

# Lecture 12: Conjugate gradients



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## 1. Idea 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

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

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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**

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- 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.

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**Algorithm:** Lanczos process generating the orthonormal basis

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

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

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

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

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

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

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

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

**end**

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- 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

$$\begin{aligned} \mathbf{P}_j &:= \mathbf{Q}_j \mathbf{U}_j^{-1} = [\mathbf{p}_0 \quad \mathbf{p}_1 \quad \cdots \quad \mathbf{p}_{j-1}], \\ \mathbf{z}_j &:= \mathbf{L}_j^{-1} (\|\mathbf{r}_0\|_2 \mathbf{e}_1) = [\zeta_1 \quad \zeta_2 \quad \cdots \quad \zeta_j]^\top, \end{aligned}$$

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

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

where  $\mathbf{D}_j$  is diagonal with scaling parameters as diagonal entries. We now derive the  $\mathbf{A}$ -conjugacy of  $\mathbf{p}_j$ , i.e., for  $i < j$ ,

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

It suffices to show that  $\mathbf{P}_j^* \mathbf{A} \mathbf{P}_j$  is diagonal. Since

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

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

- Now we can derive the scalar factors  $\alpha_j$  and  $\beta_j$  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,

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

## 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  $0 \leq i < j$ . ( *$\mathbf{A}$ -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  $k$ .

### 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

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

*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 usual Chebyshev polynomial of degree  $j$  and

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

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

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

By the change of variables

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

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

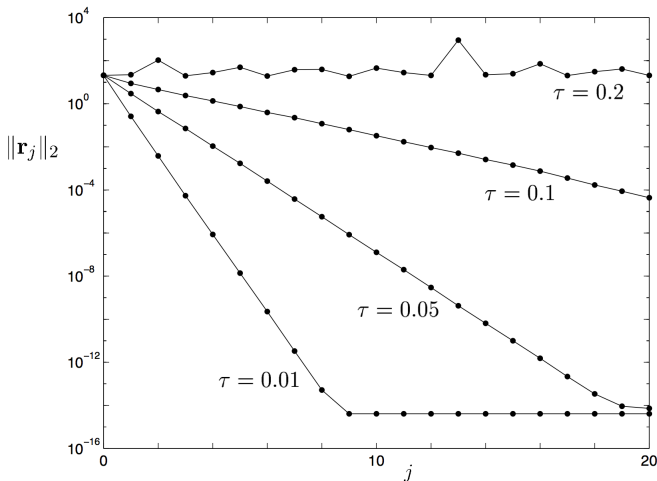
$$T_j(\gamma) = T_j \left( \frac{\kappa + 1}{\kappa - 1} \right) = \frac{1}{2} \left[ \left( \frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1} \right)^j + \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^j \right].$$

The second inequality in Theorem 5 is obvious. □



## 2.4. A numerical example

- Consider a  $500 \times 500$  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  $\tau$  is a parameter.  $\mathbf{b}$  is random,  $\mathbf{x}_0 = \mathbf{0}$ .
- For  $\tau$  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 each step, an iterate

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

is computed. The optimal step length  $\alpha_j$  is given by

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

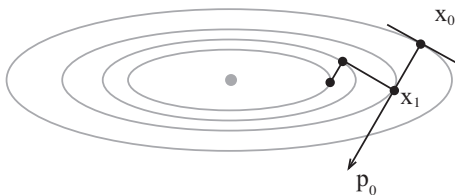
which ensures that

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

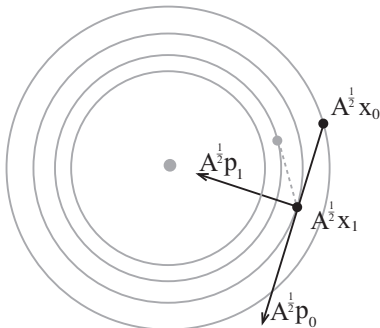
- The steepest descent iteration uses the negative gradient direction:

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

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



Steepest descent



Conjugate 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**

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

## 4. 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,

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

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

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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

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

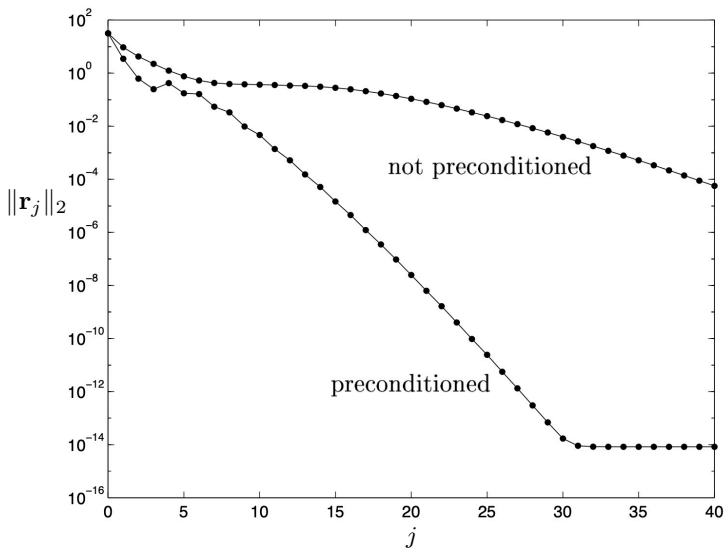
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- We now are minimizing (note that  $\mathbf{x}_0 = \mathbf{M}^{-1}\mathbf{z}_0$  and  $\mathbf{x} = \mathbf{M}^{-1}\mathbf{z}$ )

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

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  $1000 \times 1000$  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  $\mathbf{A}^*(\mathbf{A} \mathbf{v})$ .
- We have

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

and

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