

## §7.3 The Jacobi and Gauss-Siedel Iterative Techniques

- ▶ **Problem:** To solve  $A\mathbf{x} = \mathbf{b}$  for  $A \in \mathbb{R}^{n \times n}$ .
- ▶ **Methodology:** Iteratively approximate solution  $\mathbf{x}$ . No GEPP.

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MATRIX SPLITTING

$$A = \mathbf{diag}(a_{1,1}, a_{2,2}, \dots, a_{n,n}) + \begin{pmatrix} 0 & & & & \\ a_{2,1} & 0 & & & \\ \vdots & \vdots & \ddots & & \\ a_{n-1,1} & a_{n-1,2} & \cdots & 0 & \\ a_{n,1} & a_{n,2} & \cdots & a_{n,n-1} & 0 \end{pmatrix} + \begin{pmatrix} 0 & a_{1,2} & \cdots & a_{1,n-1} & a_{1,n} \\ & 0 & \cdots & a_{2,n-1} & a_{2,n} \\ & & \ddots & \vdots & \vdots \\ & & & 0 & a_{n-1,n} \\ & & & & 0 \end{pmatrix}$$

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$$\stackrel{\text{def}}{=} D - L - U = \begin{pmatrix} \diagdown & & & & \\ & \square & & & \\ & & \square & & \\ & & & \square & \\ & & & & \square \end{pmatrix} - \begin{pmatrix} \square & & & & \\ \diagdown & & & & \\ & \square & & & \\ & & \square & & \\ & & & \square & \end{pmatrix} - \begin{pmatrix} \square & & & & \\ & \square & & & \\ & & \square & & \\ & & & \square & \\ & & & & \square \end{pmatrix}.$$

**Ex:** Matrix splitting for  $A = \begin{pmatrix} 10 & -1 & 2 & 0 \\ -1 & 11 & -1 & 3 \\ 2 & -1 & 10 & -1 \\ 0 & 3 & -1 & 8 \end{pmatrix}$

$$\begin{aligned}
 A &= \begin{pmatrix} \diagdown & & & \\ & \diagdown & & \\ & & \diagdown & \\ & & & \diagdown \end{pmatrix} - \begin{pmatrix} \square & & & \\ & \square & & \\ & & \square & \\ & & & \square \end{pmatrix} - \begin{pmatrix} \square & & & \\ & \square & & \\ & & \square & \\ & & & \square \end{pmatrix} \\
 &= \mathbf{diag}(10, 11, 10, 8) - \begin{pmatrix} 0 & & & \\ 1 & 0 & & \\ -2 & 1 & 0 & \\ 0 & -3 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 & -2 & 0 \\ & 0 & 1 & -3 \\ & & 0 & 1 \\ & & & 0 \end{pmatrix}
 \end{aligned}$$

# The Jacobi and Gauss-Siedel Methods for solving $A\mathbf{x} = \mathbf{b}$

JACOBI METHOD: With matrix splitting  $A = D - L - U$ , rewrite

$$\mathbf{x} = D^{-1}(L + U)\mathbf{x} + D^{-1}\mathbf{b}.$$

Jacobi iteration with given  $\mathbf{x}^{(0)}$ ,

$$\mathbf{x}^{(k+1)} = D^{-1}(L + U)\mathbf{x}^{(k)} + D^{-1}\mathbf{b}, \quad \text{for } k = 0, 1, 2, \dots .$$

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GAUSS-SIEDEL METHOD: Rewrite

$$\mathbf{x} = (D - L)^{-1} U\mathbf{x} + (D - L)^{-1} \mathbf{b}.$$

Gauss-Siedel iteration with given  $\mathbf{x}^{(0)}$ ,

$$\mathbf{x}^{(k+1)} = (D - L)^{-1} U\mathbf{x}^{(k)} + (D - L)^{-1} \mathbf{b}, \quad \text{for } k = 0, 1, 2, \dots.$$

**Ex:** Jacobi Method for  $A\mathbf{x} = \mathbf{b}$ , with

$$A = \begin{pmatrix} 10 & -1 & 2 & 0 \\ -1 & 11 & -1 & 3 \\ 2 & -1 & 10 & -1 \\ 0 & 3 & -1 & 8 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 6 \\ 25 \\ -11 \\ 15 \end{pmatrix}$$

$$A = D - L - U$$

$$= \mathbf{diag}(10, 11, 10, 8) - \begin{pmatrix} 0 & & & \\ 1 & 0 & & \\ -2 & 1 & 0 & \\ 0 & -3 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 & -2 & 0 \\ & 0 & 1 & -3 \\ & & 0 & 1 \\ & & & 0 \end{pmatrix}$$

