CG: Conjugate Gradient method for $Ax = b$, $A \succ 0$

When A symmetric, Lanczos gives $AQ_k = Q_k T_k + q_{k+1}[0, \ldots, 0, 1]$, T_k: tridiagonal

$Q_k^T(Ax - b) = 0$ — residual. $[1, 0, \ldots, 0]^T \|b\|$

CG: when $A \succ 0$ PD, solve $Q_k^T(AQ_k y - b) = T_k y - Q_k^T b = 0$, and $x = Q_k y$

$\rightarrow$"Galerkin orthogonality": residual $Ax - b$ orthogonal to Q_k

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→"Galerkin orthogonality": residual $Ax - b$ orthogonal to Q_k

- $T_k y = Q_k^T b$ is tridiagonal linear system, $O(k)$ operations to solve
- three-term recurrence reduces cost to $O(k)$ A-multiplications
- minimises A-norm of error $x_k = \text{argmin}_{x \in Q_k} \|x - x_*\|_A$ $(Ax_* = b)$:

GMRES: $\min_{x \in Q_k} \|Ax - b\|_2$

$$(x - x_*)^T A(x - x_*) = (Q_k y - x_*)^T A(Q_k y - x_*)$$
$$= y^T (Q_k^T A Q_k) y - 2b^T Q_k y + b^T x_*,$$

: "convex"

$\succ 0$

minimiser is $y = (Q_k^T A Q_k)^{-1} Q_k^T b$, so $Q_k^T(AQ_k y - b) = 0$

$\langle x, y \rangle_A = x^T A y$

- Note $\|x\|_A = \sqrt{x^T A x}$ defines a norm (exercise)
- More generally, for inner-product norm $\|z\|_M = \sqrt{< z, z >_M}$, $\min_{x = Qy} \|x_* - x\|_M$ attained when $< q_i, x_* - x >_M = 0$, $\forall q_i$ (cf. Part A NA) $Q = [q_1 \cdots q_k]$

CG algorithm for $Ax = b$, $A \succ 0$

Set $x_0 = 0$, $r_0 = -b$, $p_0 = r_0$ and do for $k = 1, 2, 3, \ldots$

$$\begin{aligned}
\alpha_k &= \langle r_k, r_k \rangle / \langle p_k, Ap_k \rangle \\
x_{k+1} &= x_k + \alpha_k p_k \quad \leftarrow \text{soln at } k\text{th step} \\
r_{k+1} &= r_k - \alpha_k \underline{Ap_k} \\
\beta_k &= \langle r_{k+1}, r_{k+1} \rangle / \langle r_k, r_k \rangle \\
p_{k+1} &= r_{k+1} + \beta_k p_k
\end{aligned}$$

where $r_k = Ax_k - b$ (residual) and p_k (search direction).

One can show among others (exercise/sheet)

- $\mathcal{K}_k(A, b) = \text{span}(r_0, r_1, \ldots, r_{k-1}) = \text{span}(x_1, x_2, \ldots, x_k)$ (also equal to span$(p_0, p_1, \ldots, p_{k-1})$) $\forall k$
- $r_j^T r_k = 0$, $j = 0, 1, 2, \ldots, k-1$

Thus x_k is kth CG solution, satisfying orthogonality $Q_k^T(Ax_k - b) = 0$

CG convergence

Let $e_k := x_* - x_k$. We have $e_0 = x_*$ ($x_0 = 0$), and

$$
\begin{aligned}
\frac{\|e_k\|_A}{\|e_0\|_A} &= \min_{x \in \mathcal{K}_k(A,b)} \|x_k - x_*\|_A / \|x_*\|_A \\
&= \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|p_{k-1}(A)b - A^{-1}b\|_A / \|e_0\|_A \\
&= \min_{p_{k-1} \in \mathcal{P}_{k-1}} \|(p_{k-1}(A)A - I)e_0\|_A / \|e_0\|_A \\
&= \min_{p \in \mathcal{P}_k, p(0)=1} \|p(A)e_0\|_A / \|e_0\|_A \\
&= \min_{p \in \mathcal{P}_k, p(0)=1} \left\| V \begin{bmatrix} p(\lambda_1) & & \\ & \ddots & \\ & & p(\lambda_n) \end{bmatrix} V^T e_0 \right\|_A / \|e_0\|_A
\end{aligned}
$$

$$A = V \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} V^T$$

Now (blue)$^2 = \sum_i \lambda_i p(\lambda_i)^2 (V^T e_0)_i^2 \le \max_j p(\lambda_j)^2 \sum_i \lambda_i (V^T e_0)_i^2 = \max_j p(\lambda_j)^2 \|e_0\|_A^2$

