On singular values of parameter dependent matrices

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Harrachov, August 23, 2007

Outline:

- **ASVD** concept
- **Non-generic points on the path**
  structural stability? ... a motivation
- **Pathfollowing the simple singular values**
- **An application: computation of pseudospectra**
- **Singularities on the path**
  an analysis via Singularity Theory
  - nonzero multiple singular value
  - zero simple singular value
  - zero multiple singular value
- **Conclusions**

SVD ... *Singular Value Decomposition*

$A \in \mathbb{R}^{m \times n}$, $m \geq n$: $A = U \Sigma V^T$,

- $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ ... orthogonal matrices
- $\Sigma = \mathrm{diag}(s_1, \ldots, s_n) \in \mathbb{R}^{m \times n}$ ... diagonal matrix

s_i ... *singular values,*
$U_i \in \mathbb{R}^m$, $V_i \in \mathbb{R}^n$ ... *left/right singular vectors*

ASVD ... *Analytic Singular Value Decomposition*

= a version of SVD for
parameter dependent matrices

Kato, *Perturbation Theory for Linear Operators*, 1976.
Bunse-Gerstner, Byers, Mehrmann and Nichols: Numer.Math. 60 (1991)

Let $A = A(t)$, $A \in C^\omega([a,b], \mathbb{R}^{m\times n})$ ... real analytic

Construct a factorisation

$$A(t) = U(t)\Sigma(t)V(t)^T$$

such that

- U, V and Σ are real analytic on $[a,b]$

For each $t \in [a,b]$:

- $U(t) \in \mathbb{R}^{m\times m}$, $V(t) \in \mathbb{R}^{n\times n}$ ... orthogonal matrices
- $\Sigma(t) = \mathrm{diag}(s_1(t), \ldots, s_n(t)) \in \mathbb{R}^{m\times n}$ ... diagonal matrix

At $t = a$:

- $U(a)$, $\Sigma(a)$, $V(a)$ ... via SVD of $A(a)$

Specific properties:

The smoothness of $A(t) \Longrightarrow$ the singular values $s_i(t)$

- may be negative
- their ordering may by arbitrary

Example 1:

$$A(t) = \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix}$$

ASVD: $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \leq t \leq 1.5$.

e.g.

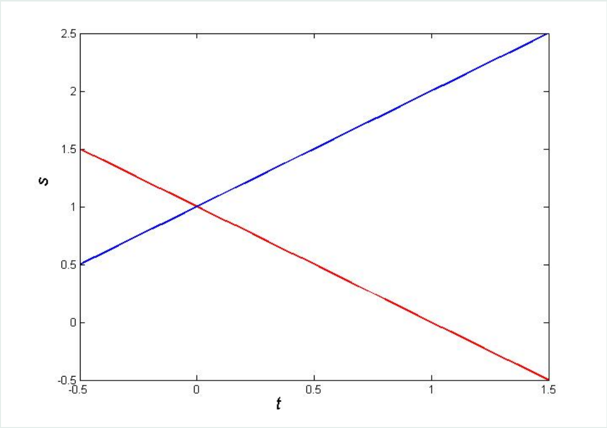
$$U(t) = V(t) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad s_1(t) = 1-t\,, \quad s_2(t) = 1+t\,.$$

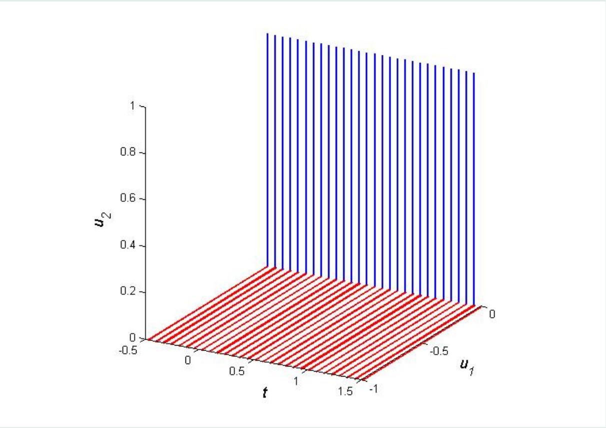
$$A(t) = s_1(t)U_1(t)V_1(t)^T + s_2(t)U_2(t)V_2(t)^T$$