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Jacobi iteration with  $\mathbf{x}^{(0)} = \mathbf{0}$ , for  $k = 0, 1, 2, \dots$

$$\begin{aligned} \mathbf{x}_J^{(k+1)} &= D^{-1}(L + U)\mathbf{x}_J^{(k)} + D^{-1}\mathbf{b} \\ &= \begin{pmatrix} 0 & \frac{1}{10} & -\frac{2}{10} & 0 \\ \frac{1}{11} & 0 & \frac{1}{11} & -\frac{3}{11} \\ -\frac{2}{10} & \frac{1}{10} & 0 & \frac{1}{10} \\ 0 & -\frac{3}{8} & \frac{1}{8} & 0 \end{pmatrix} \mathbf{x}_J^{(k)} + \begin{pmatrix} \frac{6}{10} \\ \frac{25}{11} \\ -\frac{11}{10} \\ \frac{15}{8} \end{pmatrix} \end{aligned}$$



## Ex: Gauss-Siedel Method for $Ax = b$

$$\begin{aligned} A &= D - L - U \\ &= \begin{pmatrix} 10 & & & \\ -1 & 11 & & \\ 2 & -1 & 10 & \\ 0 & 3 & -1 & 8 \end{pmatrix} - \begin{pmatrix} 0 & 1 & -2 & 0 \\ 0 & 1 & -3 & \\ & 0 & 1 & \\ & & & 0 \end{pmatrix}. \end{aligned}$$

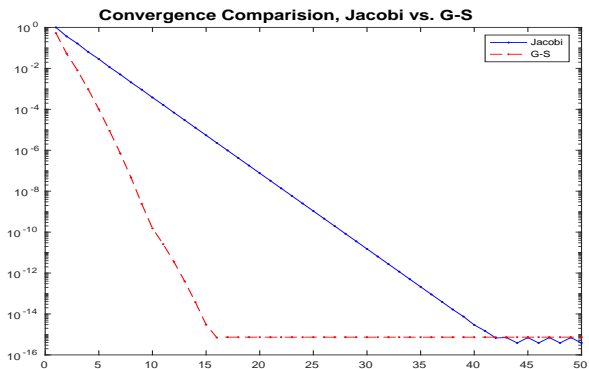
## Ex: Gauss-Siedel Method for $Ax = b$

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Gauss-Siedel iteration with  $\mathbf{x}^{(0)} = \mathbf{0}$ , for  $k = 0, 1, 2, \dots$

$$\begin{aligned} \mathbf{x}_{\text{GS}}^{(k+1)} &= (D - L)^{-1} U \mathbf{x}_{\text{GS}} + (D - L)^{-1} \mathbf{b} \\ &= \begin{pmatrix} 10 & & & \\ -1 & 11 & & \\ 2 & -1 & 10 & \\ 0 & 3 & -1 & 8 \end{pmatrix}^{-1} \left( \begin{pmatrix} 0 & 1 & -2 & 0 \\ & 0 & 1 & -3 \\ & & 0 & 1 \\ & & & 0 \end{pmatrix} \mathbf{x}_{\text{GS}}^{(k)} \right) \\ &\quad + \begin{pmatrix} \frac{6}{10} \\ \frac{10}{25} \\ \frac{11}{11} \\ -\frac{15}{10} \\ \frac{15}{8} \end{pmatrix}. \end{aligned}$$

Jacobi vs. Gauss-Siedel: **solution**  $x = \begin{pmatrix} 1 \\ 2 \\ -1 \\ 1 \end{pmatrix}$ .



# General Iteration Methods

To solve  $A\mathbf{x} = \mathbf{b}$  with matrix splitting  $A = D - L - U$ ,

- ▶ JACOBI METHOD:

$$\mathbf{x}_J^{(k+1)} = D^{-1}(L + U)\mathbf{x}_J^{(k)} + D^{-1}\mathbf{b}.$$

- ▶ GAUSS-SIEDEL METHOD:

$$\mathbf{x}_{GS}^{(k+1)} = (D - L)^{-1} U\mathbf{x}_{GS}^{(k)} + (D - L)^{-1}\mathbf{b}.$$

GENERAL ITERATION METHOD: for  $k = 0, 1, 2, \dots$

$$\mathbf{x}^{(k+1)} = T\mathbf{x}^{(k)} + \mathbf{c}.$$

Next: convergence analysis on General Iteration Method

General Iteration:  $\mathbf{x}^{(k+1)} = T \mathbf{x}^{(k)} + \mathbf{c}$  for  $k = 0, 1, 2, \dots$

**Thm:** The following statements are equivalent

- ▶  $\rho(T) < 1$ .
- ▶ The equation

$$\mathbf{x} = T \mathbf{x} + \mathbf{c} \quad (1)$$

has a unique solution and  $\{\mathbf{x}^{(k)}\}$  converges to this solution from any  $\mathbf{x}^{(0)}$ .