CG convergence cont'd

We've shown

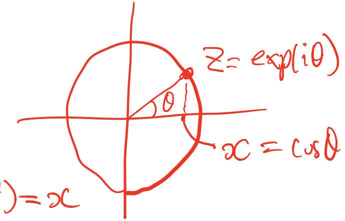
$$\frac{\|e_k\|_A}{\|e_0\|_A} \le \min_{p\in\mathcal{P}_k, p(0)=1} \max_j |p(\lambda_j)| \le \min_{p\in\mathcal{P}_k, p(0)=1} \max_{x\in[\lambda_{\min}(A), \lambda_{\max}(A)]} |p(x)|$$

Now

$$\min_{p\in\mathcal{P}_k, p(0)=1} \max_{x\in[\lambda_{\min}(A), \lambda_{\max}(A)]} |p(x)| \le 2\left(\frac{\sqrt{\kappa_2(A)}-1}{\sqrt{\kappa_2(A)}+1}\right)^k$$

- note $\kappa_2(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} (=: \frac{b}{a})$
- above bound obtained by Chebyshev polynomials on $[\lambda_{\min}(A), \lambda_{\max}(A)]$

Chebyshev polynomials

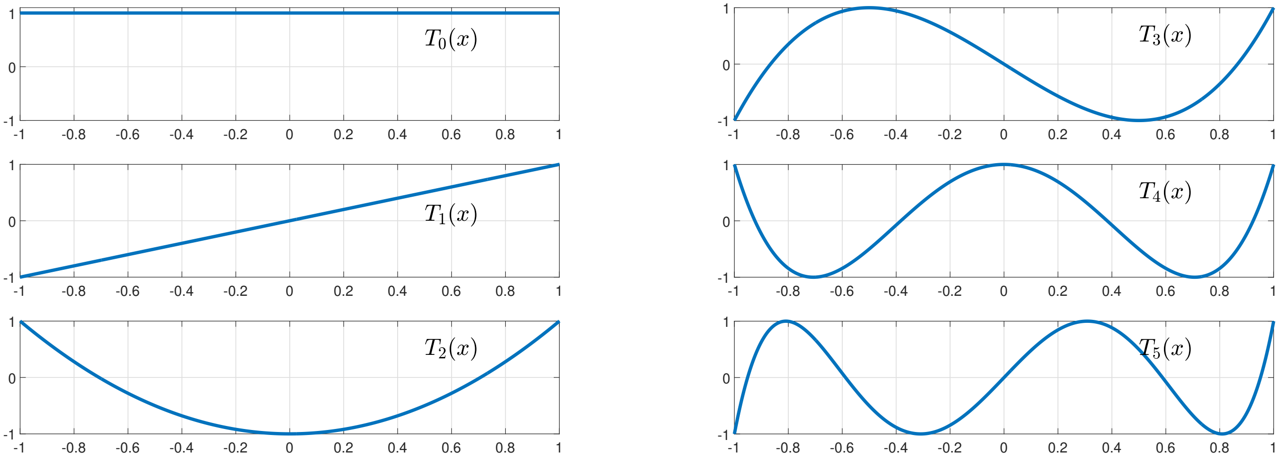


For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta = \text{acos}(x)$,

$T_k(x) = \frac{1}{2}(z^k + z^{-k}) = \cos(k\theta)$. $T_k(x)$ is a polynomial in x:

$= \mathrm{Re}(z^k)$ $\quad T_0(x) = 1 \quad T_1(x) = \frac{1}{2}(z + z^{-1}) = x$

$$\frac{1}{2}(z+z^{-1})(z^k+z^{-k}) = \frac{1}{2}(z^{k+1}+z^{-(k+1)})+\frac{1}{2}(z^{k-1}+z^{-(k-1)}) \Leftrightarrow \underbrace{2xT_k(x) = T_{k+1}(x) + T_{k-1}(x)}_{\text{3-term recurrence}}$$



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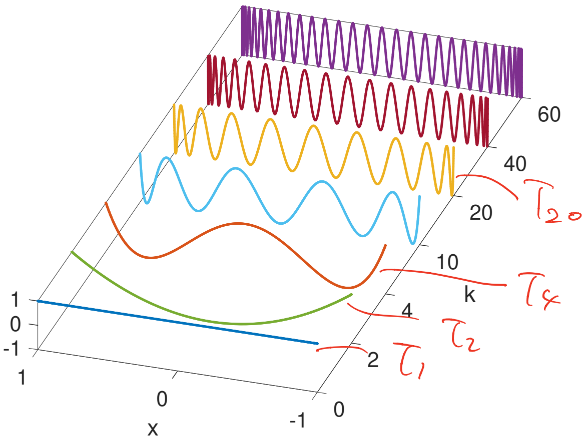

