Remark: minimization $\begin{cases} \text{if } \nabla f(x^*) = 0 \rightarrow \text{Newton (Hessian required)} \\ \text{descent method} \\ \text{trust region method} \end{cases}$

Gradient descent method

1. search direction $\vec{d}_n$ s.t. $\nabla f \cdot d < 0$

   eg. $d_n := -\nabla f$ (steepest)

2. step length λ_n s.t. $f(x_n + \lambda_n d_n) < f(x_n)$

   eg. $\lambda := \arg\min_t f(x_n + t \cdot d_n)$

Grad. desc. for $f \in P^2(\mathbb{R}^d)$ $\quad f(x) = \gamma + c^T x + \frac{1}{2} x^T Q x$, $\quad Q$.. SPD

$$\Rightarrow \lambda = \arg\min_t f(x + td) = - \frac{f(x) \cdot d_n}{d^T Q d}$$

$$x_{n+1} = x_n + \lambda_n d_n$$

Lemma (conditioning) $\quad f(x_{n+1}) - f(x_*) \leq \left(\frac{K-1}{K+1}\right)^2 \cdot \left[f(x_n) - f(x^*)\right]$

$K := \frac{\lambda_{max}}{\lambda_{min}}$ ... cond. (Q)

No proof.

Mitigate by choosing $d := -H \nabla f \Rightarrow f(x_{n+1}) - f(x^*) \leq \frac{\lambda_{max}(H^{-1}Q) - \lambda_{min}}{\lambda_{max} + \lambda_{min}} \cdot \Delta f$

$\Rightarrow$ if $H = Q$: convergence in 1 step!

(equivalent to Newton method for ∇f)

Trust region method: realize, that quadratic approx of f is only accurate close to x^*.

One tries to minimize $q_k(x)$ under constraint $\|x_{n+1} - x_n\| \leq \Delta k$

(q_k.. quadratic model of f)

model is good? check: $\rho_k := \frac{\Delta f}{\Delta q}$ $\quad$ (good: $\rho_k \approx 1$)

7) Eigenvalue problems

find eval and evec of $A \in \mathbb{R}^{n \times n}$

Power method

1. init guess $\vec{x}_0$
2. $\vec{x}_0 := \frac{x_0}{\|x_0\|}$, $\quad \tilde{\lambda}_0 := x_0^H A x_0$
3. $x_{\ell+1} := \frac{A x_\ell}{\|A x_\ell\|}$, $\quad \tilde{\lambda}_{\ell+1} := x_{\ell+1}^H A x_{\ell+1}$

Does not converge if $\lambda_1 \neq \lambda_2$ but $|\lambda_1| = |\lambda_2|$, slow conv if $\lambda_1 \approx \lambda_2$

Theorem (conv. of power meth. to eval)

$$\begin{cases} A \text{ ... diagonalizable} \\ |\lambda_1| > |\lambda_2| \geq \dots \geq \\ x_0 \text{ has component } \neq 0 \text{ in direct. of } \vec{v}_1 \end{cases}$$

$\Rightarrow$ x_ℓ is well defined and $|\tilde{\lambda}_\ell - \lambda_1| \leq C \cdot \left|\frac{\lambda_2}{\lambda_1}\right|^\ell$

Proof: $x_0 = \sum \alpha_i \vec{v}_i \Rightarrow A^\ell x_0 = \sum \alpha_i \lambda_i^\ell v_i$

$$\Rightarrow x_\ell = c_\ell \alpha_1 \lambda_1^\ell \cdot \Big[v_1 + \underbrace{\sum \frac{\alpha_i}{\alpha_1} \left(\frac{\lambda_i}{\lambda_1}\right)^\ell v_i}_{=: \varepsilon_\ell} \Big] \quad , \quad c_\ell := \frac{1}{\|A^\ell x_0\|}$$

$$\varepsilon_\ell \leq C \left|\frac{\lambda_2}{\lambda_1}\right|^\ell \Rightarrow \tilde{\lambda}_\ell = x_\ell^H A x_\ell = \dots = \lambda_1 + \mathcal{O}(\|\varepsilon\|) \qquad \blacksquare$$

Def $S := \operatorname{span}\{x\}$, $T := \operatorname{span}\{y\}$: distance $d(S,T) := |\sin\varphi|$

with $\cos\varphi := \frac{x \cdot y}{\|x\| \|y\|}$

$$\Rightarrow \begin{cases} x \parallel y \Leftrightarrow d = 0 \\ x \perp y \Leftrightarrow d = 1 \end{cases}$$

Theorem (conv. of pow. meth. to evec) $d(\operatorname{span} v_1, \operatorname{span} x_\ell) \leq \left(\frac{\lambda_2}{\lambda_1}\right)^\ell \cdot C$

Proof: $\operatorname{span}\{x_\ell\} = \operatorname{span}\{v_1 + \varepsilon_\ell\} \Rightarrow d(\dots) \leq C \cdot \left(\frac{\lambda_2}{\lambda_1}\right)^\ell$ $\blacksquare$

