Lecture 12: Conjugate gradients

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1. Idea of conjugate gradient

- Consider a Hermitian positive definite linear system

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

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

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

where

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

- Note that the residual of GMRES satisfies

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

2. Conjugate gradient

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

Choose arbitrary $\mathbf{x}_0$;
Set $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ and $\mathbf{p}_0 = \mathbf{r}_0$;
for $j = 1, 2, \dots,$ **do** until convergence:

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

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

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

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

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

end

- M.R. Hestenes and E. Stiefel
  Methods of conjugate gradients for solving linear systems
  J. Research Nat. Bur. Standards 49 (1952), 409436

Theorem 1

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

(1) *The* j*th residual* $\mathbf{r}_j$ *satisfies* $\mathbf{r}_i^*\mathbf{r}_j = 0$ *for* $0 \le i < j$. (*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* $0 \le i < j$. ($\mathbf{A}$*-conjugate or* $\langle\cdot,\cdot\rangle_{\mathbf{A}}$*-orthogonal*)

(3) *The Krylov subspace*

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

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

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

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*

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

3. Numerical example

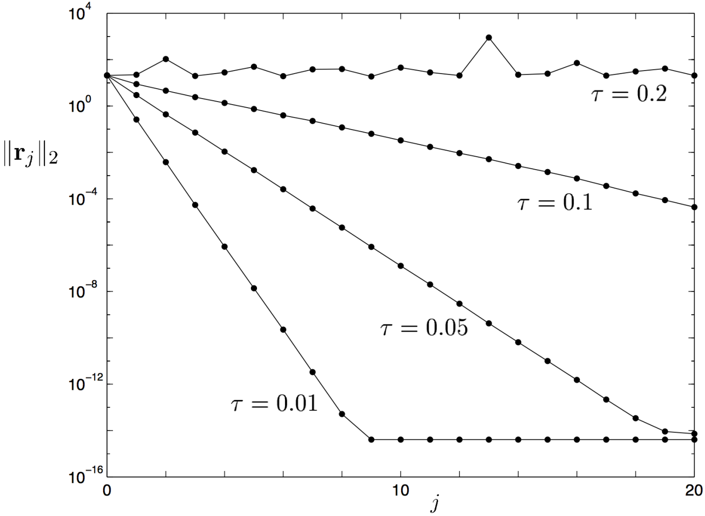
- Consider a 500×500 sparse matrix $\mathbf{A}$ constructed as follows.

  (i) 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 $\mathbf{A} = \mathbf{A}^\top$)

  (ii) 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

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

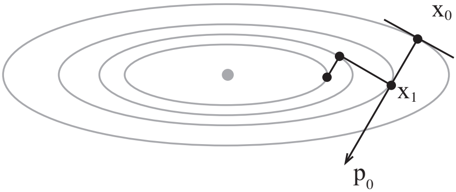
  which ensures that

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

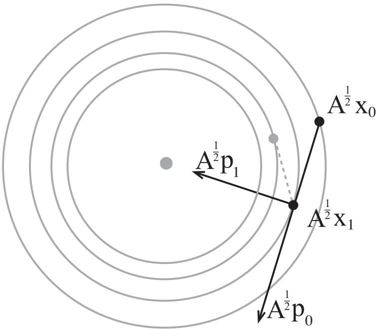
- The steepest descent iteration uses the negative gradient direction:

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

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



Steepest descent



Conjugate gradient

- CG uses the **A**-conjugate direction

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

which has the special property

$$\mathbf{x}_j = \operatorname*{arg\,min}_{\mathbf{x}\in\mathbf{x}_{j-1}+\mathrm{span}\{\mathbf{p}_{j-1}\}} \varphi(\mathbf{x}) = \operatorname*{arg\,min}_{\mathbf{x}\in\mathbf{x}_0+\mathrm{span}\{\mathbf{p}_0,\mathbf{p}_1,\cdots,\mathbf{p}_{j-1}\}} \varphi(\mathbf{x}).$$

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

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

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

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

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

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 $j = 1, 2, \ldots,$ **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

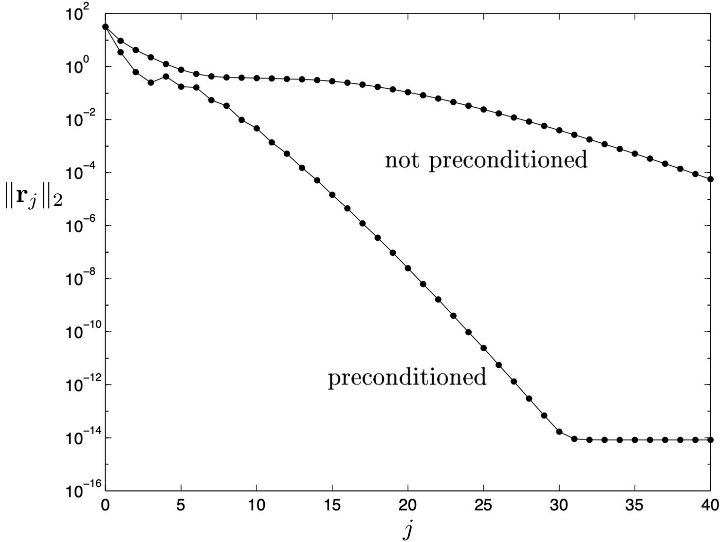
$$\alpha_j = \frac{\mathbf{r}_{j-1}^* \mathbf{M}^{-1}\mathbf{r}_{j-1}}{\mathbf{p}_{j-1}^* \mathbf{A}\mathbf{p}_{j-1}}; \quad \beta_j = \frac{\mathbf{r}_j^* \mathbf{M}^{-1}\mathbf{r}_j}{\mathbf{r}_{j-1}^* \mathbf{M}^{-1}\mathbf{r}_{j-1}}.$$

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

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

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

- 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

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

and

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