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

CG: when $A \succ 0$ PD, solve $Q_k^T(AQ_k y - b) = T_k y - Q_k^T b = 0$, and $x = Q_k y$
→"Galerkin orthogonality": residual $Ax - b$ orthogonal to Q_k

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

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

CG: when $A \succ 0$ PD, solve $Q_k^T(AQ_k y - b) = T_k y - Q_k^T b = 0$, and $x = Q_k y$
→"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 $x_k = \text{argmin}_{x \in Q_k} \|x - x_*\|_A$ $(Ax_* = b)$:

$$
\begin{aligned}
(x - x_*)^T A(x - x_*) &= (Q_k y - x_*)^T A(Q_k y - x_*) \\
&= y^T (Q_k^T A Q_k) y - 2b^T Q_k y + b^T x_*,
\end{aligned}
$$

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

- 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)

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

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

$$
\begin{aligned}
\alpha_k &= \langle r_k, r_k \rangle / \langle p_k, Ap_k \rangle \\
x_{k+1} &= x_k + \alpha_k p_k \\
r_{k+1} &= r_k - \alpha_k A p_k \\
\beta_k &= \langle r_{k+1}, r_{k+1} \rangle / \langle r_k, r_k \rangle \\
p_{k+1} &= r_{k+1} + \beta_k p_k
\end{aligned}
$$

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 $\text{span}(p_0, p_1, \ldots, p_{k-1})$)
- $r_j^T r_k = 0$, $j = 0, 1, 2, \ldots, k-1$

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

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

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

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

Now

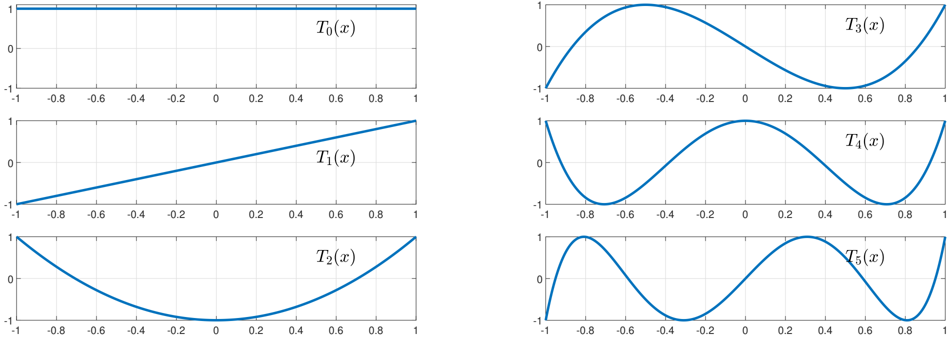
$$\min_{p \in \mathcal{P}_k, p(0)=1} \max_{x \in [\lambda_{\min}(A), \lambda_{\max}(A)]} |p(x)| \leq 2 \left(\frac{\sqrt{\kappa_2(A)} - 1}{\sqrt{\kappa_2(A)} + 1} \right)^k$$

- 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:

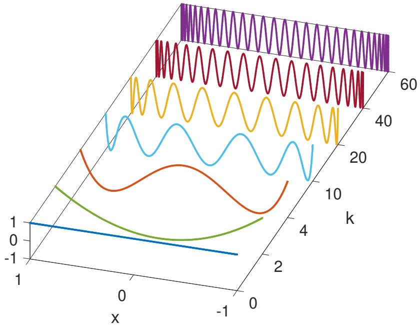
$$\frac{1}{2}(z+z^{-1})(z^k+z^{-k}) = \frac{1}{2}(z^{k+1}+z^{-(k+1)})+\frac{1}{2}(z^{k-1}+z^{-(k-1)}) \Leftrightarrow \underbrace{2xT_k(x) = T_{k+1}(x) + T_{k-1}(x)}_{\text{3-term recurrence}}$$

