The Secular Equation

My First Encounter with

Prof. Gene H. Golub (1932 – 2007)

Walter Gander, ETH and HKBU

International Workshop on Matrix Computations
Gene Golub Memorial Day 2018

Hangzhou

April 20 – 24, 2018

Least Squares with Rank Deficient Matrix

- Consider the least squares problem
  $\|A\mathbf{x} - \mathbf{b}\|^2 = \min$ with $A \in \mathbb{R}^{m \times n}$, $m > n$, $\mathrm{rank}(A) = r < n$.
- Many solutions, want minimal norm solution $\mathbf{x}_{\mathsf{min}}$
- Today $\mathbf{x}_{\mathsf{min}}$ is computed most conveniently by the SVD
  - decompose $A = U\Sigma V^\top$ with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$
  - determine rank r, $\sigma_r \neq 0, \quad \sigma_k = 0,\ k = r+1, \ldots, n$
  - form $U_r := U(:, 1:r)$, $V_r := V(:, 1:r)$, $\Sigma_r := \Sigma(1:r, 1:r)$
- $\implies \mathbf{x}_{\mathsf{min}} = V_r \Sigma_r^{-1} U_r^\top \mathbf{b}$

Solution without using SVD ?

- Use extrapolation! Don't need to know the rank.
  I presented this idea 1974 in a talk in the Numerical Analysis Colloquium at ETH.

- Choose $\varepsilon > 0$ and consider

$$\begin{pmatrix} A \\ \varepsilon I \end{pmatrix} \mathbf{x}(\varepsilon) \approx \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix}$$

- Matrix has now full rank, can show

$$\mathbf{x}(\varepsilon) = (A^\top A + \varepsilon^2 I)^{-1} A^\top \mathbf{b} = \mathbf{x}_{\mathsf{min}} + \mathbf{c}_1 \varepsilon^2 + \mathbf{c}_2 \varepsilon^4 + \cdots$$

  Using $\varepsilon_{k+1} = \varepsilon_k / 2$ and Romberg-extrapolation we get $\lim_{\varepsilon \to 0} \mathbf{x}(\varepsilon) = \mathbf{x}_{\mathsf{min}}$.

- Can speed up computing of $\mathbf{x}(\varepsilon_k)$ by first computing $A = QR$ or by bidiagonalization.

Example: $A \in \mathbb{R}^{40\times 8}$, $\text{rank}(A) = 3$

SolByExtra

```
m=40; A=magic(m); n=m/5; A=A(:,1:n); b=A*rand(n,1);
```

Solutions :

Matlab $A\backslash\mathbf{b}$	Using SVD	Extrapolation
Warning: Rank deficient	with rank $r = 3$	4 iterations
1.846673326583244	0.457727535991772	0.457727535991773
2.459131966980111	0.747175086297768	0.747175086297764
0	0.694218248476673	0.694218248476673
0	0.616598049455061	0.616598049455064
0	0.669554887276158	0.669554887276158
0	0.535347735013380	0.535347735013383
0	0.482390897192287	0.482390897192288
0.725632546879197	0.828425400739452	0.828425400739448

Norm of solutions:

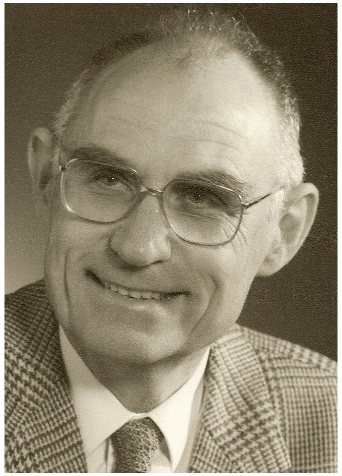
3.159758693196030	1.812127976894189	1.812127976894188

Norm of residuals:

1.0e-10 *		
0.055694948577711	0.136651389778460	0.064150008164078

My Way to Stanford

- In the audience of my 1974-talk were



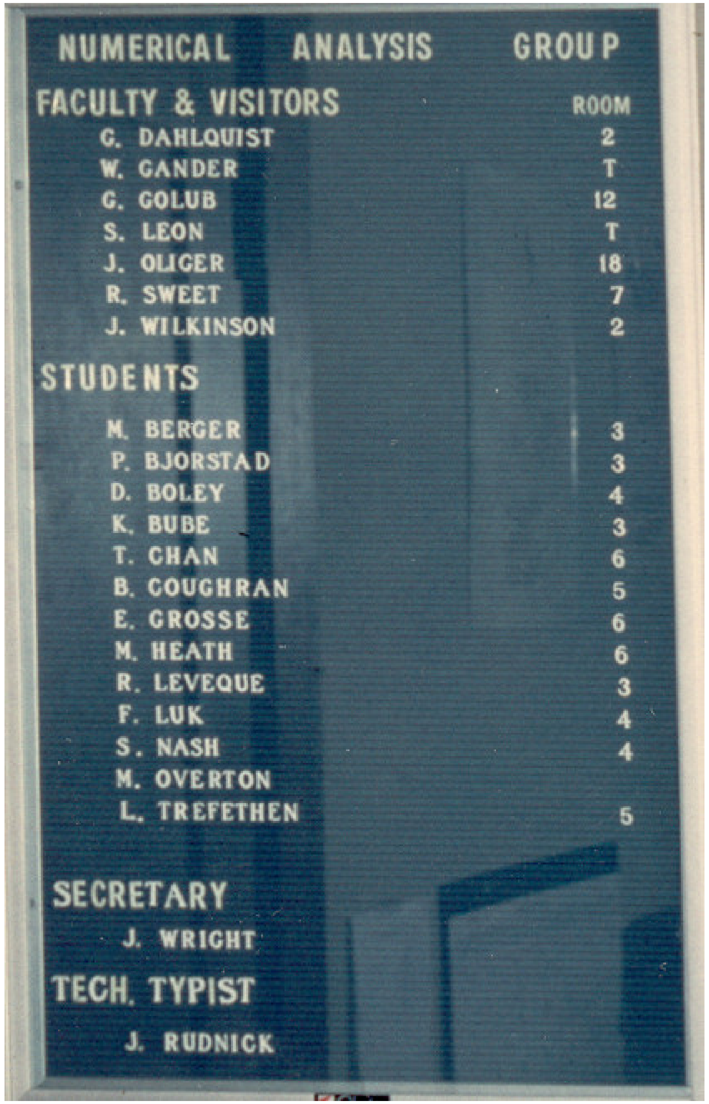
Peter Henrici
1923 – 1987

Rudolf Kalman
1930 – 2016

- Kalman gave me one of his papers containing a proof (using only the Penrose Equations) that the pseudo-inverse is unique.
- Henrici encouraged me to apply for a NSF grant to continue the research with the "master of least squares algorithms": Gene Golub.

The Golden Year 1977-1978

- Research proposal accepted by the Swiss NSF, got a grant.
- We spent a year at Stanford University. I worked as postdoc in Serra House in the numerical analysis group of Prof. Gene H. Golub.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L. TREFETHEN 5
SECRETARY
J. WRIGHT
TECH. TYPIST
J. RUDNICK

Gene gave me one of his papers:

J. Soc. Indust. Appl. Math.
Vol. 13, No. 4, December, 1965
Printed in U.S.A.

ON THE STATIONARY VALUES OF A SECOND-DEGREE POLYNOMIAL ON THE UNIT SPHERE*

GEORGE E. FORSYTHE AND GENE H. GOLUB†

1. The problem. Let A be a Hermitian square matrix of complex elements and order n. Let b be a known n-vector of complex numbers. For each complex n-vector x, the nonhomogeneous quadratic expression

$$\Phi(x) = (x - b)^H A(x - b) \tag{1.1}$$

(H denotes complex conjugate transpose) is a real number. C. R. Rao of the Indian Statistical Institute, Calcutta, suggested to us the problem of maximizing (or minimizing) $\Phi(x)$ for complex x on the unit sphere $S = \{x: x^H x = 1\}$. Since Φ is a continuous function on the compact set S, such maxima and minima always exist. We here extend the problem to include finding all stationary values of Φ.

In summary, our problem is:

(1.2) find all x which make $\Phi(x)$ stationary for $x^H x = 1$.

Quotes from Paper

- No consideration to a practical computer algorithm is given here.
- As an abstraction from optimal control theory, Balakrishnan [1] studies the minimization of $\|C\mathbf{y} - \mathbf{f}\|^2$, subject to the quadratic inequality constraint $\mathbf{y}^\top \mathbf{y} \leq 1$ ...
- THEOREM. If $\mathbf{x}$ is any vector in S at which $\Phi(\mathbf{x})$ is stationary with respect to S, then there exists a real number $\lambda = \lambda(\mathbf{x})$ such that

$$\begin{aligned} (1.5) \qquad A(\mathbf{x} - \mathbf{b}) &= \lambda \mathbf{x} \\ (1.6) \qquad \mathbf{x}^H \mathbf{x} &= 1 \end{aligned}$$

  Conversely, if any real λ and vector $\mathbf{x}$ satisfy (1.5)–(1.6), then $\mathbf{x}$ renders $\Phi(\mathbf{x})$ stationary with respect to S.
- Then the requirement that $\mathbf{x}^H \mathbf{x} = \sum_{i=1}^{n} |x_i|^2 = 1$ is equivalent to the condition

$$(2.3) \qquad g(\lambda) = \sum_{i=1}^{n} \frac{\lambda_i |b_i|^2}{|\lambda_i - \lambda|^2} = 1$$

(2.3) is now called a secular equation!

Secular Equation – One of the Favorite Topics of Gene

- Conference on *Computational Methods with Applications*, August 19 - 25, 2007, Harrachov, Czech Republic [a].
- Gene's talk is available on-line:

Matrix Computations
and
the Secular Equation

Gene H. Golub

Stanford University

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[a] `http://www.cs.cas.cz/~harrachov`

One of the Many Examples in Gene's Talk

Constrained Eigenvalue Problem

$$A = A^T$$

$$\max_{\mathbf{x}\neq\mathbf{0}} \quad \mathbf{x}^T A\mathbf{x}$$

$$\text{s.t.} \quad \mathbf{x}^T\mathbf{x} = 1, \quad \mathbf{c}^T\mathbf{x} = 0$$

$$\phi(\mathbf{x};\lambda,\mu) = \mathbf{x}^T A\mathbf{x} - \lambda(\mathbf{x}^T\mathbf{x} - 1) + 2\mu\mathbf{x}^T\mathbf{c}$$

$$\text{grad } \phi = 0 \implies A\mathbf{x} - \lambda\mathbf{x} + \mu\mathbf{c} = \mathbf{0}$$

$$\mathbf{x} = -\mu(A - \lambda I)^{-1}\mathbf{c}$$

$$\mathbf{c}^T\mathbf{x} = 0 \implies \mathbf{c}^T(A - \lambda I)^{-1}\mathbf{c} = 0$$