Inverse Iteration

$$\begin{cases} 1. \text{ init guess } x_0 \\ 2. \text{ solve } A x_{\ell+1} = x_\ell \\ 3. \; x_{\ell+1} := \frac{x_{\ell+1}}{\|x_{\ell+1}\|} \quad , \quad \lambda_{\ell+1} = \dots \end{cases}$$

converges to largest value of $\frac{1}{|\lambda|}$

Inverse with shift

1. init guess
2. solve $(A - \lambda) x_{\ell+1} = x_\ell$
3. normalize x, find $\lambda_{\ell+1}$

converges to eval closest to shift parameter λ

faster conv, if λ is close to an eval $\rightsquigarrow$ use the new $\lambda_{\ell+1}$ as shift parameter

Rayleigh quotient iteration

$$\begin{cases} 1. \text{ init guess} \\ 2. \; \lambda_\ell := x_\ell^H A x_\ell \\ 3. \text{ solve } (A - \lambda_\ell) x_{\ell+1} = x_\ell \text{ , normalize } x \end{cases}$$

Theorem. Rayleigh quot. iter converg.

$$d(\operatorname{span} x, \operatorname{span} v) \leq C \varepsilon^3$$

$$\left| \frac{x_0^H A x_0}{\|x_0\|^2} - \lambda \right| \leq C \varepsilon^2$$

No proof

(Error estimates & stopping crit.: we need Bauer-Fike)

Theorem (Bauer-Fike) relation of $\sigma(A)$ and $\sigma(A+\Delta A)$?

A .. diagonalizable : $A = TDT^{-1}$

$$\forall \mu \in \sigma(A+\Delta A) \Rightarrow \min_i |\mu - \lambda_i| \leq \operatorname{cond}(T) \|\Delta A\|$$

Proof: ~~assume~~ wlog : $\mu \in \sigma(A+\Delta A) \setminus \sigma(A)$ ... usw. ∎

Remark: 1. $\operatorname{cond}(T)$ large if evecs of A close to lin dependent

2. A self adjoint $\Rightarrow A = Q^H D Q$ with Q orthog. : $\operatorname{cond}(Q) = 1$

Now:

Stopping crit

$(\vec{x}, \lambda)$ ... eigenpair if $Ax - \tilde{\lambda} x = 0$

Hope: residual $Ax - \lambda x =: r$ is good measure for deviation from eigenpair

Theorem A .. diagon. : $A = TDT^{-1}$, $\|x\| = 1$

$\Rightarrow \begin{cases} 1. \ \min_\lambda |\lambda - \tilde{\lambda}| \leq \operatorname{cond}(T) \cdot \|r\| \\ 2. \ \text{if } \tilde{\lambda} = x^H A x, \ A \text{ self adj.}, \ \tilde{\lambda} \text{ close to eval of } A: \end{cases}$

$$\min_\lambda |\lambda - \tilde{\lambda}| \leq C \|r\|^2$$

Proof: 1. set $A + \Delta A := A - r x^H$ and use Bauer Feike ∎

2. Literature

We now want to find all evals! $\rightsquigarrow$ construct sequence of $A_e \rightarrow$ upper triangular

Instead of diagonal, we use Schur-Form

Theorem (Schur-representation) $A \in \mathbb{C}^{n \times n}$, Q orthogonal $\exists R$ upper triangle st.

$$A = Q R Q^H$$

Proof: for $n=1$ trivial, $A\vec{v} = \lambda \vec{v}$

Let $V' \in \mathbb{C}^{n \times n-1}$ s.t $V := (\vec{v}, V')$ is unitary

(Now because $A\vec{v} = \lambda \vec{v} \Rightarrow V^H A \vec{v} = V^H \lambda \vec{v} = \begin{pmatrix} \vec{v}^H \\ V'^H \end{pmatrix} \lambda \vec{v} = \begin{pmatrix} \lambda \\ 0 \end{pmatrix}$)

$$\Rightarrow V^H A V = \begin{pmatrix} \lambda & w^T \\ 0 & C \end{pmatrix}$$

By induction, C can also be written in upper triangl. form ∎

Jacobi method

Find upper tri. matrix by Givens rotations

(only symmetric A considered here)

$$A := G(i,j,\theta)^T A\, G(i,j,\theta)$$

choose i,j,θ st. A is diagonalized

off-diag entries

Lemma $B := G^T A G$ st. $B_{ij} = B_{ji} = 0 \Rightarrow \text{off}(B)^2 = \text{off}(A) - 2A_{ij}^2$

Proof: $\text{off}(B)^2 = \|B\|_F^2 - \sum_k |B_{kk}|^2 = \|A\|^2 - \sum_{k \in \{i,j\}} |B_{kk}|^2 - |B_{ii}|^2 - |B_{jj}|^2$

$$= \dots \overset{\text{Bauer-Fike}}{\overset{!}{=}} \text{off}(A)^2 - 2|A_{ij}|^2$$