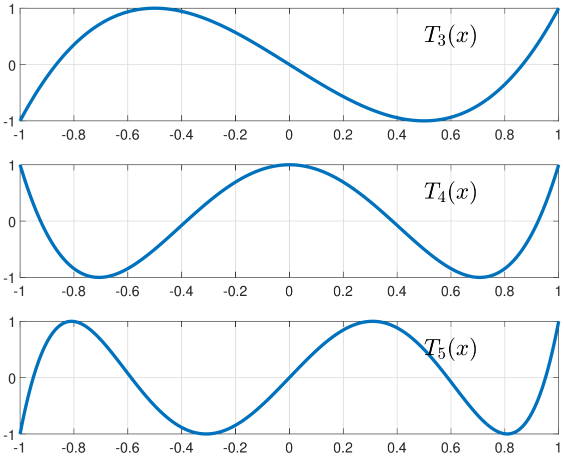

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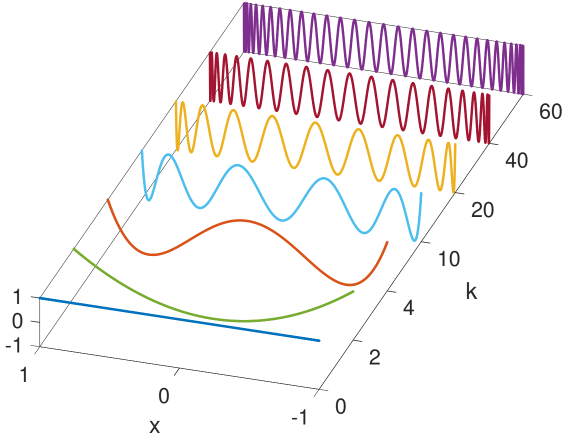

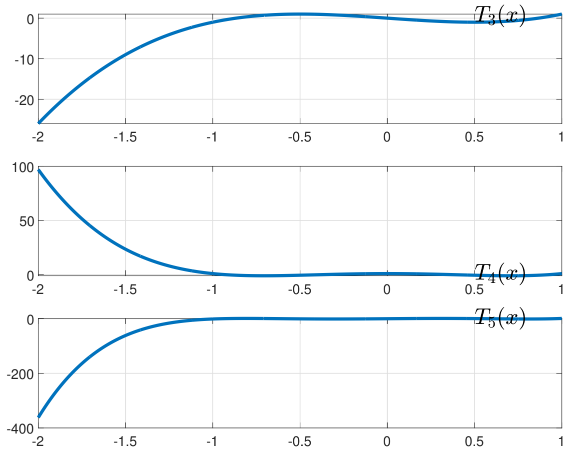

Chebyshev polynomials cont'd

For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta = \text{acos}(x)$,
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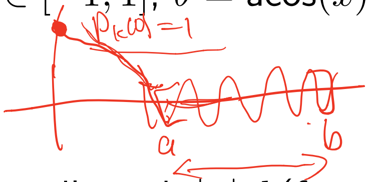


- Inside $[-1, 1]$, $|T_k(x)| \le 1$
- Outside $[-1, 1]$, $|T_k(x)| \gg 1$ grows rapidly with $|x|, k$(fastest growth among $\mathcal{P}_k$)

Shift+scale s.t. $p(x) = c_k T_k(\frac{2x-b-a}{b-a})$ where $c_k = 1/T_k(\frac{-(b+a)}{b-a})$ so $p(0) = 1$. Then

- $|p(x)| \le 1/|T_k(\frac{b+a}{b-a})|$ on $x \in [a, b]$
- $T_k(z) = \frac{1}{2}(z^k + z^{-k})$ with $\frac{1}{2}(z + z^{-1}) = \frac{b+a}{b-a} \Rightarrow z = \frac{\sqrt{b/a}+1}{\sqrt{b/a}-1} = \frac{\sqrt{\kappa_2(A)}+1}{\sqrt{\kappa_2(A)}-1}$, so

$$|p(x)| \le 1/T_k(\frac{b+a}{b-a}) \le 2\left(\frac{\sqrt{\kappa}+1}{\sqrt{\kappa}+1}\right)^k$$

For much more about T_k, see C6.3 Approximation of Functions

MINRES: symmetric (indefinite) version of GMRES

$\lambda_i(A) < 0$ allowed.

