

Numerical Linear Algebra

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Direct and iterative methods for linear systems

- ▶ Termination criteria
- ▶ Quadratic functional and linear systems
- ▶ Method of minimal residuals
- ▶ CP2
- ▶ Q & A

Recap of Previous Lecture

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- ▶ Convergence of Richardson's iterations
- ▶ Optimal parameter parameter of Richardson's iterations
- ▶ Sufficient condition $P > 0.5A$
- ▶ Preconditioning matrices

Termination criteria, 1

Definition 11.1

Iteration method is linear convergent if

$$\|x^{(k+1)} - x^{(k)}\| \leq r \|x^{(k)} - x^{(k-1)}\|, \quad r < 1$$
$$\lim_{k \rightarrow \infty} x^{(k)} = A^{-1}b$$

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▶
$$\lim_{k \rightarrow \infty} \frac{\|x^{(k+1)} - x^{(k)}\|}{\|x^{(k)} - x^{(k-1)}\|} = r$$

Theorem 11.2

linear convergent iteration method satisfy

$$\|x - x^{(k)}\| \leq \frac{r}{1-r} \|x^{(k)} - x^{(k-1)}\|$$

Termination criteria, 2

Proof.

$$\begin{aligned} & \|x^{(k+m)} - x^{(k)}\| \leq \\ & \|x^{(k+m)} - x^{(k+m-1)}\| + \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \end{aligned}$$

Termination criteria, 2

Proof.

$$\begin{aligned} \|x^{(k+m)} - x^{(k)}\| &\leq \\ \|x^{(k+m)} - x^{(k+m-1)}\| &+ \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \\ \|x^{(k+m)} - x^{(k)}\| &\leq \\ r\|x^{(k+m-1)} - x^{(k+m-2)}\| &+ \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \end{aligned}$$

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Proof.

$$\begin{aligned} & \|x^{(k+m)} - x^{(k)}\| \leq \\ & \|x^{(k+m)} - x^{(k+m-1)}\| + \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \\ & \|x^{(k+m)} - x^{(k)}\| \leq \\ & r\|x^{(k+m-1)} - x^{(k+m-2)}\| + \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \\ & \|x^{(k+m)} - x^{(k)}\| \leq \\ & (r+1)\|x^{(k+m-1)} - x^{(k+m-2)}\| + \|x^{(k+m-2)} - x^{(k+m-3)}\| + \dots + \|x^{(k+1)} - x^{(k)}\| \\ & \|x^{(k+m)} - x^{(k)}\| \leq (r^{m-1} + r^{m-2} + \dots + r + 1)\|x^{(k+1)} - x^{(k)}\| \\ & \|x^{(k+m)} - x^{(k)}\| \leq \frac{1 - r^{m-1}}{r - 1}\|x^{(k+1)} - x^{(k)}\| \leq \frac{1 - r^{m-1}}{r - 1}r\|x^{(k)} - x^{(k-1)}\| \end{aligned}$$

Termination criteria, 2

Proof.

$$\|x^{(k+m)} - x^{(k)}\| \leq$$

$$\|x^{(k+m)} - x^{(k+m-1)}\| + \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\|$$

$$\|x^{(k+m)} - x^{(k)}\| \leq$$

$$r\|x^{(k+m-1)} - x^{(k+m-2)}\| + \|x^{(k+m-1)} - x^{(k+m-2)}\| + \dots + \|x^{(k+1)} - x^{(k)}\|$$

$$\|x^{(k+m)} - x^{(k)}\| \leq$$

$$(r+1)\|x^{(k+m-1)} - x^{(k+m-2)}\| + \|x^{(k+m-2)} - x^{(k+m-3)}\| + \dots + \|x^{(k+1)} - x^{(k)}\|$$

$$\|x^{(k+m)} - x^{(k)}\| \leq (r^{m-1} + r^{m-2} + \dots + r + 1)\|x^{(k+1)} - x^{(k)}\|$$

$$\|x^{(k+m)} - x^{(k)}\| \leq \frac{1 - r^{m-1}}{r - 1} \|x^{(k+1)} - x^{(k)}\| \leq \frac{1 - r^{m-1}}{r - 1} r \|x^{(k)} - x^{(k-1)}\|$$

$$m \rightarrow \infty \Rightarrow \|x - x^{(k)}\| \leq \frac{r}{1-r} \|x^{(k)} - x^{(k-1)}\|$$