$\Rightarrow$ branches

$$t \quad \longmapsto \quad (s_1(t); -1; 0; -1; 0)$$
$$t \quad \longmapsto \quad (s_2(t); 0; 1; 0; 1)$$

Example 1 continued:





$t \longrightarrow s_1(t), s_2(t)$ $\qquad$ $t \longrightarrow U_1(t), U_2(t)$

Non-generic points on the path ($\equiv$ branch):

at $t = 0$: $s_1(0) = s_2(0)$ ... nonsimple (multiple) singular value of $A(0)$

at $t = 1$: $s_1(1) = 0$ ... zero singular value of $A(1)$

Branching scenario at non-generic points:

... the branches $t \longmapsto s_i(t)$ of singular values, $i = 1, \ldots, p$, may intersect at isolated points only, namely, at the points where

$$s_i(t) = s_j(t) \quad \text{or} \quad s_i(t) = -s_j(t)$$

for $i \neq j$

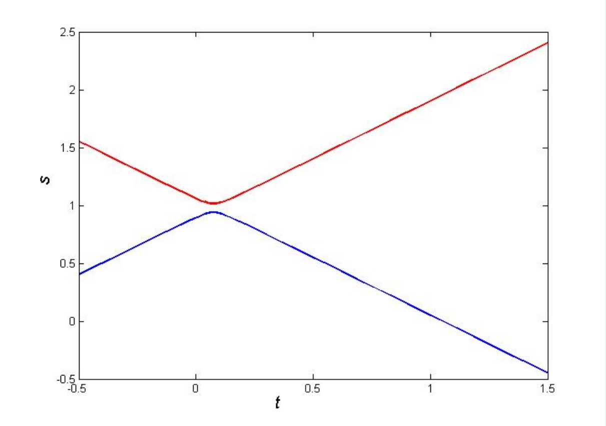
Bunse-Gerstner, Byers, Mehrmann and Nichols: Numer.Math. 60 (1991)
Wright: Numer.Math. 60 (1992)

Is it generic?

Example 1 continued:

$$A(t) = \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} + \varepsilon \begin{bmatrix} 1/2 & 1 \\ -1/4 & 0 \end{bmatrix}$$

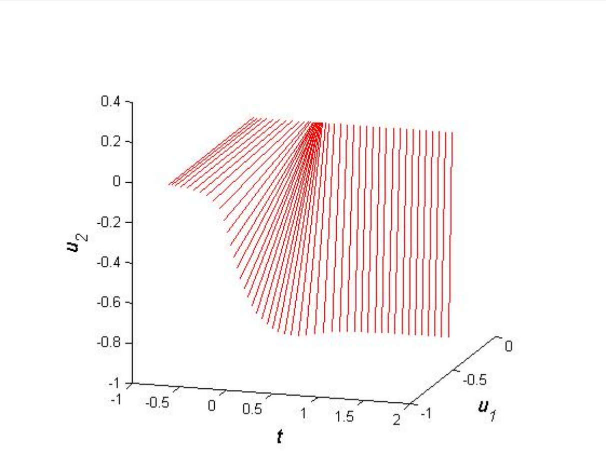
ASVD: $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \le t \le 1.5$.



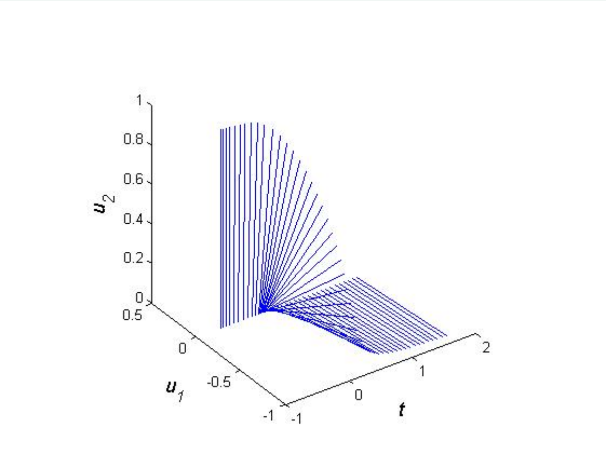
$$t \longrightarrow s_1(t), s_2(t)$$

the case: $\varepsilon = 0.1$.