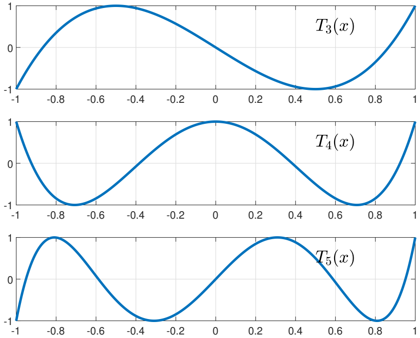


Chebyshev polynomials

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:

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

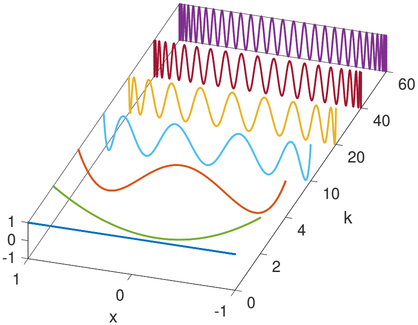


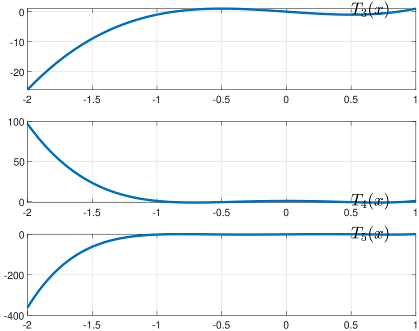


Chebyshev polynomials

For $z = \exp(i\theta)$, $x = \frac{1}{2}(z + z^{-1}) = \cos\theta \in [-1, 1]$, $\theta =$ acos(x),
$T_k(x) = \frac{1}{2}(z^k + z^{-k}) = \cos(k\theta)$. $T_k(x)$ is a polynomial in x:

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





Chebyshev polynomials cont'd

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

- Inside $[-1, 1]$, $|T_k(x)| \leq 1$
- 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

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

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

MINRES: symmetric (indefinite) version of GMRES

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

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

(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

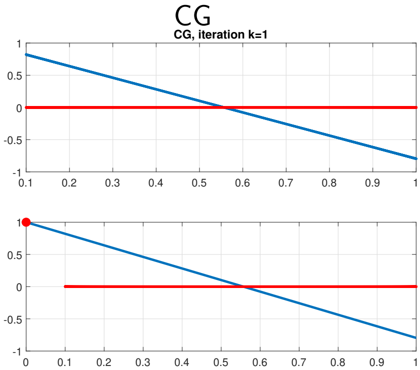
$$\frac{\|Ax-b\|_2}{\|b\|_2} \leq \min_{p \in \mathcal{P}_k, p(0)=1} \max |p(\lambda_i)|$$

One can prove (nonexaminable)

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

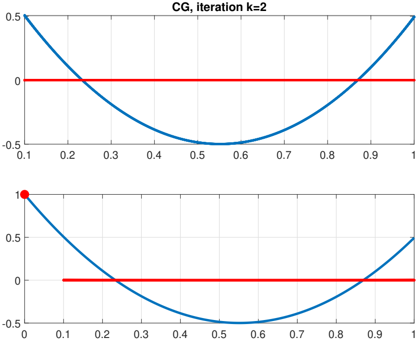
- obtained by Chebyshev+Möbius change of variables [Greenbaum's book 97]
- minimisation needed on positive **and** negative sides, hence slower convergence when A indefinite