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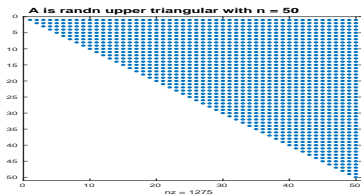
**Proof:** Assume  $\rho(T) < 1$ . Then (1) has unique solution  $\mathbf{x}^{(*)}$ .

$$\begin{aligned} \mathbf{x}^{(k+1)} - \mathbf{x}^{(*)} &= T \left( \mathbf{x}^{(k)} - \mathbf{x}^{(*)} \right) = T^2 \left( \mathbf{x}^{(k-1)} - \mathbf{x}^{(*)} \right) \\ &= \dots = T^{k+1} \left( \mathbf{x}^{(0)} - \mathbf{x}^{(*)} \right) \implies \mathbf{0}. \end{aligned}$$

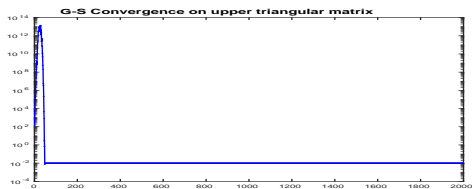
**Conversely,** if  $\dots$  (omitted)

# Jacobi on random upper triangular matrix

- ▶  $A = D - U$ .  $T = D^{-1}U$  with  $\rho(T) = 0$ .



- ▶ Convergence plot



## §7.4 Relaxation Techniques for Solving Linear Systems

To solve  $A\mathbf{x} = \mathbf{b}$  with matrix splitting  $A = D - L - U$ , rewrite

$$\begin{aligned} D\mathbf{x} &= D\mathbf{x}, \\ \omega L\mathbf{x} &= \omega(D - U)\mathbf{x} - \omega\mathbf{b}, \quad \text{for any } \omega. \end{aligned}$$



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**Successive Over-Relaxation (SOR)**, for  $k = 0, 1, 2, \dots$

$$\begin{aligned} \mathbf{x}_{\text{SOR}}^{(k+1)} &= (D - \omega L)^{-1} ((1 - \omega)D + \omega U)\mathbf{x}_{\text{SOR}}^{(k)} + \omega(D - \omega L)^{-1}\mathbf{b} \\ &\stackrel{\text{def}}{=} T_{\text{SOR}}\mathbf{x}_{\text{SOR}}^{(k)} + \mathbf{c}_{\text{SOR}}. \end{aligned}$$

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converges if  $\rho(T_{\text{SOR}}) < 1$ .

Good choice of  $\omega$  is tricky, but critical for accelerated convergence

## Optimal **SOR** parameters

**Thm:** If  $A$  is symmetric positive definite and tridiagonal, then

$$\rho(T_{GS}) = (\rho(T_J))^2 < 1,$$

and the optimal choice of  $\omega$  for the **SOR** method is

$$\omega_{\text{OPT}} = \frac{2}{1 + \sqrt{1 - (\rho(T_J))^2}}$$

with

$$\rho(T_{\text{SOR}}) = \omega_{\text{OPT}} - 1 = \left( \frac{\rho(T_J)}{1 + \sqrt{1 - (\rho(T_J))^2}} \right)^2. \quad \square$$

$$A = \begin{pmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{x} = \frac{1}{3} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

► If  $A$  is symmetric positive definite and tridiagonal,

$$\det(A) = 24, \quad \det \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix} = 7, \quad 4 > 0.$$

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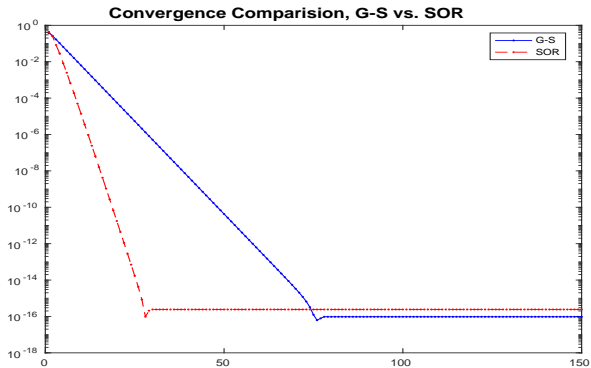
- ▶  $\rho(T_J) = \sqrt{0.625}$

$$T_J = D^{-1}(L + U) = \frac{1}{4} \begin{pmatrix} 0 & -3 & 0 \\ -3 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

- ▶ Optimal  $\omega$ :

$$\omega_{\text{OPT}} = \frac{2}{1 + \sqrt{1 - (\rho(T_J))^2}} = \omega_{\text{OPT}} = \frac{2}{1 + \sqrt{0.375}} \approx 1.24.$$

$$A = \begin{pmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{x} = \frac{1}{3} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$



## §7.5 Error Bounds and Iterative Refinement

Assume that  $\hat{\mathbf{x}}$  is an approximation to the solution  $\mathbf{x}$  of  $A\mathbf{x} = \mathbf{b}$ .

- ▶ RESIDUAL  $\hat{\mathbf{r}} \stackrel{\text{def}}{=} \mathbf{b} - A\hat{\mathbf{x}} = A(\mathbf{x} - \hat{\mathbf{x}})$ . Thus small  $\|\mathbf{x} - \hat{\mathbf{x}}\|$  implies small  $\|\hat{\mathbf{r}}\|$ .