Constrained Eigenvalue Secular Equation

$$A = Q\Lambda Q^T, \mathbf{d} = Q^T\mathbf{c}$$

$$\sum_{i=1}^{n} \frac{d_i^2}{(\lambda_i - \lambda)} = 0$$

Least Squares with Quadratic Constraint

- 1977 Gene Golub suggested to me to work on this problem [a]

$$\|A\mathbf{x}-\mathbf{b}\|^2 = \min \text{ s.t. } \|C\mathbf{x}-\mathbf{d}\|^2 = \delta^2.$$

- Lagrange function: $L(\mathbf{x},\lambda) = \|A\mathbf{x}-\mathbf{b}\|^2 + \lambda\left(\|C\mathbf{x}-\mathbf{d}\|^2 - \delta^2\right)$
- The solution is a stationary points of $L \iff$ a solution of $\partial L/\partial \mathbf{x} = 0$ and $\partial L/\partial \lambda = 0$

$$\left.\begin{array}{lrcl} (1) & \left(A^\top A + \lambda C^\top C\right)\mathbf{x} & = & A^\top \mathbf{b} + \lambda C^\top \mathbf{d} \\ (2) & \|C\mathbf{x}-\mathbf{d}\|^2 & = & \delta^2 \end{array}\right\} \quad \text{“Normal Equations”}.$$

- Solving (1) for $\mathbf{x}(\lambda)$, inserting in (2) we get $f(\lambda) = \|C\mathbf{x}(\lambda)-\mathbf{d}\|^2$ and the secular equation

$$f(\lambda) = \delta^2$$

[a] He also encouraged Lars Eldén to work on the same as I found out later!

Secular Equation Represented by BSVD

- BSVD (generalized SVD, also GSVD) for pair of matrices $A^{m\times n}$, $C^{p\times n}$:

$$U^\top AX = D_A = \mathrm{diag}(\alpha_1,\dots,\alpha_n),\ \alpha_i \geq 0$$
$$V^\top CX = D_C = \mathrm{diag}(\gamma_1,\dots,\gamma_q),\ \gamma_i \geq 0,\ q = \min(n,p)$$

where $U^{m\times m}$ and $V^{p\times p}$ orthogonal and $X^{n\times n}$ nonsingular.

- If $\gamma_1 \geq \dots \geq \gamma_r > \gamma_{r+1} = \dots = \gamma_q = 0$ then $\mu_i = \dfrac{\alpha_i^2}{\gamma_i^2}$, $i = 1,\dots,r$ are the eigenvalues of generalised EV-Problem

$$A^\top A\mathbf{x} = \mu C^\top C\mathbf{x}.$$

- With $\mathbf{c} := U^\top \mathbf{b}$ and $\mathbf{e} := V^\top \mathbf{d}$ the secular equation becomes

$$f(\lambda) = \sum_{1=1}^{r} \alpha_i^2 \left(\frac{\gamma_i c_i - \alpha_i e_i}{\alpha_i^2 + \lambda\gamma_i^2}\right)^2 + \sum_{i=r+1}^{p} e_i^2 = \delta^2$$

f has at most r poles for $\lambda = -\mu_i$ and $f(\lambda) = \delta^2$ at most $2r$ solutions

Characterization of the Solution

If $(\mathbf{x}_1, \lambda_1)$ and $(\mathbf{x}_2, \lambda_2)$ are solutions of the normal equations, then

Thm 1

$$\|A\mathbf{x}_2 - \mathbf{b}\|^2 - \|A\mathbf{x}_1 - \mathbf{b}\|^2 = \frac{\lambda_1 - \lambda_2}{2}\|C(\mathbf{x}_1 - \mathbf{x}_2)\|^2.$$

If $\lambda_1 > \lambda_2 \implies \|A\mathbf{x}_1 - \mathbf{b}\| < \|A\mathbf{x}_2 - \mathbf{b}\|$

$\implies$ the largest solution λ determines solution

Thm 2

$$-\frac{\lambda_1 + \lambda_2}{2}\|C(\mathbf{x}_1 - \mathbf{x}_2)\|^2 = \|A(\mathbf{x}_1 - \mathbf{x}_2)\|^2.$$

$\implies \lambda_1 + \lambda_2 < 0 \implies$ At most one $\lambda > 0$

Geometric Interpretation for $n = 2$

$$\|A\mathbf{x} - \mathbf{b}\|^2 = \min \text{ subject to } \|C\mathbf{x} - \mathbf{d}\|^2 = \delta^2$$

