Iterative methods for symmetric positive matrices

Solving the linear system $Ax = b$ is the same as minimizing the function

$$\phi(x) = \frac{1}{2} x^T A x - x^T b; \qquad \nabla\phi(x) = Ax - b.$$

All iterative methods are of the form $x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$. The optimum α on the line $x^{(k)} + \alpha p^{(k)}$, for a given $p^{(k)}$, is given by

$$\alpha_k = \frac{p^{(k)T} r^{(k)}}{p^{(k)T} A\, p^{(k)}}, \quad r^{(k)} = b - Ax^{(k)}, \quad x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

The $p^{(k)}$ direction satisfies $p^{(k)T} r^{(k+1)} = 0$. Choosing $p^{(k)}$ fixes the method.

Gradient method: $p^{(k)} = r^{(k)} = -\nabla\phi(x^{(k)})$. Converges for any $x^{(0)}$ and

$$\|e^{(k+1)}\|_A \leq \frac{K_2(A) - 1}{K_2(A) + 1} \|e^{(k)}\|_A, \quad e^{(k)} = x^{(k)} - x, \quad \|x\|_A = \left(x^T A\, x\right)^{1/2}.$$

Convergence is very slow for $K_2(A) \gg 1$.

If $p^{(k)} = 0$ then $x^{(k)}$ is the exact solution.

Conjugate gradient method

We say $x^{(k+1)}$ is optimal with respect to a direction p if

$$\phi(x^{(k+1)}) \leq \phi(x^{(k+1)} + \lambda p),\ \forall \lambda \qquad \Leftrightarrow \qquad p^T r^{(k+1)} = 0.$$

The conjugate gradient method is optimal with respect all previous directions:

$$p^{(j)T} r^{(k+1)} = 0, \quad j = 0, 1, \ldots, k$$

The directions are chosen as

$$p^{(k+1)} = r^{(k+1)} - \beta_k p^{(k)}, \quad \beta_k = \frac{p^{(k)T} A\, r^{(k+1)}}{p^{(k)T} A\, p^{(k)}}.$$

The method produces the **exact solution in at most n steps**, and

$$\|e^{(k)}\|_A \leq \frac{2c^k}{1 + c^{2k}} \|e^{(0)}\|_A, \quad c = \frac{\sqrt{K_2(A)} - 1}{\sqrt{K_2(A)} + 1}.$$

If $p^{(k)} = 0$ then $x^{(k)}$ is the exact solution.

Krylov methods

Given $A \in \mathbb{R}^{n \times n}$ and $v \in \mathbb{R}^n$ we define the m-dimensional Krylov subspace

$$\mathcal{K}_m(A, v) = \langle v, Av, \ldots, A^{m-1}v \rangle.$$

An orthonormal basis of $\mathcal{K}_m(A, v)$ can be found by the Gram-Schmidt method:

$$v_1 = \frac{v}{\|v\|_2}, \; w_k = Av_k - \sum_{i=1}^{k} h_{ik} v_i, \; v_{k+1} = \frac{w_k}{\|w_k\|_2}, \; k = 1 : m$$

where $h_{ik} = v_i^T A v_k$, $i = 1 : k$, $h_{k+1,k} = \|w_k\|_2$. The method can be written

$$V_k = [v_1 | \ldots | v_k], \quad AV_m = V_{m+1}\hat{H}_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T \,.$$

As $V_k^T V_k = I_k$, $V_{m+1}^T A V_m = \hat{H}_m$ and $V_m^T A V_m = H_m$. $H_m \in \mathbb{R}^{m \times m}$ and $\hat{H}_m \in \mathbb{R}^{(m+1) \times m}$ are upper Hessenberg matrices with elements h_{ij}, $i \leq j + 1$ or zero.

Instead of solving $Ax = b$ in $\mathbb{R}^n$, we put $x^{(m)} - x^{(0)} \in \mathcal{K}_m(A, r^{(0)})$, where $r^{(0)} = b - Ax^{(0)}$ is the initial residual. $x^{(m)} = x^{(0)} + V_m z^{(m)}$, and we look for the iterates $z^{(m)} \in \mathbb{R}^m$, $m = 1, 2, 3, \ldots$

Strategies for finding $z^{(m)}$: FOM and GMRES

FOM – Full Orthogonalization Method

$z^{(m)}$ is fixed by the condition $r^{(m)} \perp \mathcal{K}_m(A, r^{(0)})$. In terms of $z^{(m)}$,

$$H_m z^{(m)} = \|r^{(0)}\|_2 e_1 ,$$

that can be solved by a QR decomposition of H_m.