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- ▶ However, big  $\|\mathbf{x} - \hat{\mathbf{x}}\|$  can still lead to small  $\|\hat{\mathbf{r}}\|$ . **Ex:**

$$\begin{pmatrix} 1 & 2 \\ 1 + 10^{-\tau} & 2 \end{pmatrix} \mathbf{x} = \begin{pmatrix} 3 \\ 3 + 10^{-\tau} \end{pmatrix}.$$

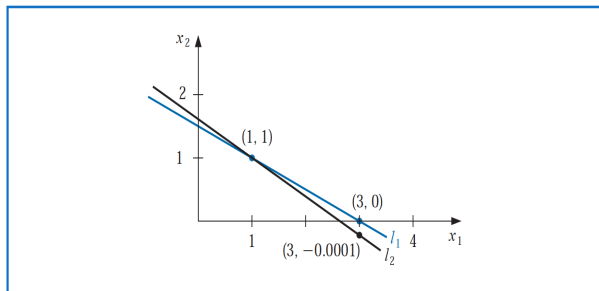
Exact solution  $\mathbf{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ . Bad approximation  $\hat{\mathbf{x}} = \begin{pmatrix} 3 \\ 0 \end{pmatrix}$   
has a small residual for large  $\tau$ :

$$\hat{\mathbf{r}} = \begin{pmatrix} 3 \\ 3 + 10^{-\tau} \end{pmatrix} - \begin{pmatrix} 1 & 2 \\ 1 + 10^{-\tau} & 2 \end{pmatrix} \begin{pmatrix} 3 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -2 \times 10^{-\tau} \end{pmatrix}.$$

# Near Linear Dependence

For  $\tau = 4$ , equations define two *nearly* parallel lines

$$\ell_1: x_1 + 2x_2 = 3, \quad \text{and} \quad \ell_2: 1.0001x_1 + 2x_2 = 3.0001.$$



Parallel lines do not have intersections.

Let  $A\mathbf{x} = \mathbf{b}$  with non-singular  $A$  and non-zero  $\mathbf{b}$

Thm: Assume  $\hat{\mathbf{x}}$  is an approximate solution with  $\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}}$ . Then for any natural norm,

$$\begin{aligned}\|\hat{\mathbf{x}} - \mathbf{x}\| &\leq \|A^{-1}\| \|\hat{\mathbf{r}}\|, \\ \frac{\|\hat{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} &\leq \kappa(A) \frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|},\end{aligned}$$

where  $\kappa(A) \stackrel{\text{def}}{=} \|A\| \|A^{-1}\|$  is the CONDITION NUMBER of  $A$  □

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- ▶  $A$  is WELL-CONDITIONED if  $\kappa(A) = O(1)$ :

small residual implies small solution error.

- ▶  $A$  is ILL-CONDITIONED if  $\kappa(A) \gg 1$ :

small residual may still allow large solution error.

**Ex:** Condition Number for  $A = \begin{pmatrix} 1 & 2 \\ 1 + 10^{-\tau} & 2 \end{pmatrix}$

**Solution:** For  $\tau > 0$ ,  $\|A\|_{\infty} = 3 + 10^{-\tau}$ . Since

$$A^{-1} = -\frac{10^{\tau}}{2} \begin{pmatrix} 2 & -2 \\ -(1 + 10^{-\tau}) & 1 \end{pmatrix},$$

we have  $\|A^{-1}\|_{\infty} = 2 \times 10^{\tau}$ . Thus

$$\kappa(A) = \|A\|_{\infty} \|A^{-1}\|_{\infty} = 6 \times 10^{\tau} + 2.$$

$\kappa(A)$  grows exponentially in  $\tau$ .  $A$  is ill-conditioned for large  $\tau$ .

## ITERATIVE REFINEMENT (I)

- ▶ Let  $A\mathbf{x} = \mathbf{b}$  with non-singular  $A$  and non-zero  $\mathbf{b}$ .
- ▶ Let  $\mathcal{F}(\cdot)$  be an in-exact equation solver, so  $\mathcal{F}(\mathbf{b})$  is approximate solution.
- ▶ Assume  $\mathcal{F}(\cdot)$  is accurate enough that there exists a  $\rho < 1$  so

$$\frac{\|\mathbf{b} - A\mathcal{F}(\mathbf{b})\|}{\|\mathbf{b}\|} \leq \rho \quad \text{for any } \mathbf{b} \neq \mathbf{0}.$$