$\rightsquigarrow$ should choose (i,j) st. $|A_{ij}|$ is as large as possible. Then:

Lemma $$\text{off}(A)^2 \le \overbrace{\frac{n(n-1)}{2}}^{=:N} \cdot 2A_{ij}^2 = n(n-1)A_{ij}^2$$

and $\Rightarrow \text{off}(B)^2 = \text{off}(A)^2 - 2|A_{ij}|^2 \le \left(1 - \frac{1}{N}\right) \text{off}(A)^2$

Converg: linear, but faster for A close to diagonal!
Jacobi touches less entries of A than QR

Orthog. iteration

recall: power iter generates sequence $\{A^l \operatorname{span} \vec{x}_0\}$ to eigenspace of largest eval

idea: sequence $(A^l X_0)$ of k-dim space to k-dominant evals
instead of normalizing $\vec{x}_0$, make $A^l X_0$ orthonormal basis

1. init $X_0 = Q_0 R_0$, Q_0 orthog., R upper tri.
2. $X_{l+1} := A Q_l$
3. $Q_{l+1} R_{l+1} := X_{l+1}$ (QR-fact.)

Remark: without QR-fact, one gets only 1 eval

Theorem (conv.) the k evals $\{\tilde{\lambda}_{i,l}\}_{i=1,\dots,k}$ of $Q_l^H A Q_l$ satisfy

$$\min_{\lambda \in \sigma(A)} |\tilde{\lambda}_{i,l} - \lambda| \le C \cdot \underbrace{\left|\frac{\lambda_{k+1}}{\lambda_k}\right|}_{<1}^{l}$$

No proof.

QR-Algorithm (viewed as orth. iter)

1. $X_0 := \mathbb{I} \in \mathbb{R}^{n\times n}$ and $X_0 := Q_0 R_0$
2. $X_{l+1} := A Q_l$
3. $Q_{l+1} R_{l+1} := X_{l+1}$ (QR-fact.)

it performs n orth. iter simultaneously

QR-Algo (basic form)

$$\begin{cases} 1.\ A_0 := A \\ 2.\ A_\ell =: Q_\ell R_\ell \quad \text{(QR-decomp.)} \\ 3.\ A_{\ell+1} := R_\ell Q_\ell \quad (\rightarrow \text{conv to upper tri. form}) \end{cases}$$

efficiency:
$\mathcal{O}(n^3)$ for each ℓ
so $\mathcal{O}(n^4)$ in total $\rightarrow$ combine w. shift parameter to make more efficient

QR-Algo (Hessenberg form)
(A)

if A has Hessenb. form
$\Rightarrow$ cost of QR: $\mathcal{O}(n^2)$
$\Rightarrow$ cost of multiplication with RQ: $\mathcal{O}(n^2)$

QR-Algo (Deflation)
(B)

if $A = \begin{pmatrix} x & x & \cdots & & x \\ x & & & & \vdots \\ & \ddots & & & x \\ 0 & 0 & \cdots & 0 & \mu \end{pmatrix}$, $x \neq 0$, μ .. eval(A)

now one can look for λ_i on the submatrix

QR-Algo (with shift)
(tries to accelerate Deflation)
(C)

$$\begin{cases} 1.\ \text{init } A_0 := A \\ 2.\ \text{choose } \mu^{(\ell)} \\ 3.\ A_\ell - \mu^{(\ell)} := Q \cdot R \\ 4.\ A_{\ell+1} := R \cdot Q + \mu^{(\ell)} \end{cases}$$

$\mu^{(\ell)}$ can be chosen as $A_\ell(n,n)$.

The QR-Algo does implicitly an invers iter. for a certain starting value.
A good choice for μ is therefore a Rayleigh-quotient $\rightsquigarrow A_\ell(n,n)$

QR-Algo (combining (A)(B)(C))

$$\begin{cases} 1.\ \text{make } A \text{ Hessenberg}, \quad \mu^{(\ell)} := A_\ell(n,n) \\ \left.\begin{array}{l} 2.\ A_\ell - \mu^{(\ell)} := Q \cdot R \\ 3.\ A_{\ell+1} = R \cdot Q + \mu \end{array}\right\} \text{until } A(n,n-1) \text{ is small} \\ 4.\ \text{recursion on sub matrix } A(1{:}n-1,\ 1{:}n-1) \end{cases}$$

8) Conjugate Gradient Method

iterative sol for $Ax^* = b$, A .. SPD
rule: dont compute A^{-1}, only use $x \mapsto A \cdot x$

Def.: $\begin{cases} (x,y)_A := x^T A y \\ K_\ell := \{r_0, Ar_0, \ldots A^{\ell-1} r_0\} \end{cases}$

$Ax^* = b \Leftrightarrow Ae_0 = r_0$

goal: approx x^* by $x_\ell = x_0 + e_\ell$

$\Rightarrow$ find $x_\ell \in x_0 + K_\ell$ st. $\|x^* - x_\ell\|_A \leq \|x^* - x\|_A \quad \forall x$