Example 1 continued:

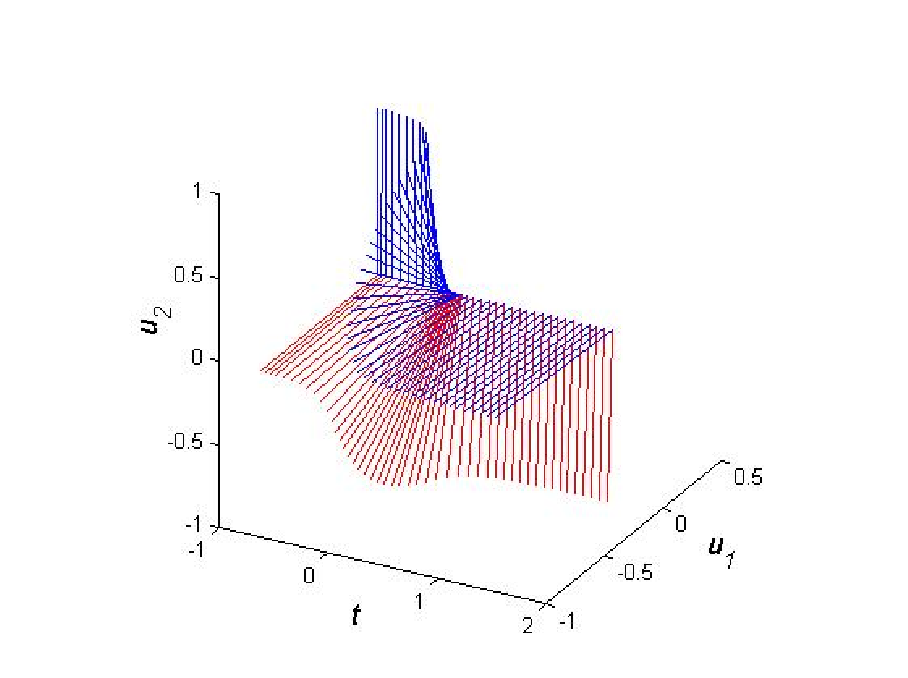


$t \longrightarrow U_1(t)$



$t \longrightarrow U_2(t)$

Example 1 continued:



$$t \longrightarrow U_1(t),\ U_2(t)$$

Reducing the problem

ASVD: $A(t) = U(t)\Sigma(t)V(t)^T = \sum s_i(t)U_i(t)V_i(t)^T$

... the left/right singular vectors $U_i(t)$, $V_i(t)$
and corresponding singular values $s_i(t)$

Note: Redundancy in scalling
either $U_i(t)^T U_i(t) = 1$ or $V_i(t)^T V_i(t) = 1$, or a combination,
become redundant
provided that $s_i(t) \neq 0$

Question: $\exists$ branch of
$s(t) \in \mathbb{R}$, $u(t) \in \mathbb{R}^m$, $v(t) \in \mathbb{R}^n$ ...
singular value, left/right singular vectors

Let

$$f : \mathbb{R} \times \mathbb{R}^{1+m+n} \rightarrow \mathbb{R}^{1+m+n}$$

$$t \in \mathbb{R}\,, \quad x = (s, u, v) \in \mathbb{R}^1 \times \mathbb{R}^m \times \mathbb{R}^n \longmapsto f(t, x) \in \mathbb{R}^{1+m+n}$$

$$f(t, x) \equiv \begin{pmatrix} -su + A(t)v \\ A^T(t)u - sv \\ v^T v - 1 \end{pmatrix}$$

alternative:

$$f(t, x) \equiv \begin{pmatrix} -su + A(t)v \\ A^T(t)u - sv \\ u^T u + v^T v - 2 \end{pmatrix}$$

Problem 1 *Let* $t^0 \in \mathcal{J}$ *and*

$$x^0 = (s^0, u^0, v^0) : f(t^0, x^0) = 0\,.$$

Find all $(t, x) \in \mathbb{R} \times \mathbb{R}^{1+m+n}$: $f(t, x) = 0$.