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In practice,

- ▶  $\mathcal{F}(\cdot)$  could be from an (in-exact) LU factorization,

$$\mathcal{F}(\mathbf{b}) = U^{-1}(L^{-1}\mathbf{b}).$$

- ▶ Inaccuracies in LU factorization could be due to rounding-error,

$$A \approx LU.$$

**Ex:**  $A = \text{randn}(n, n)$ ,  $\mathbf{b} = \text{randn}(n, 1)$ ,  $n = 3000$

- ▶ **LU factorize**  $A$  to get  $L, U$ , (LU without pivoting)
- ▶  $\mathbf{x}_0 = U^{-1}(L^{-1}\mathbf{b})$ ,
- ▶  $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}_0$ ,
- ▶  $\Delta\mathbf{x}_1 = U^{-1}(L^{-1}\mathbf{r}_0)$ ,
- ▶  $\mathbf{r}_1 = \mathbf{r}_0 - A\Delta\mathbf{x}_1$ ,
- ▶  $\mathbf{x} = \mathbf{x}_0 + \Delta\mathbf{x}_1$
- ▶ `disp(norm(r0), norm(r1))`

2.6606e-07

1.0996e-16



## ITERATIVE REFINEMENT (II)

Given a tolerance  $\tau > 0$  and  $\mathbf{x}^{(0)}$

- ▶ Initialize  $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$ .
- ▶ for  $k = 0, 1, \dots$ 
  - ▶ Compute

$$\begin{aligned}\Delta\mathbf{x}^{(k)} &= \mathcal{F}(\mathbf{r}^{(k)}), \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \Delta\mathbf{x}^{(k)}, \\ \mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - A\Delta\mathbf{x}^{(k)}.\end{aligned}$$

- ▶ If  $\|\mathbf{r}^{(k+1)}\| \leq \tau \|\mathbf{b}\|$  **stop**.

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**Convergence Proof:**

$$\|\mathbf{r}^{(k+1)}\| \leq \rho \|\mathbf{r}^{(k)}\| \leq \rho^2 \|\mathbf{r}^{(k-1)}\| \leq \dots \leq \rho^{k+1} \|\mathbf{r}^{(0)}\|.$$

# PERTURBATION THEORY

**Thm:** Let  $\mathbf{x}$  and  $\hat{\mathbf{x}}$  be solutions to

$$A\mathbf{x} = \mathbf{b} \quad \text{and} \quad (A + \Delta A)\hat{\mathbf{x}} = \mathbf{b} + \Delta\mathbf{b}$$

with PERTURBATIONS  $\Delta A$  and  $\Delta\mathbf{b}$ . Then

$$\frac{\|\hat{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \frac{\kappa(A)}{1 - \kappa(A) \frac{\|\Delta A\|}{\|A\|}} \left( \frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta\mathbf{b}\|}{\|\mathbf{b}\|} \right).$$

with  $\kappa(A) = \|A\| \|A^{-1}\| \quad \square$ .

## §7.6 The Conjugate Gradient Method (CG) for $A\mathbf{x} = \mathbf{b}$

**Assumption:**  $A$  is SYMMETRIC POSITIVE DEFINITE (SPD)

- ▶  $A^T = A$ ,
- ▶  $\mathbf{x}^T A\mathbf{x} \geq 0$  for any  $\mathbf{x}$ ,
- ▶  $\mathbf{x}^T A\mathbf{x} = 0$  if and only if  $\mathbf{x} = \mathbf{0}$ .

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**Proof:** Let  $A\mathbf{x}^* = \mathbf{b}$ . Then

$$\begin{aligned} g(\mathbf{x}) &= \mathbf{x}^T A\mathbf{x} - 2\mathbf{x}^T A\mathbf{x}^* \\ &= (\mathbf{x} - \mathbf{x}^*)^T A(\mathbf{x} - \mathbf{x}^*) - (\mathbf{x}^*)^T A(\mathbf{x}^*) \\ &= (\mathbf{x} - \mathbf{x}^*)^T A(\mathbf{x} - \mathbf{x}^*) + g(\mathbf{x}^*). \end{aligned}$$

Thus,  $g(\mathbf{x}) \geq g(\mathbf{x}^*)$  for all  $\mathbf{x}$ ; and  $g(\mathbf{x}) = g(\mathbf{x}^*)$  iff  $\mathbf{x} = \mathbf{x}^*$ . □

## CG for $A\mathbf{x} = \mathbf{b}$

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## SEARCH DIRECTION and LINE SEARCH

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$$\begin{aligned} 0 &= \frac{d}{dt} g(\mathbf{x}^{(k-1)} + t\mathbf{v}^{(k)}) = (\mathbf{v}^{(k)})^T \nabla g(\mathbf{x}^{(k-1)} + t\mathbf{v}^{(k)}) \\ &= (\mathbf{v}^{(k)})^T (2A(\mathbf{x}^{(k-1)} + t\mathbf{v}^{(k)}) - 2\mathbf{b}), \end{aligned}$$

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## SEARCH DIRECTION choices

For a small step-size  $t$ :

$$g\left(\mathbf{x}^{(k-1)} + t\mathbf{v}^{(k)}\right) \approx g\left(\mathbf{x}^{(k-1)}\right) + t\left(\mathbf{v}^{(k)}\right)^T \nabla g\left(\mathbf{x}^{(k-1)}\right).$$