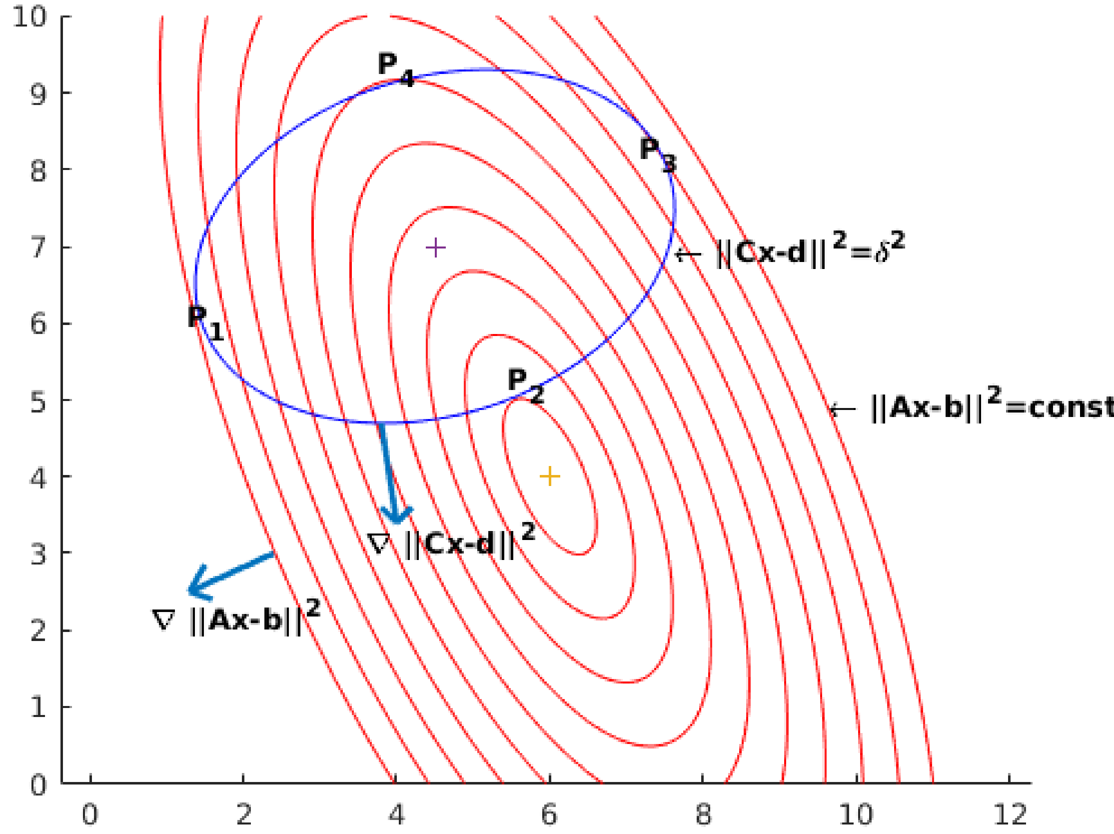
$$L(\mathbf{x}, \lambda) = \|A\mathbf{x} - \mathbf{b}\|^2 + \lambda \left(\|C\mathbf{x} - \mathbf{d}\|^2 - \delta^2\right)$$

$$\partial L / \partial \mathbf{x} = 0 \iff$$

$$\nabla \|A\mathbf{x} - \mathbf{b}\|^2 = -\lambda \nabla \|C\mathbf{x} - \mathbf{d}\|^2$$

Stationary points: gradients are parallel

- P_1, P_3, P_4: gradients have same directions: $\implies \lambda < 0$
- P_2: gradients have opposite directions: $\implies \lambda > 0$
- Solutions of the secular equation: 3 with $\lambda < 0$ and one (the minimum, the solution of the problem) with $\lambda > 0$.



Inequality Constraint

$\|A\mathbf{x} - \mathbf{b}\|^2 = \min$ subject to $\|C\mathbf{x} - \mathbf{d}\|^2 \leq \delta^2$

1. $M = \{\mathbf{x} \mid \|A\mathbf{x} - \mathbf{b}\| = \min\}$
2. If $\|C\mathbf{x}^* - \mathbf{d}\| \leq \delta$ for some $\mathbf{x}^* \in M$ then $\mathbf{x}^*$ is a solution.
   Constraint is not active.
3. If $\{\mathbf{x} \mid \|C\mathbf{x} - \mathbf{d}\| \leq \delta\} \cap M = \emptyset$ then
   constraint is active, solution on boundary: $\|C\mathbf{x} - \mathbf{d}\|^2 = \delta^2$
   (a) solve secular equation $f(\lambda) = \delta^2$ for the only $\lambda^* > 0$
   (b) $\mathbf{x}(\lambda^*)$ is the solution.

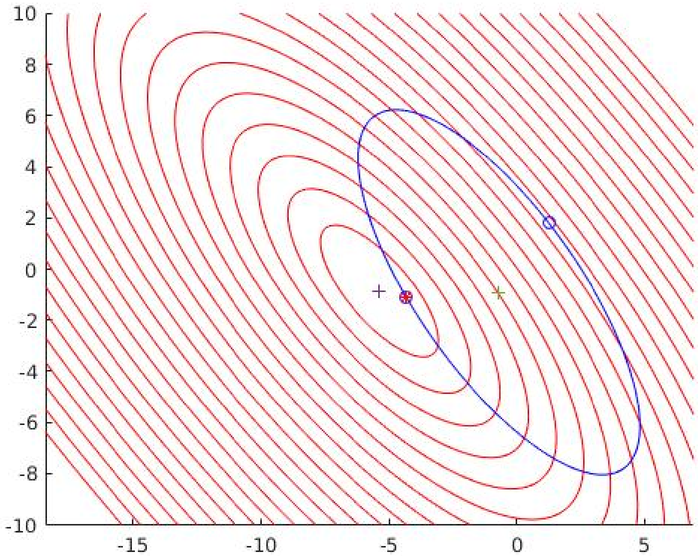
   One of the typical applications is from CHRISTIAN REINSCH, "Smoothing by Spline Functions", 1967.