Recall GMRES

$$x = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Algorithm: Given $AQ_k = Q_{k+1}\tilde{H}_k$ and writing $x = Q_k y$, rewrite as

$$\begin{aligned} \min_y \|AQ_k y - b\|_2 &= \min_y \|Q_{k+1}\tilde{H}_k y - b\|_2 \\ &= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \begin{bmatrix} Q_k^T \\ Q_{k,\perp}^T \end{bmatrix} b \right\|_2 \\ &= \min_y \left\| \begin{bmatrix} \tilde{H}_k \\ 0 \end{bmatrix} y - \|b\|_2 e_1 \right\|_2, \quad e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n \end{aligned}$$

(where $[Q_k, Q_{k,\perp}]$ orthogonal; same trick as in least-squares)

- Minimised when $\|\tilde{T}_k y - \tilde{Q}_k^T b\| \to \min$; Hessenberg least-squares problem
- Solve via QR (k Givens rotations)+triangular solve, $O(k^2)$ in addition to Arnoldi

MINRES: symmetric (indefinite) version of GMRES

MINRES (minimum-residual method) for $A = A^T$ (but not necessarily $A \succ 0$)

$$x = \text{argmin}_{x \in \mathcal{K}_k(A,b)} \|Ax - b\|_2$$

Algorithm: Given $AQ_k = Q_{k+1}\tilde{T}_k$ and writing $x = Q_k y$, rewrite as

$$\begin{aligned}
\min_y \|AQ_k y - b\|_2 &= \min_y \|Q_{k+1}\tilde{T}_k y - b\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{T}_k \\ 0 \end{bmatrix} y - \begin{bmatrix} Q_k^T \\ Q_{k,\perp}^T \end{bmatrix} b \right\|_2 \\
&= \min_y \left\| \begin{bmatrix} \tilde{T}_k \\ 0 \end{bmatrix} y - \|b\|_2 e_1 \right\|_2, \quad e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^n
\end{aligned}$$

(where $[Q_k, Q_{k,\perp}]$ orthogonal; same trick as in least-squares)

- Minimised when $\|\tilde{T}_k y - \tilde{Q}_k^T b\| \to \min$; tridiagonal least-squares problem
- Solve via QR (k Givens rotations)+tridiagonal solve, $O(k)$ in addition to Lanczos

MINRES convergence

As in GMRES,

$$\min_{x\in\mathcal{K}_k(A,b)} \|Ax-b\|_2 = \min_{p_{k-1}\in\mathcal{P}_{k-1}} \|Ap_{k-1}(A)b-b\|_2 = \min_{\tilde{p}\in\mathcal{P}_k,\tilde{p}(0)=0} \|(\tilde{p}(A)-I)b\|_2$$
$$= \min_{p\in\mathcal{P}_k,p(0)=1} \|p(A)b\|_2$$

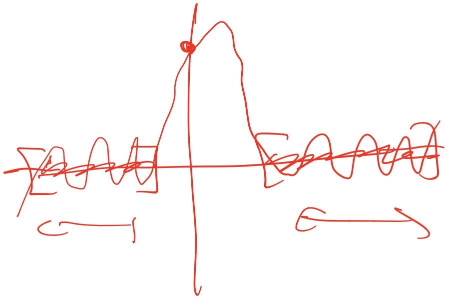
Since $A=A^T$, A is diagonalisable $A=Q\Lambda Q^T$ with Q orthogonal, so

$$\|p(A)\|_2 = \|Qp(\Lambda)Q^T\|_2 \le \|Q\|_2\|Q^T\|_2\|p(\Lambda)\|_2$$
$$= \max_{z\in\lambda(A)} |p(z)|$$

Interpretation: (again) find polynomial s.t. $p(0)=1$ and $|p(\lambda_i)|$ small

MINRES convergence cont'd

$$\frac{\|Ax-b\|_2}{\|b\|_2} \le \min_{p\in\mathcal{P}_k, p(0)=1} \max |p(\lambda_i)|$$

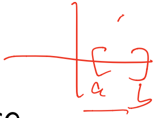


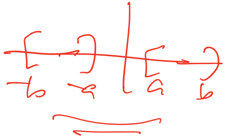
One can prove (nonexaminable)

$$\min_{p\in\mathcal{P}_k, p(0)=1} \max |p(\lambda_i)| \le 2\left(\frac{\kappa_2(A)-1}{\kappa_2(A)+1}\right)^{k/2}$$