Termination criteria, 3

$$\blacktriangleright \|x - x^{(k)}\| \leq \frac{r^k}{1-r} \|x^{(1)} - x^0\|$$

Termination criteria, 3

► $\|x - x^{(k)}\| \leq \frac{r^k}{1-r} \|x^{(1)} - x^0\|$

► Criterion 1

$$\|b - Ax^{(k)}\| < \epsilon$$

Termination criteria, 3

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Bad criterion, is not scaling invariant

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Termination criteria, 3

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Scaling invariant, drawback = depends on initial estimate $x^{(0)}$

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- Criterion 3, better termination criterion

$$\frac{\|b - Ax^{(k)}\|}{\|b\|} < \epsilon$$

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$$\frac{\|b - Ax^{(k)}\|}{\|b\|} < \epsilon$$

- Criterion 4, if $\|A^{-1}\|$ estimate available

$$\frac{\|b - Ax^{(k)}\|}{\|x^{(k)}\|} < \epsilon / \|A^{-1}\|$$

Termination criteria, 5

Proposition 11.3

if

$$\frac{\|b - Ax^{(k)}\|}{\|b\|} \leq \epsilon / \text{Cond}(A)$$

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Proof.

$Ax = b, A\tilde{x} = \tilde{b}$, *Right perturbation theorem*

Termination criteria, 5

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Proof.

$Ax = b, A\tilde{x} = \tilde{b}$, Right perturbation theorem

$$\frac{\|x - x^{(k)}\|}{\|x\|} \stackrel{\Downarrow}{\leq} \text{cond}(A) \frac{\|b - \tilde{b}\|}{\|b\|}$$

Termination criteria, 5

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if

$$\frac{\|b - Ax^{(k)}\|}{\|b\|} \leq \epsilon / \text{Cond}(A)$$

then

$$\frac{\|x - x^{(k)}\|}{\|x\|} \leq \epsilon$$

Proof.

$Ax = b, A\tilde{x} = \tilde{b}$, Right perturbation theorem



$$\frac{\|x - x^{(k)}\|}{\|x\|} \leq \text{cond}(A) \frac{\|b - \tilde{b}\|}{\|b\|}$$

$$Ax = b, Ax^{(k)} = b + (Ax^{(k)} - b)$$

Termination criteria, 5

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Termination criteria, 6

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Proof.

$$\frac{\|x - x^{(k)}\|}{\|x^{(k)}\|} = \frac{\|A^{-1}(b - Ax^{(k)})\|}{\|x^{(k)}\|}$$

Termination criteria, 6

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$$\frac{\|x - x^{(k)}\|}{\|x^{(k)}\|} \leq \frac{\|A^{-1}\| \|b - Ax^{(k)}\|}{\|x^{(k)}\|} \leq \epsilon$$



Quadratic functional & $Ax = b$, 1

Theorem 11.5

► $A \in \mathbb{R}^{n \times n}, A = A^T > 0$

Quadratic functional & $Ax = b, 1$

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Quadratic functional & $Ax = b, 1$

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- ▶ $1 \equiv (2, 3) :$

Quadratic functional & $Ax = b$, 1

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▶ $A \in \mathbb{R}^{n \times n}, A = A^T > 0$



▶ $1 \equiv (2, 3) :$

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Quadratic functional & $Ax = b$, 1

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Quadratic functional & $Ax = b$, 1

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Quadratic functional & $Ax = b$, 1

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- ▶ two steps

Quadratic functional & $Ax = b$, 1

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Quadratic functional & $Ax = b$, 1

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Proof.

- ▶ two steps
- ▶ $1 \Rightarrow (2, 3)$
- ▶ $(2, 3) \Rightarrow 1$



Quadratic functional & $Ax = b$, 2

1,2,3

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Quadratic functional & $Ax = b$, 2

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Proof.