Example 1 $\|A\mathbf{x}-\mathbf{b}\| = \min$ s.t. $\|C\mathbf{x}-\mathbf{d}\| \le 10$

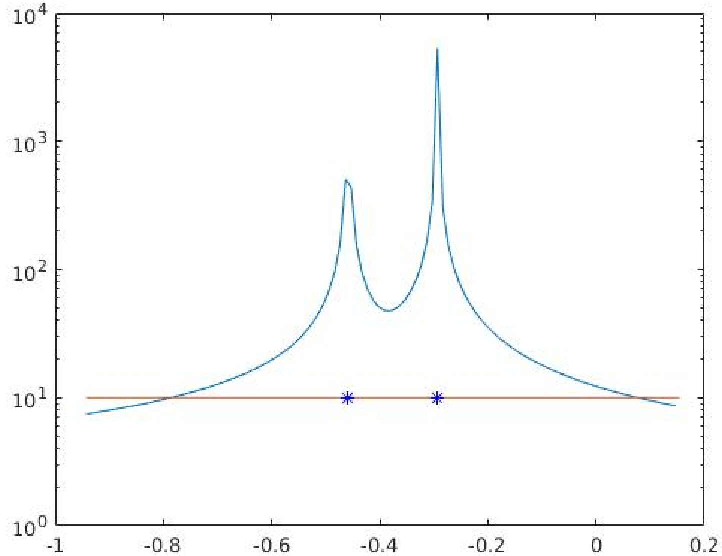
Bsp1

A		$\mathbf{b}$
0.7398	0.5244	-4.4414
0.8930	0.7545	-5.9504
0.0259	0.1698	-0.7691
0.1376	0.6727	-2.1635
0.4241	0.6187	-1.1464
0.7646	0.0068	-4.2864

C		$\mathbf{d}$
-1.6443	-1.9204	2.2650
-0.0263	-0.3913	3.0165
-1.9660	-0.2804	2.0781



$\|A\mathbf{x}-\mathbf{b}\| = \text{const}$, $\|C\mathbf{x}-\mathbf{d}\| = 10$



$f(\lambda) = \|C\mathbf{x}(\lambda)-\mathbf{d}\|$

active constraint, $\lambda_i = [-0.7857, 0.0772]$, poles$= -\mu_i = [-0.4582, -0.2935]$

Equality Constraint

$\|A\mathbf{x} - \mathbf{b}\|^2 = \min$ subject to $\|C\mathbf{x} - \mathbf{d}\|^2 = \delta^2$

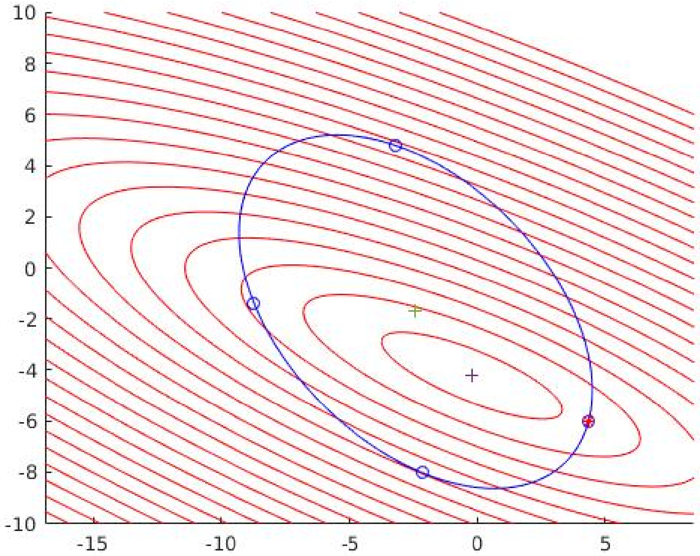
1. Constraint is always active.
2. Compute the largest solution of the secular equation: $\lambda_{\max}$
3. $\lambda_{\max}$ may be positive or negative.
4. The solution is $\mathbf{x}(\lambda_{\max})$

Example 2 $\|A\mathbf{x}-\mathbf{b}\| = \min$ s.t. $\|C\mathbf{x}-\mathbf{d}\| = 10$

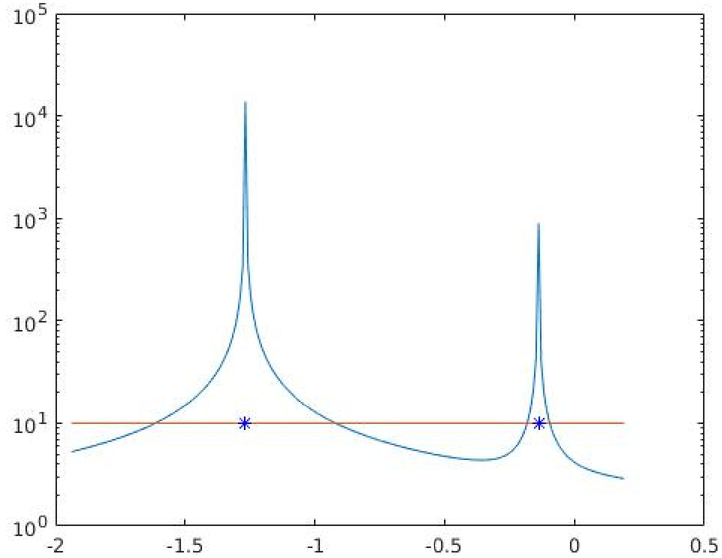
Bsp2

A		$\mathbf{b}$
0.5859	0.6309	-3.9636
0.1907	0.8920	-3.1196
0.5034	0.6734	-1.9904
0.0509	0.6853	-5.6050
0.0561	0.6957	-1.4789
0.3352	0.7998	-3.0672

C		$\mathbf{d}$
-0.5194	-0.9237	3.7413
-1.4917	-0.1797	3.7109
-0.3088	-1.2986	2.3508