. . . *solution manifold*

? ... a branch $f(t, x(t)) = 0$.

Proposition 1 *Let* $s^0 \neq 0$ *be a simple singular value of* $A(t^0)$*.*
Then there exists a smooth

$$t \in \mathcal{I} \longmapsto x(t) \in \mathbb{R}^{1+m+n}$$

such that

$f(t, x(t)) = 0$ *for all* $t \in \mathcal{I}$

$x(t^0) = x^0$.

An application: computing pseudospectra

$\forall \varepsilon > 0$, $\varepsilon-$**pseudospectrum** of $\mathbf{A}$

• the subset of the complex plane bounded by the ε^{-1} level curve of the resolvent norm:

$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : \|(z\mathbf{I} - \mathbf{A})^{-1}\| \geq \varepsilon^{-1}\}$$

• the set of all complex numbers that are in the spectrum of some matrix obtained by a perturbation of norm at most ε:

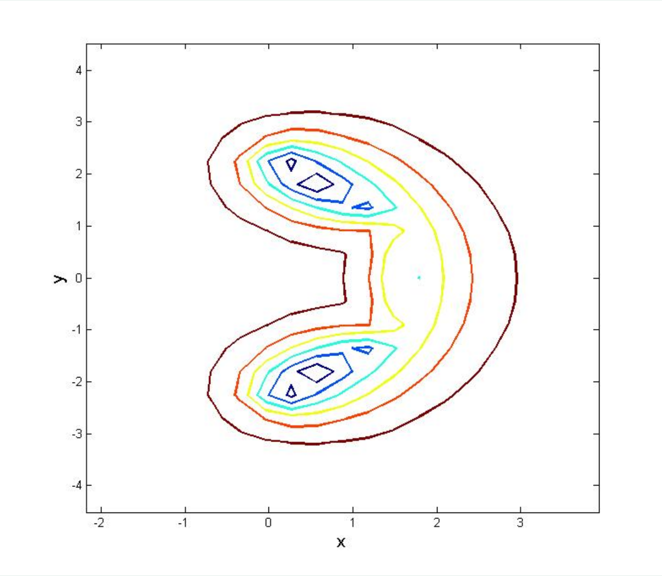
$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : z \in \Lambda(\mathbf{A} + \mathbf{E}) \text{ for some } \mathbf{E} \text{ with } \|\mathbf{E}\| \leq \varepsilon\}$$

• the sets in the $z-$plane bounded by level curves of the function $\sigma_{\min}(z\mathbf{I} - \mathbf{A})$ ($\sigma_{\min}(\mathbf{A}) \ldots$ the smallest singular value of $\mathbf{A}$):

$$\Lambda_\varepsilon(\mathbf{A}) = \{z \in \mathcal{C} : \ \sigma_{\min}(z\mathbf{I} - \mathbf{A}) \leq \varepsilon\}.$$

Example: `grcar`, n = 50

see `http://www.comlab.ox.ac.uk/pseudospectra/eigtool`




```
[U,T,eigA] = fact(A,1); ... Schur decomposition
stepx = 20, stepy = 20
Z1 = psacore(T,1,zeros(50,1),x,y,1e-5,50)
[X,Y] = meshgrid(x,y);
contour(X,Y,log10(Z1),6); ... No of isolines
```

Problem: Given $A \in \mathbb{C}^{n\times n}$, follow the contours

$$\partial\Lambda_\epsilon = \{z|\sigma_{\min}(zI - A) = \epsilon\}$$

The idea ... curve tracing algorithm:

After a "realification" and some transformations,
we consider a curve

$$f : \mathbb{R}^{2+4n} \longrightarrow \mathbb{R}^{1+4n}.$$

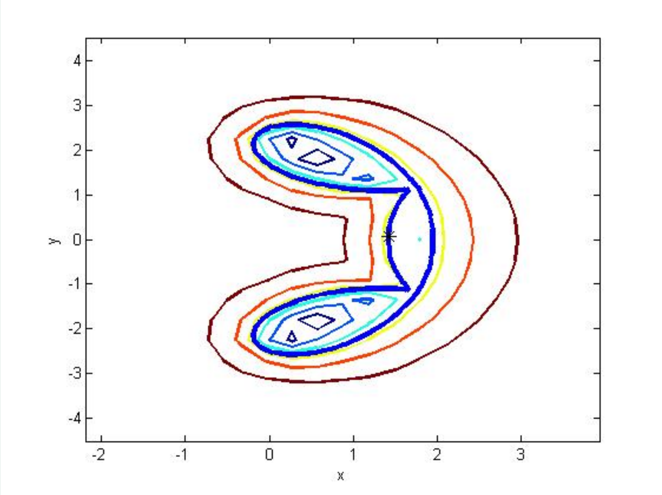
The coordinates of the state space $\mathbb{R}^{2+4n}$ are interpreted as

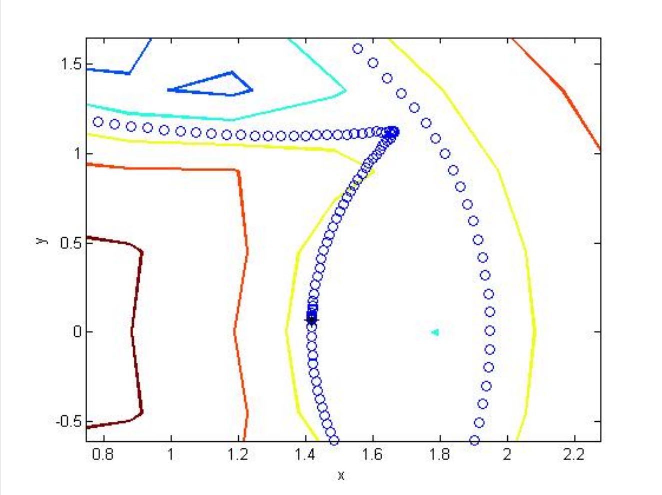
- the parameter $z \in \mathbb{C}$
- u, $v \in \mathbb{C}^n$, respectively, are the right/left singular vectors of $(zI - A)$, related to $\sigma_{\min}(zI - A) = \epsilon$.

The pathfollowing f yields the contours $\partial\Lambda_\epsilon$.

Example continued:

- pathfollowing: blue, $\varepsilon = 1.8373 \cdot 10^{-4}$

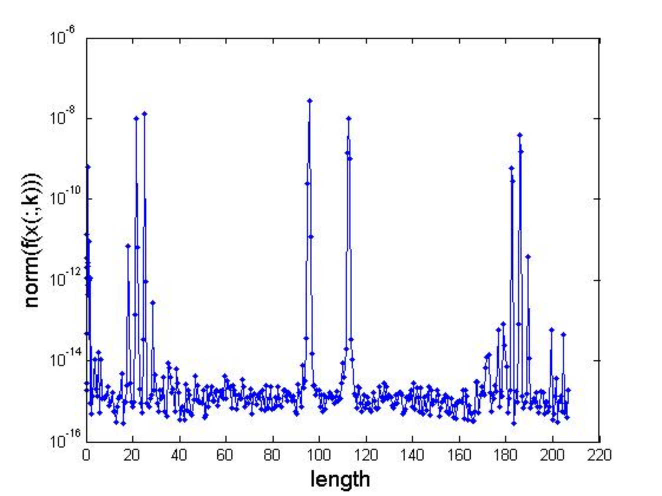




elapsed time = 13.14 secs
npoints curve = 299

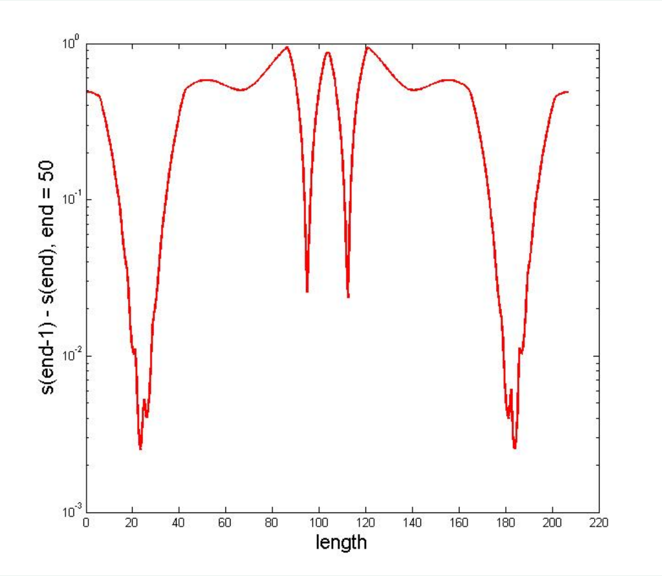
Residuum: $1 \le k \le 299$, $k \to$ arclength,

$$k \to \left\{ z \in \mathbb{C}, u \in \mathbb{C}^{50}, v \in \mathbb{C}^{50} \right\} \equiv x \to f(x) \to \text{norm}(f(x))$$




```
opt=contset(opt,'MaxStepsize', 1);
opt=contset(opt,'MinStepsize', 1e-5);
opt=contset(opt,'InitStepsize', 0.1);
etc
```

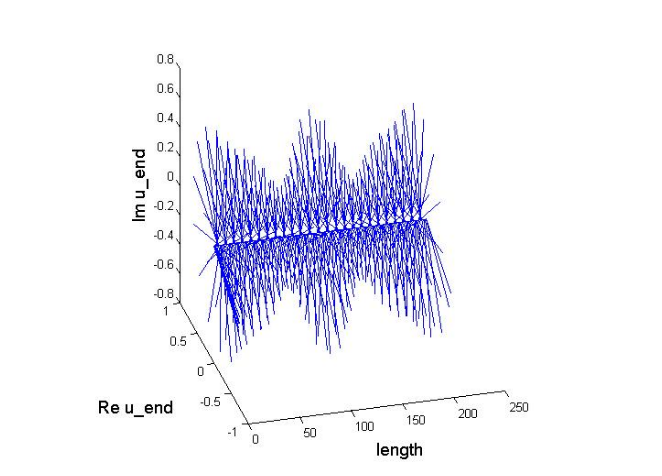
Singularities?

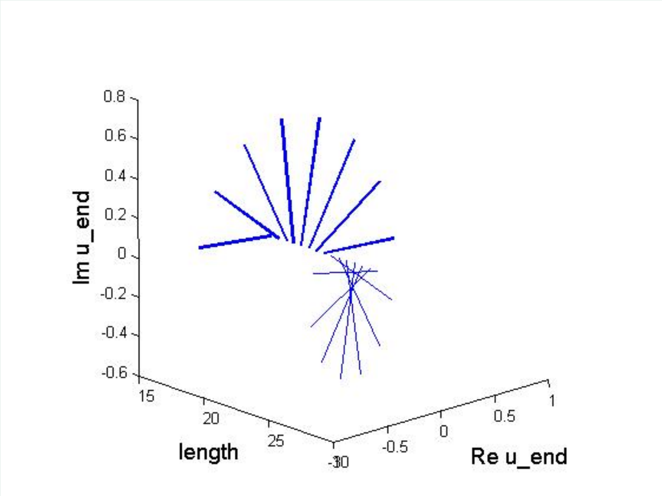


$$k \to x(:,k) \to [U,S,V] = svd(A - (x(1,k) + i * x(2,k)) * eye(n,n)) \to$$
$$\to \{s(n) \equiv \varepsilon, s(n-1)\} \to s(n-1) - s(n)$$