CG and MINRES, optimal polynomials



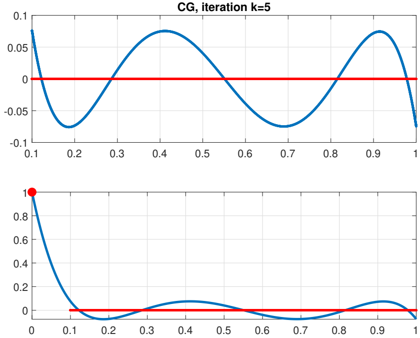
CG and MINRES, optimal polynomials

CG

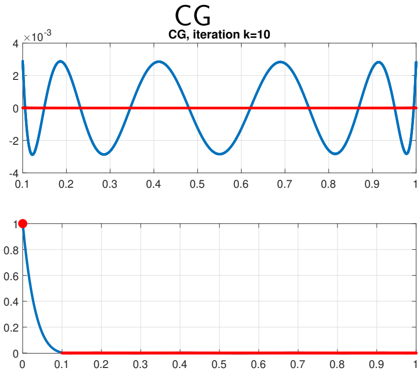


CG and MINRES, optimal polynomials

CG

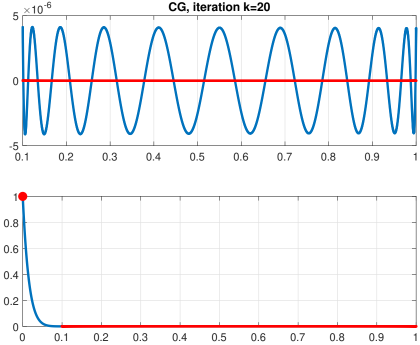


CG and MINRES, optimal polynomials

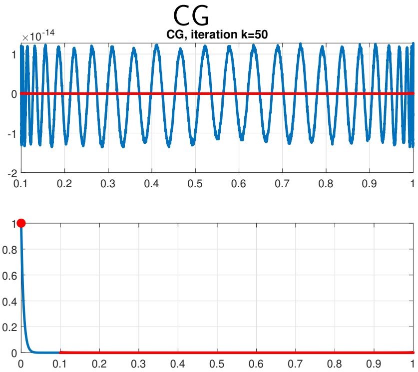


CG and MINRES, optimal polynomials

CG

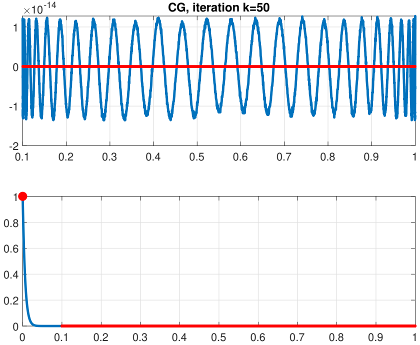


CG and MINRES, optimal polynomials

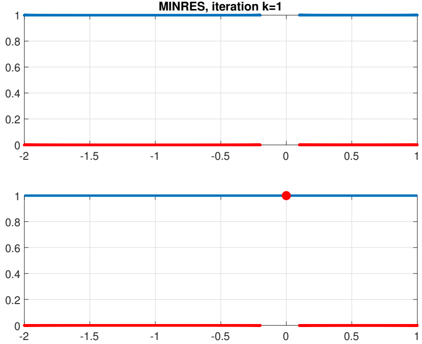


CG and MINRES, optimal polynomials

CG

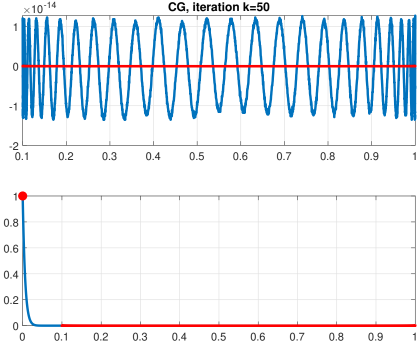


MINRES