- ▶ **STEEPEST DESCENT**: Greatest decrease in the value of  $g\left(\mathbf{x}^{(k-1)} + t\mathbf{v}^{(k)}\right)$ :

$$\mathbf{v}^{(k)} = -\nabla g\left(\mathbf{x}^{(k-1)}\right).$$

- ▶ **A-orthogonal DIRECTIONS**: non-zero vectors  $\{\mathbf{v}^{(i)}\}_{i=1}^n$

$$\left(\mathbf{v}^{(i)}\right)^T \left(A\mathbf{v}^{(j)}\right) = 0 \quad \text{for all } i \neq j.$$

**A-orthogonal** vectors associated with the positive definite matrix  $A$  is linearly independent.

# A-orthogonality Craft

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**Thm:** Let non-zero vectors  $\{\mathbf{v}^{(k)}\}$  be A-orthogonal with  $\mathbf{v}^{(1)} = -\mathbf{r}^{(0)}$  and for  $k = 1, \dots, n$

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$$\text{Magic (I): } \min_{\tau_1} g(\mathbf{x}_0 + \tau_1 \mathbf{v}^{(1)}) = g(\mathbf{x}_0 + t_1 \mathbf{v}^{(1)}).$$

$$\min_{\tau_1, \tau_2} g(\mathbf{x}_0 + \tau_1 \mathbf{v}^{(1)} + \tau_2 \mathbf{v}^{(2)}) = g(\mathbf{x}_0 + t_1 \mathbf{v}^{(1)} + t_2 \mathbf{v}^{(2)}).$$

$$\min_{\mathbf{x}} g(\mathbf{x}) =$$

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Thus  $\mathbf{x} = \mathbf{x}_0 + t_1 \mathbf{v}^{(1)} + \dots + t_n \mathbf{v}^{(n)}$  is solution to  $A \mathbf{x} = \mathbf{b}$ .

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**Proof (I):** Let  $\mathbf{t} = (\tau_1, \dots, \tau_k)$ . Then

$$\begin{aligned} g(\mathbf{x}_0 + \tau_1 \mathbf{v}_1 + \dots + \tau_k \mathbf{v}_k) &= g(\mathbf{x}_0) \\ &+ \mathbf{t}^T (\mathbf{v}_1, \dots, \mathbf{v}_k)^T A (\mathbf{v}_1, \dots, \mathbf{v}_k) \mathbf{t} - 2 \mathbf{t}^T (\mathbf{v}_1, \dots, \mathbf{v}_k)^T \mathbf{r}^{(0)}, \\ \nabla_{\mathbf{t}} g &= 2 \left( (\mathbf{v}_1, \dots, \mathbf{v}_k)^T A (\mathbf{v}_1, \dots, \mathbf{v}_k) \mathbf{t} - (\mathbf{v}_1, \dots, \mathbf{v}_k)^T \mathbf{r}^{(0)} \right) \end{aligned}$$

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$$\min_{\tau_1, \dots, \tau_k} g(\mathbf{x}_0 + \tau_1 \mathbf{v}_1 + \dots + \tau_k \mathbf{v}_k) \iff \nabla_{\mathbf{t}} g = \mathbf{0}.$$

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**Proof (II):** Since vectors  $\{\mathbf{v}^{(k)}\}$  are A-orthogonal

$$\nabla_{\mathbf{t}} g = 2 \left( \text{diag} \left( (\mathbf{v}^{(1)})^T A \mathbf{v}^{(1)}, \dots, (\mathbf{v}^{(k)})^T A \mathbf{v}^{(k)} \right) \mathbf{t} - (\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(k)})^T \mathbf{r}^{(0)} \right)$$

$$\nabla_{\mathbf{t}} g = \mathbf{0} \iff \mathbf{t} = \begin{pmatrix} \frac{(\mathbf{v}^{(1)})^T (\mathbf{r}^{(0)})}{(\mathbf{v}^{(1)})^T (A \mathbf{v}^{(1)})} \\ \vdots \\ \frac{(\mathbf{v}^{(k)})^T (\mathbf{r}^{(0)})}{(\mathbf{v}^{(k)})^T (A \mathbf{v}^{(k)})} \end{pmatrix}.$$

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**Proof (III):** Since

$$(\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)}) = (\mathbf{v}^{(k)})^T \left( \mathbf{r}^{(0)} - \sum_{j=1}^{k-1} t_j A\mathbf{v}^{(j)} \right) = (\mathbf{v}^{(k)})^T (\mathbf{r}^{(0)}), \quad \text{so}$$

$$t_k = \frac{(\mathbf{v}^{(k)})^T (\mathbf{r}^{(0)})}{(\mathbf{v}^{(k)})^T (A\mathbf{v}^{(k)})} = \frac{(\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(k)})^T (A\mathbf{v}^{(k)})}.$$

# A-orthogonality vectors (I)

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**Thm:** Set  $\mathbf{v}^{(1)} = -\mathbf{r}^{(0)}$ , and for  $k = 2, \dots, n$

$$\mathbf{v}^{(k)} = -\mathbf{r}^{(k-1)} + \sum_{j=1}^{k-1} \frac{(\mathbf{v}^{(j)})^T (A\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)})} \mathbf{v}^{(j)}.$$

Assume that  $\{\mathbf{v}^{(k)}\}$  are non-zero. Then they are A-orthogonal.