- ▶ $(2, 3) \Rightarrow 1$
- ▶ $f(x) = 0.5(Ax, x) - (b, x) = 0.5 \sum_{i=1}^n (\sum_{j=1}^n a_{ij}x_j)x_i - \sum_{i=1}^n b_i x_i$

Quadratic functional & $Ax = b$, 2

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- ▶ $\frac{\partial f(x)}{\partial x_k} = 0.5(\sum_{i=1}^n a_{ik} x_i + \sum_{j=1}^n a_{kj} x_j) - b_k$

Quadratic functional & $Ax = b$, 2

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- ▶ $\nabla f(x) = 0.5(A^T + A)x - b = Ax - b$

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- ▶ $Ay = b \Rightarrow \nabla f(y) = 0$

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- ▶ $\nabla f(x) = 0.5(A^T + A)x - b = Ax - b$
- ▶ $Ay = b \Rightarrow \nabla f(y) = 0$
- ▶ $\nabla^2 f(x) = A > 0 \Rightarrow (2, 3) \Rightarrow 1$



Quadratic functional & $Ax = b$, 3

1,2,3

1. $Ay = b$
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Quadratic functional & $Ax = b$, 3

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Proof.

► $1 \Rightarrow (2, 3)$

Quadratic functional & $Ax = b$, 3

1,2,3

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3. $f(x) = 0.5(Ax, x) - (b, x)$

Proof.

- ▶ $1 \Rightarrow (2, 3)$
- ▶ $f(x) = f(y + x - y) = f(x + z) = 0.5(A(y + z), y + z) - (b, y + z)$

Quadratic functional & $Ax = b$, 3

1,2,3

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- ▶ $f(x) = 0.5[(Ay, y) + (Az, z) + (Ay, z) + (Az, y)] - (b, y) - (b, z)$

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- ▶ $f(x) = 0.5[(Ay, y) + (Az, z) + (Ay, z) + (Az, y)] - (b, y) - (b, z)$
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Quadratic functional & $Ax = b$, 3

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- ▶ $f(x) = 0.5[(Ay, y) + (Az, z) + (Ay, z) + (Az, y)] - (b, y) - (b, z)$
- ▶ $f(x) = 0.5(Ay, y) - (b, y) + 0.5(Az, z) + (Ay, z) - (b, z)$
- ▶ $f(x) = f(y) + 0.5\|z\|_A + (Ay - b, z) = f(y) + 0.5\|z\|_A$

Quadratic functional & $Ax = b$, 3

1,2,3

1. $Ay = b$
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- ▶ $f(x) = f(y + x - y) = f(x + z) = 0.5(A(y + z), y + z) - (b, y + z)$
- ▶ $f(x) = 0.5[(Ay, y) + (Az, z) + (Ay, z) + (Az, y)] - (b, y) - (b, z)$
- ▶ $f(x) = 0.5(Ay, y) - (b, y) + 0.5(Az, z) + (Ay, z) - (b, z)$
- ▶ $f(x) = f(y) + 0.5\|z\|_A + (Ay - b, z) = f(y) + 0.5\|z\|_A$
- ▶ $f(x) = f(y) + 0.5\|z\|_A$

Quadratic functional & $Ax = b$, 3

1,2,3

1. $Ay = b$
2. $y = \arg \min_{x \in \mathbb{R}^n} f(x)$
3. $f(x) = 0.5(Ax, x) - (b, x)$

Proof.

- ▶ $1 \Rightarrow (2, 3)$
- ▶ $f(x) = f(y + x - y) = f(x + z) = 0.5(A(y + z), y + z) - (b, y + z)$
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- ▶ $f(x) - f(y) = 0.5\|z\|_A \geq 0$

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- ▶ $f(x) = f(y) + 0.5\|z\|_A$
- ▶ $f(x) - f(y) = 0.5\|z\|_A \geq 0 \Rightarrow f(x) \geq f(y) \quad \forall x$

Quadratic functional & $Ax = b$, 3

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Method of minimal residuals, Derivation, 1

► Non-stationary Richardson method

$$\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b, \quad k = 0, 1, 2, \dots$$

Method of minimal residuals, Derivation, 1

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$$\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b, \quad k = 0, 1, 2, \dots$$

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► $A \in \mathbb{R}^{n \times n}, A = A^T > 0, Ae^{(k)} = A(x - x^{(k)}) = b - Ax^{(k)} = r_k$

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Method of minimal residuals, Derivation, 1

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Method of minimal residuals, Derivation, 1

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► $\varphi(\alpha) = \|r_k - \alpha Ar_k\|_2 \Rightarrow$

Method of minimal residuals, Derivation, 1

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► What is "best" α_k ?