$\|A\mathbf{x}-\mathbf{b}\| = \text{const},\ \|C\mathbf{x}-\mathbf{d}\| = 10$



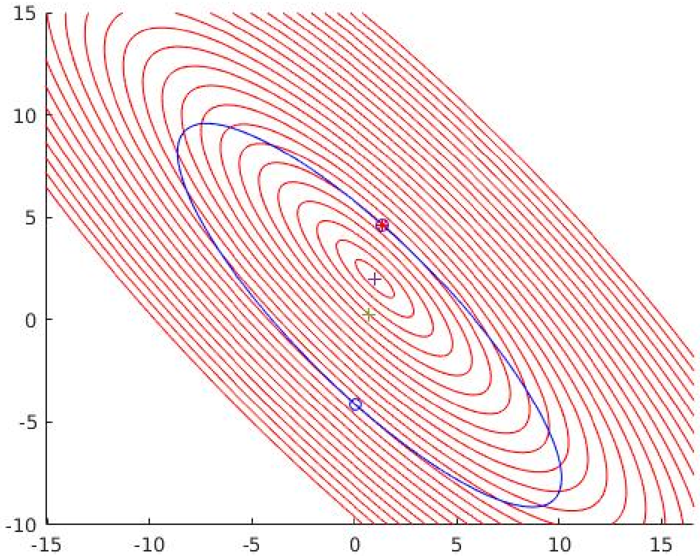
$f(\lambda) = \|C\mathbf{x}(\lambda)-\mathbf{d}\|$

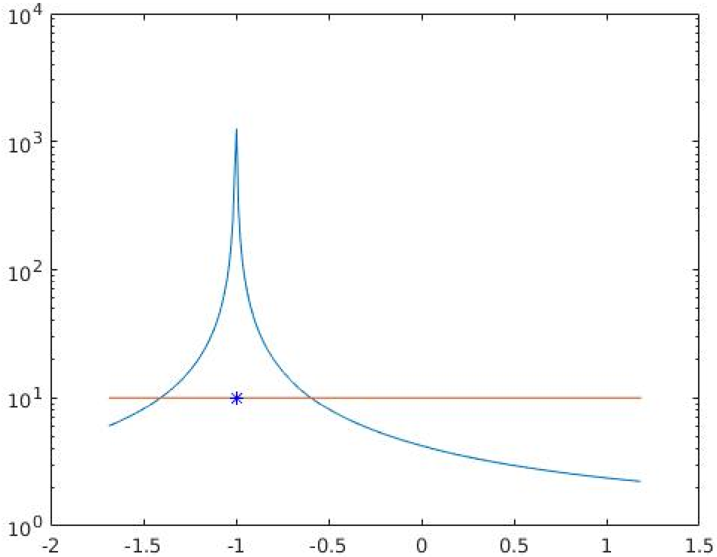
$\lambda_i = [-1.6157, -0.9211, -0.1827, -0.0962]$, poles $= -\mu_i = [-1.2686, -0.1393]$

Example 3 secular equation with one (double) pole

Bsp3

A		$\mathbf{b}$		$\mathbf{d}$
0.9200	0.9900	2.9000		0.8147
0.9800	0.8000	2.5800		0.9058
0.0400	0.8100	1.6600		0.1270
0.8500	0.8700	2.5900	$C = A$	0.9134
0.8600	0.9300	2.7200		0.6324
0.1700	0.2400	0.6500		0.0975
0.2300	0.0500	0.3300		0.2785
0.7900	0.0600	0.9100		0.5469
0.1000	0.1200	0.3400		0.9575
0.1100	0.1800	0.4700		0.9649





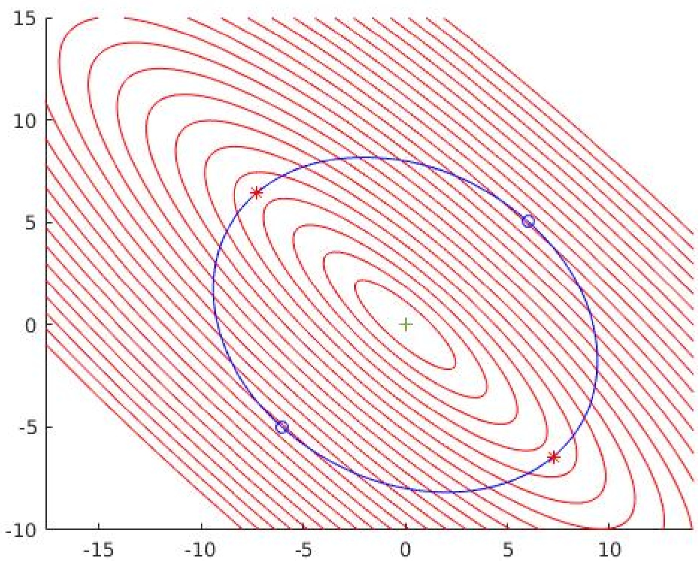
$\lambda_i = [-1.4057, -0.5943]$, $-\mu_i = [-1.0000, -1.0000]$

Example 4 Special Case: Constant secular function

Bsp4

A		$\mathbf{b}$
0.9200	0.9900	-0.7048
0.9800	0.8000	0.6638
0.0400	0.8100	0.2285
0.1100	0.1800	-0.1024

C		$\mathbf{d}$
-0.0925	-0.0088	-0.2748
-0.2666	0.1165	0.6711
0.0353	-0.3772	0.5353
-0.3109	-0.2802	-0.4330



- In this example
  $A^\top \mathbf{b} = 0$ and $C^\top \mathbf{d} = 0$
  $\Longrightarrow \left(A^\top A + \lambda C^\top C\right) \mathbf{x} = 0$
- $\mathbf{x} = 0, \; f(\lambda) = \|\mathbf{d}\|^2 = \text{const}\,.$
- Nontrivial solution of normal equations are eigenvectors for $\lambda = -\mu_i$
- $\lambda_i = [-15.3424, \; -1.8882]$
- Solution is eigenvector for eigenvalue 1.8882, scaled so that
  $\|\rho C\mathbf{x} - \mathbf{d}\| = \delta = 4.$
  $\rho = \pm 3.8730.$

Solving the Secular Equation

- Assume active constraint $\|C\mathbf{x} - \mathbf{d}\| \le \delta$
- Want compute $\lambda^* > 0$
- Consider Newton's iteration for the equations

$$g_1(\lambda) := f(\lambda) - \delta^2 = 0$$

$$g_2(\lambda) := \sqrt{f(\lambda)} - \delta = 0$$

$$g_3(\lambda) := \frac{1}{\sqrt{f(\lambda)}} - \frac{1}{\delta} = 0.$$

- Reinsch first used g_2, starting with $\lambda_0 = 0$.