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Assume that  $\{\mathbf{v}^{(k)}\}$  are non-zero. Then they are A-orthogonal.

**Induction Proof:** For all  $1 \leq i < k$ ,

$$\begin{aligned} (\mathbf{v}^{(k)})^T (A\mathbf{v}^{(i)}) &= -(\mathbf{r}^{(k-1)})^T (A\mathbf{v}^{(i)}) \\ &\quad + \sum_{j=1}^{k-1} \frac{(\mathbf{v}^{(j)})^T (A\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)})} (\mathbf{v}^{(j)})^T (A\mathbf{v}^{(i)}) \\ &= -(\mathbf{r}^{(k-1)})^T (A\mathbf{v}^{(i)}) + (\mathbf{v}^{(i)})^T (A\mathbf{r}^{(k-1)}) = 0. \end{aligned}$$

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Let  $\mathbf{x}^{(k)} = \mathbf{x}^{(0)} + t_1\mathbf{v}^{(1)} + \dots + t_k\mathbf{v}^{(k)}$  and  $\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)}$ . Then

$$(\mathbf{v}^{(j)})^T (\mathbf{r}^{(k)}) = 0, \quad j = 1, \dots, k; \quad (\mathbf{r}^{(j)})^T (\mathbf{r}^{(k)}) = 0, \quad j = 1, \dots, k-1.$$

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**Proof:** Due to optimality property of  $\mathbf{x}^{(k)}$ , for all  $\tau$  and for  $1 \leq j \leq k$ ,

$$\begin{aligned} g(\mathbf{x}^{(k)}) &\leq g(\mathbf{x}^{(k)} + \tau \mathbf{v}^{(j)}) \\ &= g(\mathbf{x}^{(k)}) - 2\tau (\mathbf{r}^{(k)})^T \mathbf{v}^{(j)} + \tau^2 (\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)}). \end{aligned}$$

This is true only when  $(\mathbf{r}^{(k)})^T \mathbf{v}^{(j)} = 0$ .

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Let  $\mathbf{x}^{(k)} = \mathbf{x}^{(0)} + t_1\mathbf{v}^{(1)} + \dots + t_k\mathbf{v}^{(k)}$  and  $\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)}$ . Then

$$(\mathbf{v}^{(j)})^T (\mathbf{r}^{(k)}) = 0, \quad j = 1, \dots, k; \quad (\mathbf{r}^{(j)})^T (\mathbf{r}^{(k)}) = 0, \quad j = 1, \dots, k-1.$$

**Proof:** Due to optimality property of  $\mathbf{x}^{(k)}$ , for all  $\tau$  and for  $1 \leq j \leq k$ ,

$$\begin{aligned} g(\mathbf{x}^{(k)}) &\leq g(\mathbf{x}^{(k)} + \tau \mathbf{v}^{(j)}) \\ &= g(\mathbf{x}^{(k)}) - 2\tau (\mathbf{r}^{(k)})^T \mathbf{v}^{(j)} + \tau^2 (\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)}). \end{aligned}$$

This is true only when  $(\mathbf{r}^{(k)})^T \mathbf{v}^{(j)} = 0$ .

Residual vector orthogonality:  $\mathbf{r}^{(j)} =$  linear combination of  $\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(j+1)}$



# A-orthogonality vectors (III)

## $A$ -orthogonality vectors (III)

**Thm:** Set  $\mathbf{v}^{(1)} = -\mathbf{r}^{(0)}$ , and for  $k = 2, \dots, n$

$$\mathbf{v}^{(k)} = -\mathbf{r}^{(k-1)} + \sum_{j=1}^{k-1} \frac{(\mathbf{v}^{(j)})^T (A\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)})} \mathbf{v}^{(j)}.$$

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$$(\mathbf{v}^{(k)})^T (\mathbf{r}^{(j)}) = -(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)}), \quad j = 1, \dots, k-1.$$

**Proof (I):** For  $j = k-1$ ,

$$\begin{aligned} (\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)}) &= \left( -\mathbf{r}^{(k-1)} + \sum_{j=1}^{k-1} \frac{(\mathbf{v}^{(j)})^T (A\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(j)})^T (A\mathbf{v}^{(j)})} \mathbf{v}^{(j)} \right)^T (\mathbf{r}^{(k-1)}) \\ &= -(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)}). \end{aligned}$$