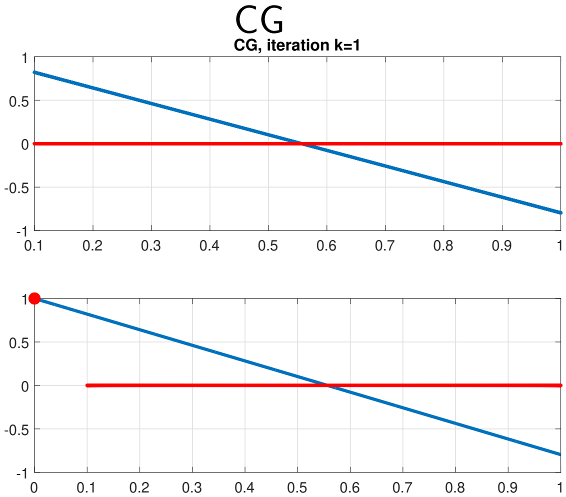
much slower than CG w/ same $\kappa_2(A)$

- obtained by Chebyshev+Möbius change of variables [Greenbaum's book 97]
- minimisation needed on positive **and** negative sides, hence slower convergence when A indefinite



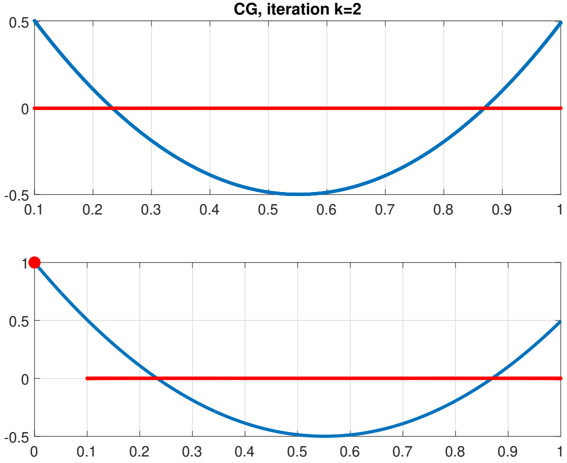


CG and MINRES, optimal polynomials



CG and MINRES, optimal polynomials

CG



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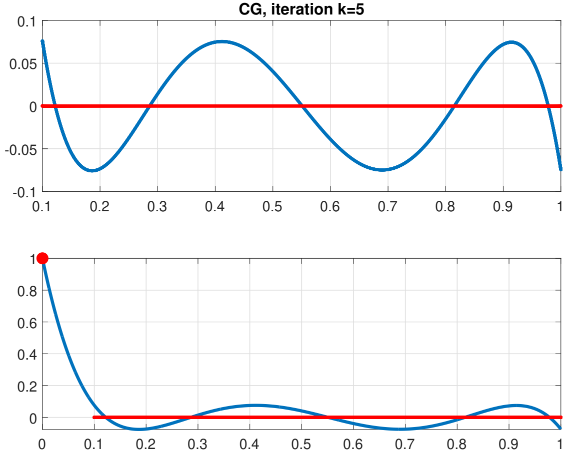

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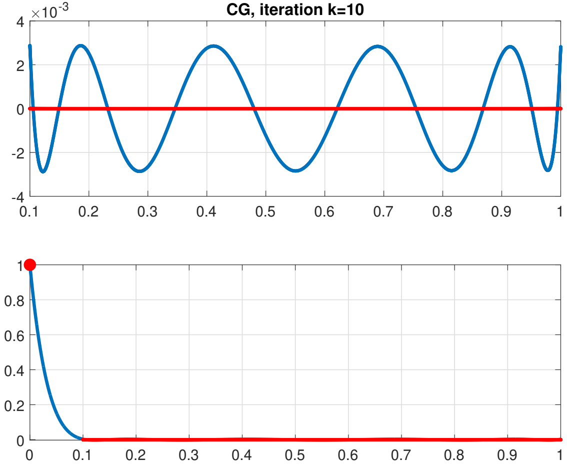

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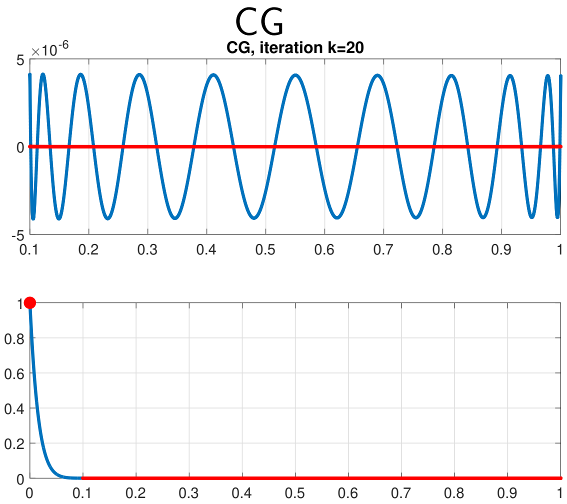

