

Lecture 12: Conjugate gradients



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1. Idea of conjugate gradient

- 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

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

2. Conjugate gradient

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

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 $0 \leq i < j$. (*\mathbf{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 .

- Let \mathbb{P}_j denote the set of polynomials p of degree $\leq j$.

Theorem 3

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} .

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)

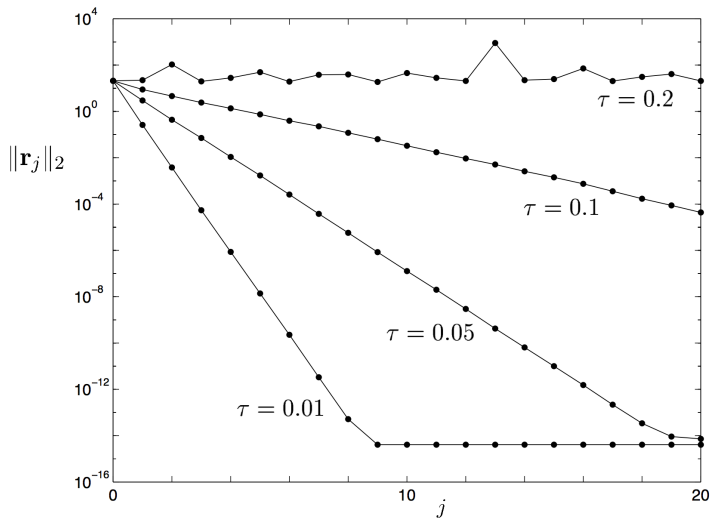
Let \mathbf{A} have the 2-norm condition number $\kappa = \lambda_{\max}(\mathbf{A})/\lambda_{\min}(\mathbf{A})$. Then the \mathbf{A} -norms of the errors satisfy

$$\frac{\|\boldsymbol{\varepsilon}_j\|_{\mathbf{A}}}{\|\boldsymbol{\varepsilon}_0\|_{\mathbf{A}}} \leq 2 / \left[\left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^j + \left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^{-j} \right] \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^j.$$

3. Numerical example

- Consider a 500×500 sparse matrix \mathbf{A} constructed as follows.
 - First we put 1 at each diagonal position and a random number from the uniform distribution on $[-1, 1]$ at each off-diagonal position (maintaining the symmetry $\mathbf{A} = \mathbf{A}^\top$)
 - Then we replace each off-diagonal entry with $|a_{ij}| > \tau$ by zero, where τ is a parameter.
- For τ close to zero, the matrix \mathbf{A} is well-conditioned positive definite.

• Convergence history of CG: \mathbf{b} random, $\mathbf{x}_0 = \mathbf{0}$



4. 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 each step, an 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

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

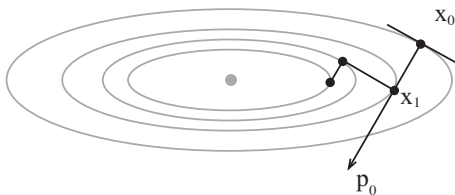
which ensures that

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

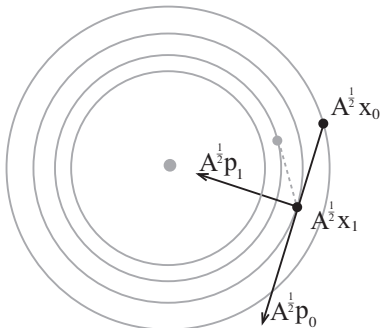
- The steepest descent iteration uses the negative gradient direction:

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

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



Steepest descent



Conjugate gradient

- 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**

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

5. Preconditioning

- A good preconditioner \mathbf{M} , which accelerates the convergence, needs to be easy to construct and 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

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

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:

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

This approach has the disadvantage that \mathbf{M} must be available in factored form.

- There is a more elegant alternative.

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

$$\langle \mathbf{x}, \mathbf{y} \rangle_{\text{L}} = \langle \mathbf{M}\mathbf{x}, \mathbf{y} \rangle \quad \text{and} \quad \langle \mathbf{x}, \mathbf{y} \rangle_{\text{R}} = \langle \mathbf{M}^{-1}\mathbf{x}, \mathbf{y} \rangle,$$

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 $\langle \cdot, \cdot \rangle_{\text{L}}$ and $\langle \cdot, \cdot \rangle_{\text{R}}$, respectively. For example,

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

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

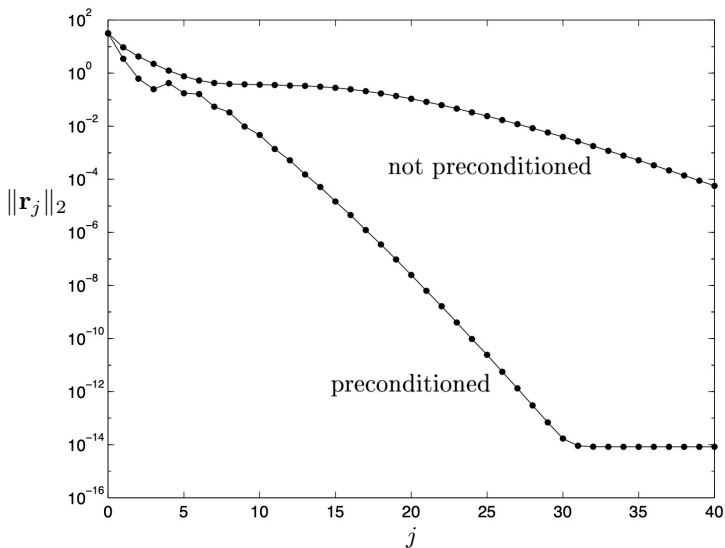
$$\alpha_j = \frac{\mathbf{r}_{j-1}^* \mathbf{M}^{-1} \mathbf{r}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{A} \mathbf{p}_{j-1}}; \quad \beta_j = \frac{\mathbf{r}_j^* \mathbf{M}^{-1} \mathbf{r}_j}{\mathbf{r}_{j-1}^* \mathbf{M}^{-1} \mathbf{r}_{j-1}}.$$

- We now are minimizing (note that $\mathbf{x}_0 = \mathbf{M}^{-1}\mathbf{z}_0$ and $\mathbf{x} = \mathbf{M}^{-1}\mathbf{z}$)

$$\begin{aligned} \langle \mathbf{A}\mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}), \mathbf{z}_\star - \mathbf{z} \rangle_{\mathbf{R}} &= \langle \mathbf{A}\mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}), \mathbf{M}^{-1}(\mathbf{z}_\star - \mathbf{z}) \rangle \\ &= \langle \mathbf{A}(\mathbf{x}_\star - \mathbf{x}), \mathbf{x}_\star - \mathbf{x} \rangle \\ &= \|\boldsymbol{\varepsilon}\|_{\mathbf{A}}^2, \end{aligned}$$

over $\mathbf{z}_0 + \mathcal{K}_j(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}_0)$ or $\mathbf{x}_0 + \mathbf{M}^{-1}\mathcal{K}_j(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}_0)$.

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



6. 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 $\mathbf{A}^*(\mathbf{A} \mathbf{v})$.
- We have

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

and

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