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$$(\mathbf{v}^{(k)})^T (\mathbf{r}^{(j)}) = -(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)}), \quad j = 1, \dots, k-1.$$

**Proof (II):** For  $j < k-1$

$$\begin{aligned}(\mathbf{v}^{(k)})^T (\mathbf{r}^{(j)}) &= (\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)}) + (\mathbf{v}^{(k)})^T (\mathbf{r}^{(j)} - \mathbf{r}^{(k-1)}) \\ &= (\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)}) + (\mathbf{v}^{(k)})^T \left( \sum_{i=j+1}^{k-1} t_i A\mathbf{v}^{(i)} \right) \\ &= -(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)}).\end{aligned}$$

# *A*-orthogonality: A Gift from Math God

## A-orthogonality: A Gift from Math God

Set  $\mathbf{v}^{(1)} = -\mathbf{r}^{(0)}$ , and for  $k = 2, \dots, n$ , write

$$\mathbf{v}^{(k)} = \sum_{j=0}^{k-1} \frac{(\mathbf{v}^{(k)})^T (\mathbf{r}^{(j)})}{(\mathbf{r}^{(j)})^T (\mathbf{r}^{(j)})} \mathbf{r}^{(j)}.$$

Then

$$\begin{aligned} \mathbf{v}^{(k)} &= -\sum_{j=0}^{k-1} \frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(j)})}{(\mathbf{r}^{(j)})^T (\mathbf{r}^{(j)})} \mathbf{r}^{(j)} \\ &= -\mathbf{r}^{(k-1)} - \frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-2)})}{(\mathbf{r}^{(k-2)})^T (\mathbf{r}^{(k-2)})} \sum_{j=0}^{k-2} \frac{(\mathbf{r}^{(k-2)})^T (\mathbf{r}^{(j)})}{(\mathbf{r}^{(j)})^T (\mathbf{r}^{(j)})} \mathbf{r}^{(j)} \\ &= -\mathbf{r}^{(k-1)} + s_{k-1} \mathbf{v}^{(k-1)}, \end{aligned}$$

with  $s_{k-1} = \frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-2)})}{(\mathbf{r}^{(k-2)})^T (\mathbf{r}^{(k-2)})}$ .



**Thm:** Let  $\{\mathbf{v}^{(i)}\}_{i=1}^n$  be  $A$ -orthogonal with  $\mathbf{v}^{(1)} = -\mathbf{r}^{(0)}$  and for  $k = 1, \dots, n$

$$t_k = \frac{(\mathbf{v}^{(k)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(k)})^T (A \mathbf{v}^{(k)})} = -\frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(k)})^T (A \mathbf{v}^{(k)})}, \quad \mathbf{x}^{(k)} \stackrel{\text{def}}{=} \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}.$$

Then  $A \mathbf{x}^{(n)} = b$  in exact arithmetic.

# Conjugate Gradient Algorithm

**Thm:** For  $k = 1, \dots, n$ , define,

$$\mathbf{v}^{(k)} = -\mathbf{r}^{(k-1)} + s_{k-1} \mathbf{v}^{(k-1)} \quad \text{with} \quad s_{k-1} = \frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{r}^{(k-2)})^T (\mathbf{r}^{(k-2)})},$$
$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)} \quad \text{with} \quad t_k = -\frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(k)})^T (A \mathbf{v}^{(k)})}.$$

Then vectors  $\{\mathbf{v}^{(k)}\}$  are A-orthogonal and  $A\mathbf{x}^{(n)} = b$  in *exact arithmetic*.

The CG Algorithm: C is for *Craft*, G is for *Gift*.

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## Algorithm 1 Conjugate Gradient Algorithm

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**Input:** Symmetric positive definite  $A \in \mathbb{R}^{n \times n}$ ,  $\mathbf{b} \in \mathbb{R}^n$ ,  
initial guess  $\mathbf{x}^{(0)} \in \mathbb{R}^n$ , and tolerance  $\tau > 0$ .

**Output:** Approximate solution  $\mathbf{x}$ .

**Algorithm:**

Initialize:  $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$ ,  $\mathbf{v}^{(0)} = -\mathbf{r}^{(0)}$ ,  $k = 1$

**while**  $\|\mathbf{r}^{(k-1)}\|_2 \geq \tau$  **do**

$$t_k = -\frac{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)})}{(\mathbf{v}^{(k)})^T (A\mathbf{v}^{(k)})}.$$

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}$$

$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - t_k A\mathbf{v}^{(k)}.$$

$$s_k = \frac{(\mathbf{r}^{(k)})^T (\mathbf{r}^{(k)})}{(\mathbf{r}^{(k-1)})^T (\mathbf{r}^{(k-1)})}.$$

$$\mathbf{v}^{(k+1)} = -\mathbf{r}^{(k)} + s_k \mathbf{v}^{(k)}.$$

$$k = k + 1.$$

**end while**

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