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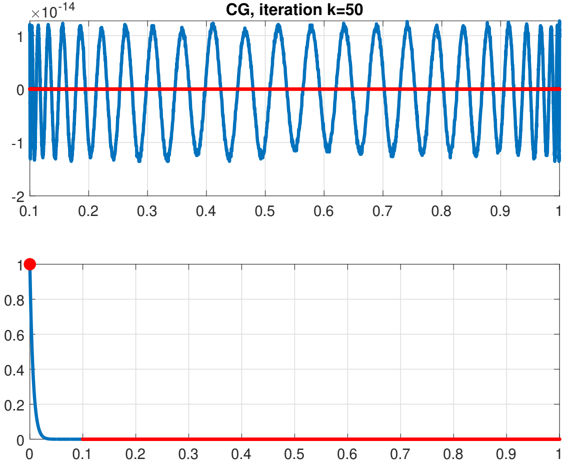

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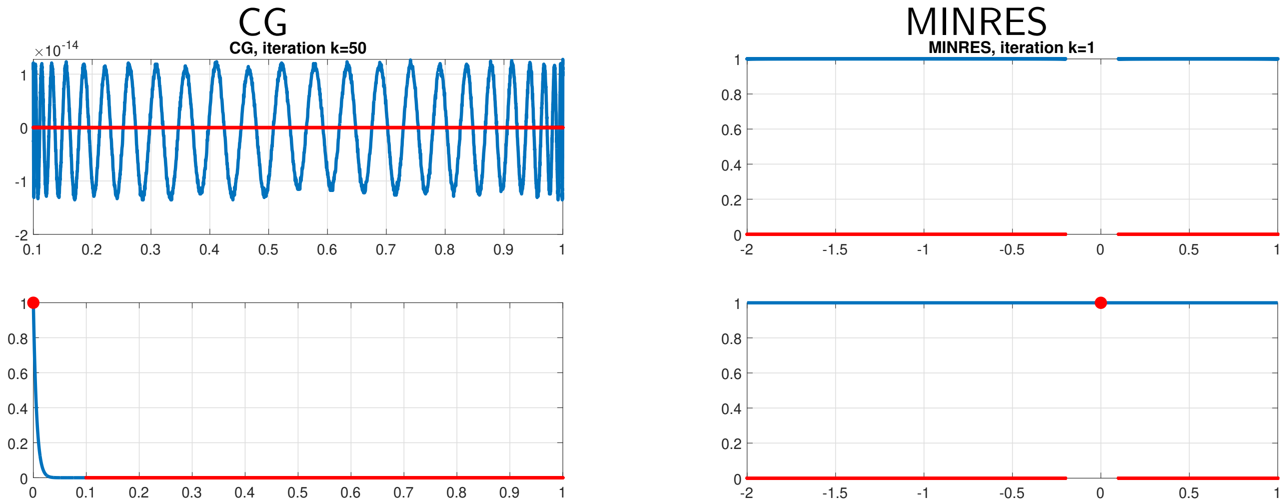

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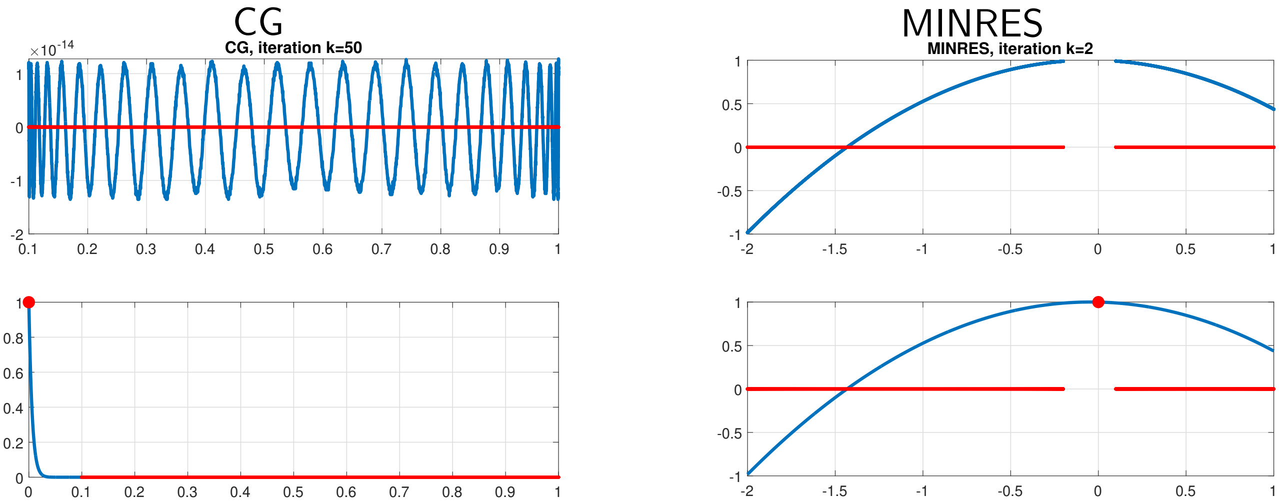