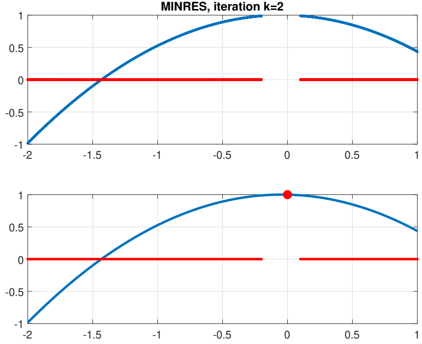


CG and MINRES, optimal polynomials

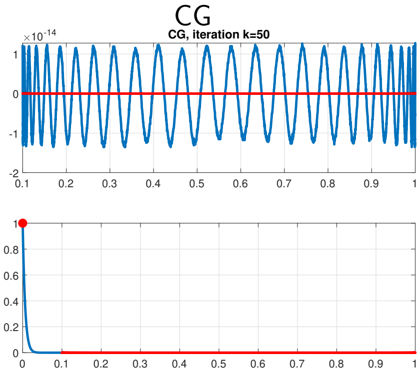
CG

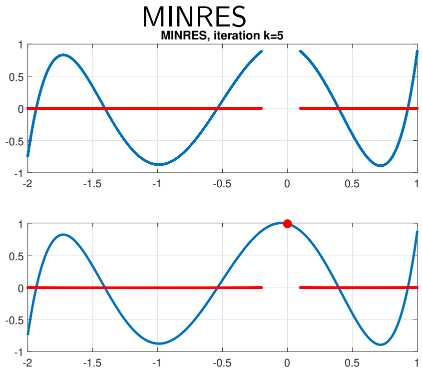


MINRES

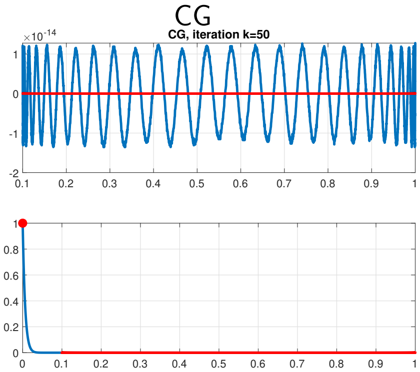


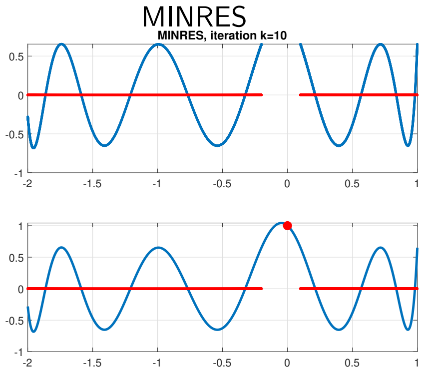
CG and MINRES, optimal polynomials



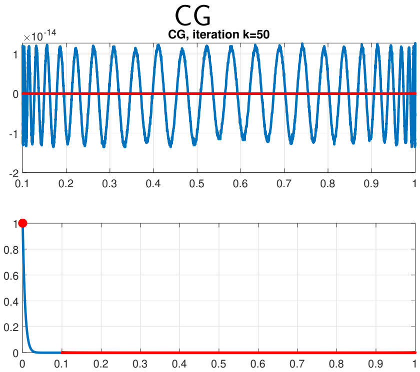


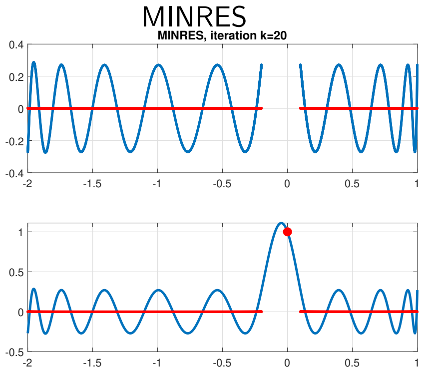
CG and MINRES, optimal polynomials



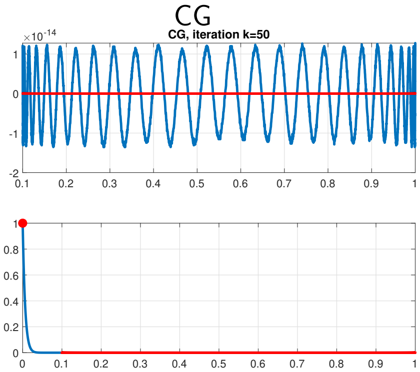


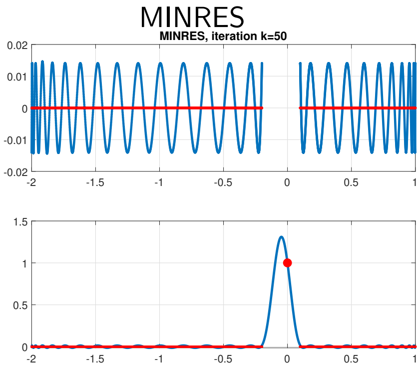
CG and MINRES, optimal polynomials





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)