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► $\varphi(\alpha) = \|r_k - \alpha Ar_k\|_2 \Rightarrow$ "Best" $\alpha_{opt} = \arg \min \varphi(\alpha)$

Method of minimal residuals, Derivation, 2

► $f(x) = 0.5(Ax, x) - (b, x), A \in \mathbb{R}^{n \times n}, A = A^T > 0$

Method of minimal residuals, Derivation, 2

► $f(x) = 0.5(Ax, x) - (b, x), A \in \mathbb{R}^{n \times n}, A = A^T > 0$



$$\begin{aligned}\varphi^2(\alpha) &= \|r_k - \alpha Ar_k\|_2 = (r_k - \alpha Ar_k, r_k - \alpha Ar_k) = \\ &= (r_k, r_k) - \alpha(r_k, Ar_k) - \alpha(Ar_k, r_k) + \alpha^2(Ar_k, Ar_k) \\ &= \|r_k\|_2^2 - 2\alpha(r_k, Ar_k) + \alpha^2\|Ar_k\|_2^2\end{aligned}$$

Method of minimal residuals, Derivation, 2

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Method of minimal residuals, Derivation, 2

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► $\varphi'_\alpha = 0 \Rightarrow \alpha_{opt} = \frac{(Ar_k, r_k)}{(Ar_k, Ar_k)}$

Method of minimal residuals, derivation, 3

Algorithm of the method of minimal residuals for solving
 $Ax = b, A = A^T > 0$

Method of minimal residuals, derivation, 3

Algorithm of the method of minimal residuals for solving
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- Choose $x^{(0)}$, set $k = 0$

Method of minimal residuals, derivation, 3

Algorithm of the method of minimal residuals for solving
 $Ax = b, A = A^T > 0$

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Method of minimal residuals, derivation, 3

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Method of minimal residuals, convergence, 1

Method of minimal residuals for solving $Ax = b$, $A = A^T > 0$ is
non-stationary Richardson

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Method of minimal residuals, convergence, 1

Method of minimal residuals for solving $Ax = b$, $A = A^T > 0$ is **non-stationary Richardson**

- ▶ Choose $x^{(0)}$, set $k = 0$
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 3. $x^{(k+1)} = x^{(k)} + \alpha_k r_k$



$$x^{(k+1)} = x^{(k)} + \alpha_k r_k = x^{(k)} + \alpha_k (b - Ax^{(k)})$$

$$\Rightarrow x^{(k+1)} - x^{(k)} = \alpha_k (b - Ax^{(k)})$$

$$\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$$

$$B_{\minres} = B_{R, \alpha_k}, \quad x^{(k+1)} = (I - \alpha_k A)x^{(k)} + b$$

Method of minimal residuals, convergence, 2

Theorem 11.6

► $Ax = b, A = A^T > 0$

Method of minimal residuals, convergence, 2

Theorem 11.6

- ▶ $Ax = b, A = A^T > 0$
- ▶ $\lambda_1(A) > \lambda_2(A) > \dots > \lambda_n(A) > 0$

Method of minimal residuals, convergence, 2

Theorem 11.6

- ▶ $Ax = b, A = A^T > 0$
- ▶ $\lambda_1(A) > \lambda_2(A) > \dots > \lambda_n(A) > 0$
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- ▶ $\lim_{k \rightarrow \infty} x_{minres}^{(k)} = A^{-1}b$

Method of minimal residuals, convergence, 2

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Method of minimal residuals, convergence, 2

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Proof.