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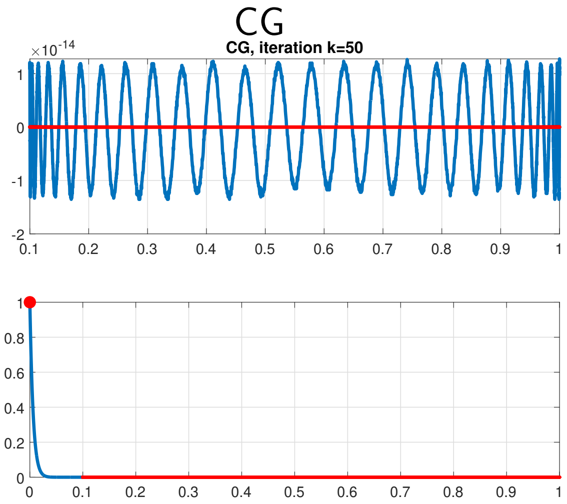

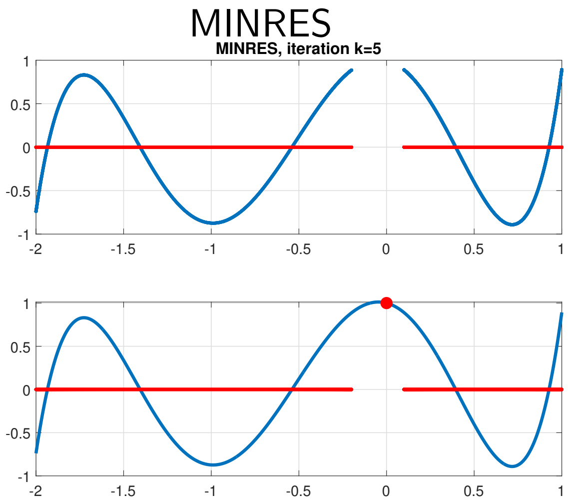

CG and MINRES, optimal polynomials

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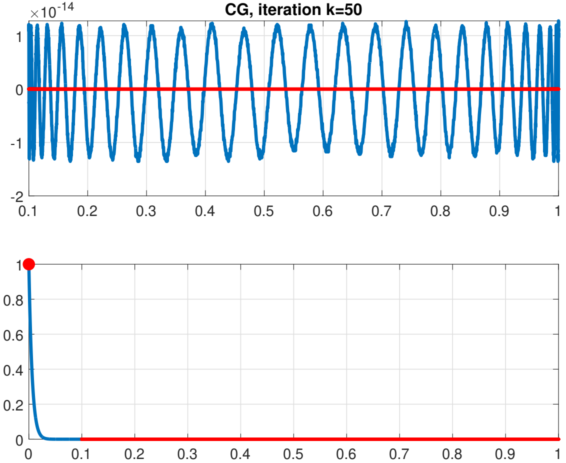
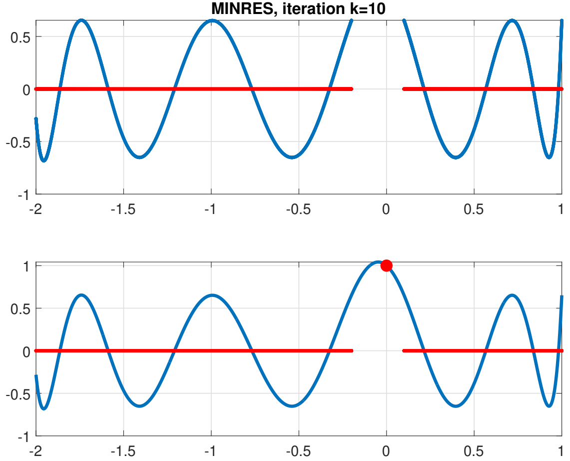
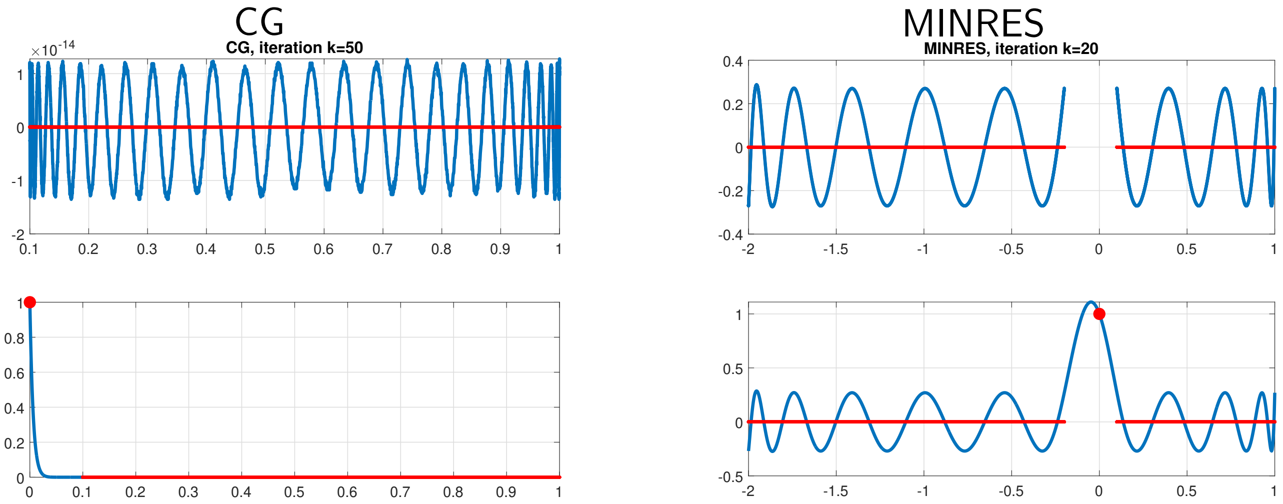