  He observed better global convergence using g_3.

  Proved also monotonic convergence.

Why Better Global Convergence for g_3 ?

Compare the Newton iteration functions

$$\lambda - \frac{f-\delta^2}{f'} \qquad \text{for } g_1$$

$$\lambda - \frac{f-\delta^2}{f'} \frac{2}{1+\frac{\delta}{\sqrt{f}}} \qquad \text{for } g_2$$

$$\lambda - \frac{f-\delta^2}{f'} \frac{2\frac{\sqrt{f}}{\delta}}{1+\frac{\delta}{\sqrt{f}}} \qquad \text{for } g_3$$

For $\sqrt{f} >> \delta$ the Newton step for g_2 is twice the step for g_1!

And for g_3 even larger, proportional to $\frac{\sqrt{f}}{\delta}$.

Geometric Argument for Reinsch's Proposal

- Geometric derivation to construct a zero finder for $f(x) = \delta^2$: Approximate f for $x = x_k$ by simpler function $h(x)$ such that $h^{(i)}(x_k) = f^{(i)}(x_k), i = 0, 1.$
- Solving $h(x) = \delta^2$ gives the new iterate x_{k+1}.
- Newton's method: $h(x) = ax + b \quad \Longrightarrow \quad x_{k+1} = x_k - \dfrac{f(x_k) - \delta^2}{f'(x_k)}$
- Reinsch's proposal: $h(x) = \dfrac{a}{(x-b)^2}$ gives

$$x_{k+1} = x_k - \frac{f(x_k) - \delta^2}{f'(x_k)} G(x_k) \qquad \text{with} \quad G(x) = \frac{2\dfrac{\sqrt{f}}{\delta}}{1 + \dfrac{\delta}{\sqrt{f}}}$$

- The secular function is much better approximated by h than by a linear function!

Computing Derivatives of the Secular Function

Derivatives can be obtained by differentiating the normal equations:

- $\left(A^\top A + \lambda C^\top C\right) \mathbf{x} = A^\top \mathbf{b} + \lambda C^\top \mathbf{d}$
  $f(\lambda) = \|C\mathbf{x} - \mathbf{d}\|^2$
- $\left(A^\top A + \lambda C^\top C\right) \mathbf{x}^{(k)} = -k\, C^\top C\mathbf{x}^{(k-1)}$
  $C\mathbf{x}^{(0)} := C\mathbf{x} - \mathbf{d}, \quad k = 1, 2, \ldots$
- $f^{(2k-1)}(\lambda) = k\, \gamma_{2k-1}\, \mathbf{x}^{(k)\top} C^\top C\mathbf{x}^{(k-1)}$
  $f^{(2k)}(\lambda) = \gamma_{2k} \|C\mathbf{x}^{(k)}\|^2$
  $\gamma_{2k} = (2k+1)\gamma_{2k-1}, \quad \gamma_{2k-1} = \dfrac{2}{k}\, \gamma_{2k-2}, \quad \gamma_1 = 2$

Effective Computation for A, C dense and $\lambda^* > 0$

- Avoid using normal equations! Rather solve the least squares problem

$$\begin{pmatrix} A \\ \sqrt{\lambda}\, C \end{pmatrix} \mathbf{x} \approx \begin{pmatrix} \mathbf{b} \\ \sqrt{\lambda}\, \mathbf{d} \end{pmatrix}$$

- Use Eldén's Transformation to simplify

$$\begin{pmatrix} A \\ \sqrt{\lambda}\, C \end{pmatrix} \mathbf{x} \approx \begin{pmatrix} \mathbf{b} \\ \sqrt{\lambda}\, \mathbf{d} \end{pmatrix} \longrightarrow \begin{pmatrix} A' \\ \sqrt{\lambda}\, I \end{pmatrix} \mathbf{x}' \approx \begin{pmatrix} \mathbf{b}' \\ \sqrt{\lambda}\, \mathbf{d}' \end{pmatrix}$$

- For P, Q orthogonal with $\mathbf{y} = Q^\top \mathbf{x}$

$$\begin{pmatrix} P^\top & 0 \\ 0 & Q^\top \end{pmatrix} \begin{pmatrix} A \\ \sqrt{\lambda}\, I \end{pmatrix} Q Q^\top \mathbf{x} \approx \begin{pmatrix} P^\top \mathbf{b} \\ Q^\top \sqrt{\lambda}\, \mathbf{d} \end{pmatrix} \iff \begin{pmatrix} P^\top A Q \\ \sqrt{\lambda}\, I \end{pmatrix} \mathbf{y} \approx \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{pmatrix}$$

Choose P and Q

1. SVD: $\Sigma = P^\top A Q \implies \begin{pmatrix} \Sigma \\ \sqrt{\lambda}\, I \end{pmatrix} \mathbf{y} \approx \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{pmatrix}$

   + Efficient iteration (n Givens rotations per step)
   - Preparation: need SVD

2. Bidiagonalization: $B = P^\top A Q \implies \begin{pmatrix} B \\ \sqrt{\lambda}\, I \end{pmatrix} \mathbf{y} \approx \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{pmatrix}$