GMRES – Generalized Minimum RESidual

In this method, $z^{(m)}$ is fixed by the condition $\min \|r^{(m)}\|_2$. In terms of $z^{(m)}$,

$$\min_{z^{(m)}} \|r^{(m)}\|_2 = \min_{z^{(m)}} \left\| \, \|r^{(0)}\|_2 e_1 - \hat{H}_m z^{(m)} \right\|_2 .$$

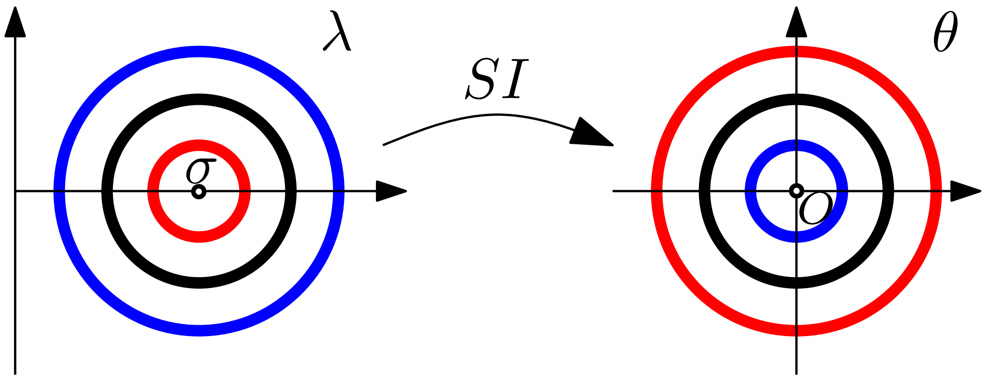
The QR decomposition of $\hat{H}_m = Q_m \tilde{R}_m$, $Q_m \in \mathbb{R}^{(m+1)\times(m+1)}$, $\tilde{R}_m \in \mathbb{R}^{(m+1)\times m}$, reduces the problem to the solution of the linear system

$$R_m z^{(m)} = f_m, \quad \tilde{R}_m = \begin{bmatrix} R^m \\ 0 \end{bmatrix}, \quad \tilde{f}_m = \begin{bmatrix} f_m \\ (\tilde{f}_m)_{m+1} \end{bmatrix} = \|r^{(0)}\|_2 Q_m^T e_1 .$$

and $\|r^{(m)}\|_2 = |(\tilde{f}_m)_{m+1}|$.

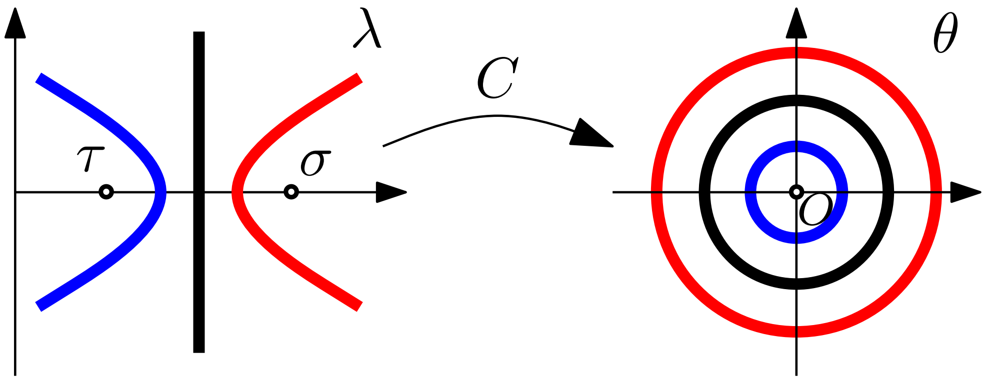
Generalized eigenvalue problem: transformations

$Ax = \lambda Bx \quad \Rightarrow \quad T(A, B)x = \theta x$



Shift-invert: $T_{SI} = (A - \sigma B)^{-1} B$

$$\lambda = \frac{1}{\theta} + \sigma, \quad \theta = \frac{1}{\lambda - \sigma}$$



Cayley: $T_C = (A - \sigma B)^{-1}(A - \tau B)$

$$\lambda = \frac{\tau - \sigma\theta}{1 - \theta}, \quad \theta = \frac{\lambda - \tau}{\lambda - \sigma}$$

Power method for $Tx = \theta x$ produces the eigenvalues with largest $|\theta|$. In the original problem $Ax = \lambda Bx$ we obtain the eigenvalues closest to σ.

Generalized eigenvalue problem: Krylov method

In order to solve $Tx = \theta x$, with $T = P^{-1}Q$, two embedded Krylov iterations are needed. The first Krylov space is

$$\mathcal{K}_m(T, v) = \langle v, Tv, \ldots, T^{m-1}v \rangle.$$

Given $v_k = T^k v$, in order to obtain $v_{k+1} = Tv_k = P^{-1}Qv_k$ we need to solve the linear system $Pv_{k+1} = Qv_k$, in

$$\mathcal{K}_k(P, r) = \langle r, Pr, \ldots, P^{k-1}r \rangle.$$

We solve for eval and evec of T in $\mathcal{K}_m(T, v)$, increasing k to check convergence. If

$$TQ_m = Q_m H_m + w_m e_m^T, \quad \text{and} \quad H_m u = \theta u,$$

$$\text{then} \quad \tilde{u} = Q_m u \quad \text{satisfies} \quad T\tilde{u} \approx \theta \tilde{u}.$$

Theorem. If the eigenvalues of T satisfy

$$|\mu_1| \geq |\mu_2| \geq \ldots \geq |\mu_k| > |\mu_{k+1}| \geq \ldots$$

$$\text{then} \quad |\theta_i - \mu_i| = 0\left(\left|\frac{\mu_{k+1}}{\mu_k}\right| + \epsilon_i\right)^m, \quad \lim_{m\to\infty} \epsilon_i = 0\,.$$