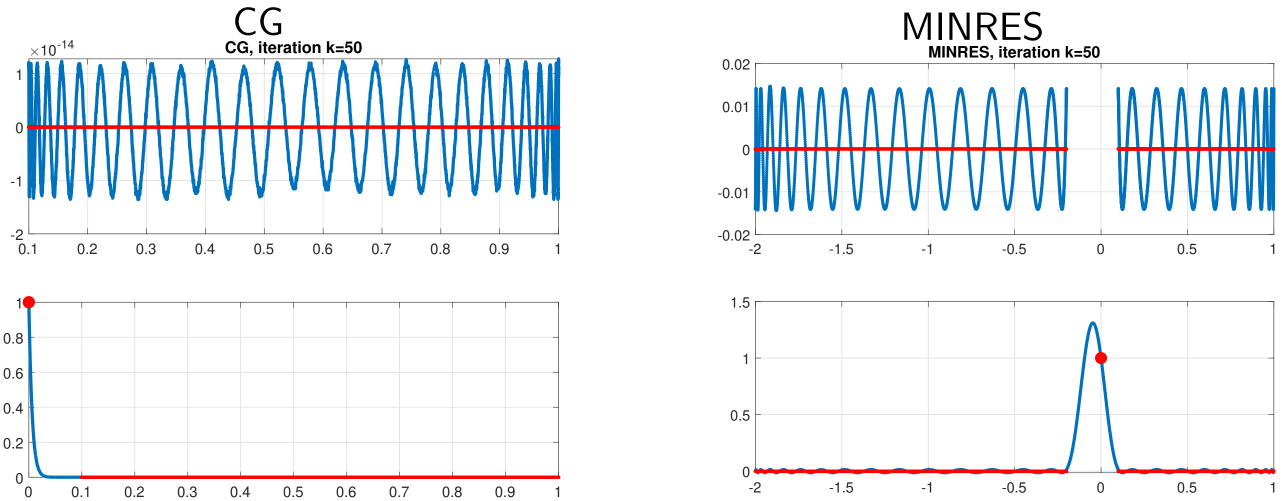
MINRES



CG and MINRES, optimal polynomials



CG and MINRES, optimal polynomials



- CG employs Chebyshev polynomials
- MINRES is more complicated+slower convergence

Preconditioned CG/MINRES

$$Ax = b, \quad A \succ 0$$

Find preconditioner M s.t. "$M^T M \approx A^{-1}$" and solve

$$M^T A M y = M^T b, \quad My = x$$

As before, desiderata of M:

- $M^T A M$ simple to apply
- $M^T A M$ has clustered eigenvalues

Note that reducing $\kappa_2(M^T A M)$ directly implies rapid convergence

- Possible to implement with just $M^T M$ (no need to find M)