- ▶ Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$

Method of minimal residuals, convergence, 2

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Method of minimal residuals, convergence, 2

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Method of minimal residuals, convergence, 2

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- ▶ Approach: $\alpha_{minres,k}$ vs α_{opt}

Method of minimal residuals, convergence, 3

Proof.

► Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$

Method of minimal residuals, convergence, 3

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Method of minimal residuals, convergence, 3

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Method of minimal residuals, convergence, 3

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- ▶ Approach: $\alpha_{minres,k}$ vs α_{opt} for the same r_k, x_k

Method of minimal residuals, convergence, 3

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- ▶ Approach: $\alpha_{\minres,k}$ vs α_{opt} for the same r_k, x_k
- ▶ $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} = b - Ax^{(k)}$

Method of minimal residuals, convergence, 3

Proof.

- ▶ Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$
- ▶ **Minimal residuals** $\alpha_k = \alpha_{\minres,k} = \frac{(Ar_k, r_k)}{(Ar_k, Ar_k)}$
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- ▶ Approach: $\alpha_{\minres,k}$ vs α_{opt} for the same r_k, x_k
- ▶ $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} = b - Ax^{(k)} \Rightarrow x^{(k+1)} - x^{(k)} = \alpha_k r_k$

Method of minimal residuals, convergence, 3

Proof.

- ▶ Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$
- ▶ **Minimal residuals** $\alpha_k = \alpha_{minres,k} = \frac{(Ar_k, r_k)}{(Ar_k, Ar_k)}$
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- ▶ $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} = b - Ax^{(k)} \Rightarrow x^{(k+1)} - x^{(k)} = \alpha_k r_k \Rightarrow$
 $Ax^{(k+1)} - Ax^{(k)} = \alpha_k Ar_k$

Method of minimal residuals, convergence, 3

Proof.

- ▶ Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$
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 $Ax^{(k+1)} - Ax^{(k)} = \alpha_k Ar_k \Rightarrow -(b - Ax^{(k+1)}) + (b - Ax^{(k)}) = \alpha_k Ar_k$

Method of minimal residuals, convergence, 3

Proof.

- ▶ Richardson: $\frac{x^{(k+1)} - x^{(k)}}{\alpha_k} + Ax^{(k)} = b$
- ▶ **Minimal residuals** $\alpha_k = \alpha_{minres,k} = \frac{(Ar_k, r_k)}{(Ar_k, Ar_k)}$
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- ▶ $r_{minres,k+1} = (I - \alpha_{minres,k} A)r_{minres,k} = B_{R_{minres,k}} r_{minres,k}$

Method of minimal residuals, convergence, 3

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Method of minimal residuals, convergence, 3

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Method of minimal residuals, convergence, 3

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- ▶ $\rho_{opt} = \frac{\lambda_1(A) - \lambda_n(A)}{\lambda_1(A) + \lambda_n(A)} < 1$

Method of minimal residuals, convergence, 3

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- ▶ $\rho_{opt} = \frac{\lambda_1(A) - \lambda_n(A)}{\lambda_1(A) + \lambda_n(A)} < 1$
- ▶ $\|r_{\minres,k+1}\|_2 \leq \|r_{opt,k+1}\|_2 \leq \rho_{opt} \|r_k\|_2$

Method of minimal residuals, convergence, 3

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- ▶ $\|r_{\minres,k+1}\|_2 \leq \rho_{opt} \|r_{\minres,k}\|_2$

Method of minimal residuals, convergence, 4

Proof.

$$\blacktriangleright \|r_{opt,k+1}\|_2 = \|B_{R_{opt,k}} r_{opt,k}\|_2 \leq \|B_{R_{opt,k}}\|_2 \|r_{opt,k}\|_2 = \rho_{opt} \|r_k\|_2$$

Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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- ▶ $\|r_{minres,k+1}\|_2 \leq \rho_{opt}^2 \|r_{minres,k-1}\|_2$

Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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Method of minimal residuals, convergence, 4

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- ▶ $\|e_{minres}^{(k)}\|_2 \leq \|A^{-1}\|_2 \|r_{minres,k}\|_2 \xrightarrow{k \rightarrow \infty} 0$

Method of minimal residuals, convergence, 4

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Q & A