbf{x}_j = \mathbf{M}^{-1}\mathbf{z}_j$, $\mathbf{x}_\star = \mathbf{M}^{-1}\mathbf{z}_\star$,

$$\mathbf{z}_j = \underset{\mathbf{z} \in \mathbf{z}_0 + \mathcal{K}_j(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}_0)}{\operatorname{argmin}} \quad \langle \mathbf{A}\mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}), \mathbf{z}_\star - \mathbf{z} \rangle_{\mathbf{R}},$$

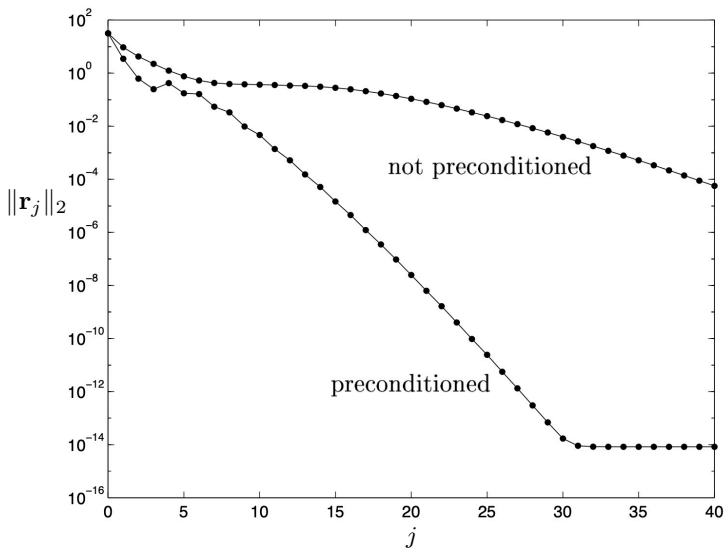
and

$$\begin{aligned}\langle \mathbf{A}\mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}), \mathbf{z}_\star - \mathbf{z} \rangle_{\mathbf{R}} &= \langle \mathbf{A}\mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}), \mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}) \rangle \\ &= \langle \mathbf{A}(\mathbf{x}_\star - \mathbf{x}), \mathbf{x}_\star - \mathbf{x} \rangle,\end{aligned}$$

we have

$$\mathbf{x}_j = \underset{\mathbf{x} \in \mathbf{x}_0 + \mathbf{M}^{-1}\mathcal{K}_j(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}_0)}{\operatorname{argmin}} \quad \langle \mathbf{A}(\mathbf{x}_\star - \mathbf{x}), \mathbf{x}_\star - \mathbf{x} \rangle.$$

- CG and PCG convergence curves for a 1000×1000 matrix



5. CGN = CG applied to the normal equations

- Let $\mathbf{A} \in \mathbb{C}^{m \times m}$ be nonsingular but not necessarily Hermitian. We can solve the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ via applying the CG method to the normal equations

$$\mathbf{A}^* \mathbf{A} \mathbf{x} = \mathbf{A}^* \mathbf{b}.$$

- The matrix $\mathbf{A}^* \mathbf{A}$ is not formed explicitly. Instead, each matrix-vector product $\mathbf{A}^* \mathbf{A} \mathbf{v}$ is evaluated in two steps as $\mathbf{A}^* (\mathbf{A} \mathbf{v})$.
- Let $\mathbf{r}_j := \mathbf{b} - \mathbf{A} \mathbf{x}_j$ and $\boldsymbol{\varepsilon}_j := \mathbf{x}_* - \mathbf{x}_j$. We have

$$\begin{aligned} \|\mathbf{r}_j\|_2 &= \|\boldsymbol{\varepsilon}_j\|_{\mathbf{A}^* \mathbf{A}} = \|\mathbf{x}_* - \mathbf{x}_j\|_{\mathbf{A}^* \mathbf{A}} \\ &= \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}^* \mathbf{A}, \mathbf{A}^* \mathbf{r}_0)} \|\mathbf{x}_* - \mathbf{x}\|_{\mathbf{A}^* \mathbf{A}}, \end{aligned}$$

and

$$\frac{\|\mathbf{r}_j\|_2}{\|\mathbf{r}_0\|_2} \leq 2 \left(\frac{\kappa - 1}{\kappa + 1} \right)^j, \quad \text{where} \quad \kappa = \frac{\sigma_{\max}(\mathbf{A})}{\sigma_{\min}(\mathbf{A})}.$$