   + cheaper preparation

   $\pm$ still efficient iteration using $2n$ Givens rotations per step followed by backsolve with bidiagonal matrix

$$
\begin{bmatrix}
\color{red}{x} & \color{red}{x} & & \\
 & x & x & \\
 & & x & x \\
 & & & x \\
\color{red}{x} & & & \\
 & x & & \\
 & & x & \\
 & & & x
\end{bmatrix}
\rightarrow
\begin{bmatrix}
\color{blue}{0} & \color{red}{x} & & \\
 & x & x & \\
 & & x & x \\
 & & & x \\
\color{blue}{x} & \color{blue}{x} & & \\
 & \color{red}{x} & & \\
 & & x & \\
 & & & x
\end{bmatrix}
\rightarrow
\begin{bmatrix}
\color{blue}{0} & \color{blue}{0} & & \\
 & x & x & \\
 & & x & x \\
 & & & x \\
\color{blue}{x} & \color{blue}{x} & & \\
 & \color{blue}{x} & & \\
 & & x & \\
 & & & x
\end{bmatrix}
$$

One-point Iteration Methods

- Every fixed point iteration $x_{n+1} = F(x_n)$ can be seen as a Newton iteration to some $g(x) = 0$

$$x - \frac{g(x)}{g'(x)} = F(x) \iff g(x) = c \cdot \left(\int \frac{dx}{x - F(x)} \right).$$

- Example Halley's iteration $F(x) = x - \frac{2f(x)f'(x)}{2f'(x)^2 - f''(x)f(x)}$

$$g(x) = \exp\left(\int \left(\frac{f(x)}{f'(x)} - \frac{f''(x)}{2f'(x)} \right) dx \right) = \frac{f(x)}{\sqrt{f'(x)}}$$

  Thus Halley for $f(x) = 0$ is Newton for $g(x) = \frac{f(x)}{\sqrt{f'(x)}} = 0$.

- Motivated by the secular equation I became interested in studiying fixed point iterations $x_{n+1} = F(x_n)$, where

$$F(x) = x - \frac{f(x)}{f'(x)} G(x)$$

Third Order Iterative Methods

Assume s is a simple zero of f. Consider

- $x_{n+1} = F(x_n) = x_n - \frac{f(x_n)}{f'(x_n)} G(x_n)$
- Let $u(x) := \frac{f(x)}{f'(x)}$ then $F(x) = x - u(x)G(x)$
- We wish to have $F'(s) = F''(s) = 0$ for cubic convergence

$$F' = 1 - u'G - uG', \quad F'' = -u''G - 2u'G' - uG''$$

$$u = f/f', \quad u' = 1 - \frac{ff''}{f'^2}$$

$$u'' = -\frac{f''}{f'} + 2\frac{ff''}{f'^3} - \frac{ff'''}{f'^2}.$$

- Since $u(s) = 0$, $u'(s) = 1$, $u''(s) = -\frac{f''(s)}{f'(s)}$

$\implies F'(s) = 0$ if $G(s) = 1$ and $F''(s) = 0$ if $G'(s) = \frac{1}{2}\frac{f''(s)}{f'(s)}$

Third Order Iterative Methods (cont.)

- $G(s) = 1,\ G'(s) = \frac{1}{2}\frac{f''(s)}{f'(s)}$ not helpful since we do not know s.
- $t(x) := \frac{f(x)f''(x)}{f(x)^2} = 1 - u'(x) \implies t(s) = 0, \quad t'(s) = -u''(s) = \frac{f''(s)}{f'(s)}$
- Consider $G(x) = H(t(x)), \quad G(s) = H(0)$

$$G'(x) = H'(t(x))t'(x) \implies G'(s) = H'(0)\frac{f''(s)}{f'(s)}$$

Theorem Let s be a simple zero of f and H any function with $H(0) = 1$, $H'(0) = 1/2$ and $|H''(0)| < \infty$. The iteration $x_{n+1} = F(x_n)$, with

$$F(x) = x - \frac{f(x)}{f'(x)}H(t(x)) \quad \text{where} \quad t(x) = \frac{f(x)f''(x)}{f'(x)^2}$$

is of third order.

Many iterative methods are special cases of theorem

1. Euler's formula $H(t) = \frac{2}{1+\sqrt{1-2t}} = 1 + \frac{1}{2}t + \frac{1}{2}t^2 + \frac{5}{8}t^3 + \dots$
2. Halley's formula $H(t) = \frac{1}{1-\frac{1}{2}t} = 1 + \frac{1}{2}t + \frac{1}{4}t^2 + \frac{1}{8}t^3 + \dots$
3. Quadratic inverse interpolation $H(t) = 1 + \frac{1}{2}t$
4. Ostrowski's square root iteration
$$H(t) = \frac{1}{\sqrt{1-t}} = 1 + \frac{1}{2}t + \frac{3}{8}t^2 + \frac{5}{16}t^3 + \dots$$
5. Hansen-Patrick family $H(t) = \frac{\alpha+1}{\alpha+\sqrt{1-(\alpha+1)t}} = 1 + \frac{1}{2}t + \frac{\alpha+3}{8}t^2 + \dots$

Result by Schröder: all third order iteration formula have the form

$$G(x) = H(t(x)) + f(x)^2 b(x)$$

with b arbitrary bounded for $x \to s$

Summary

- My first encounter with Prof. Gene H. Golub was very fruitful
- it was the start in a new world for me
- it was the start of my academic career
- it was the start of deep friendship with Gene and with international colleagues

Thank you Gene!

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