$k \to$ arclength

Twisting of $u's$, $v's$

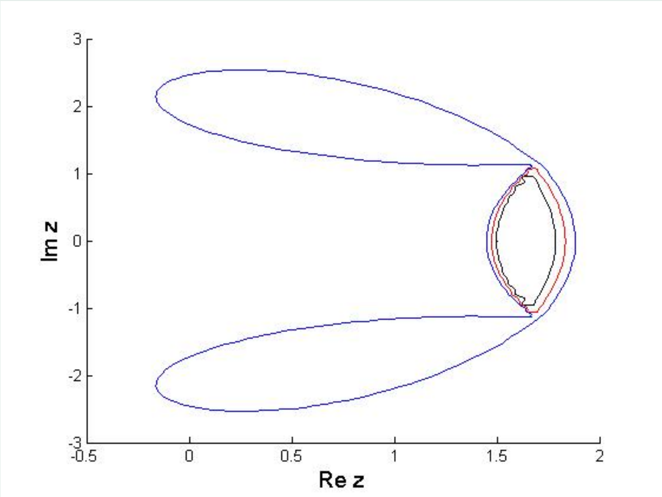


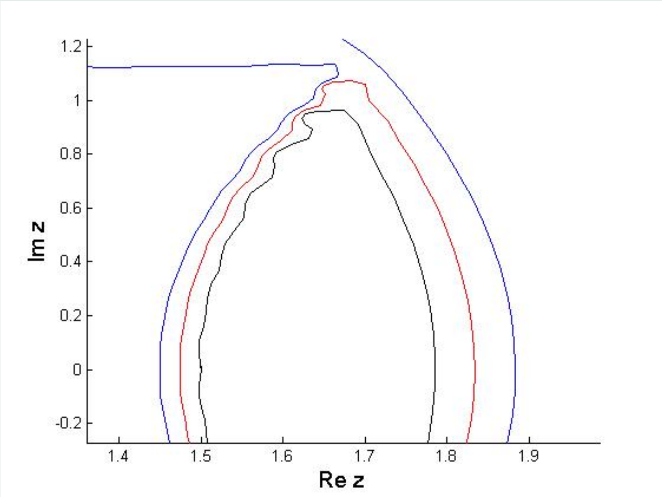


$k \to x(:,k) \in \mathbb{R}^{2+4n} \to u \in \mathbb{C}^n \to u_n \in \mathbb{C}$

$k \to$ arclength

contours:





$\varepsilon = 9.588746417274005e - 005$ ... blue
$\varepsilon = 5.808753134673688e - 005$ ... red
$\varepsilon = 3.534213595315432e - 005$ ... black

Non-generic point = a singular point of the branch

Case: $s^0 \neq 0$ ... nonsimple singular value of $A(t^0)$
i.e.,
$f(t^0, x^0) = 0,\ x^0 = (s^0, u^0, v^0),\ s^0 \neq 0,$
$\dim \mathrm{Ker}\, f_x(t^0, x^0) \geq 1.$
Let $\dim \mathrm{Ker}\, f_x(t^0, x^0) = 1$
$\Rightarrow$
$$\mathrm{Ker}\, f_x(t^0, x^0) = \mathrm{span}\left\{ \begin{pmatrix} 0 \\ \delta u \\ \delta v \end{pmatrix} \right\},\ \|\delta u\| = \|\delta v\| = 1$$

Idea: apply **Singularity Theory**

Govaerts: Numerical Methods for Bifurcation ... , 2000

(t^0, x^0) ... **singular point** of the mapping f
... corank $= 1$

Ingredients: dimensional reduction
expanding bifurcation equation

The solution manifold $f(t,x) = 0$ is, locally, parametrisable via $\tau \in \mathbb{R}$, $\xi \in \mathbb{R}$ ... observable such that

$$f(t^0 + \tau, x^0 + \Delta x) = 0\,, \qquad \Delta x = \Delta x(\tau, \xi) \tag{1}$$

Moreover, (1) if and only if

$$\varphi(\tau, \xi) = 0 \tag{2}$$

The scalar equation (2) ... **bifurcation equation**

Ad **Dimensional reduction:**
Fix matrices $B \in \mathbb{R}^{m+n+1}$, $C \in \mathbb{R}^{1+m+n}$.
Find $\xi \in \mathbb{R}$, $\tau \in \mathbb{R}$, $\Delta x \in \mathbb{R}^{1+m+n}$ and $\varphi \in \mathbb{R}$ such that

$$\begin{array}{rcl} f(t^0+\tau, x^0+\Delta x)+\varphi B & = & 0 \\ C^T \Delta x & = & \xi \end{array}$$

Requirement:

$$\det \begin{pmatrix} f_x(t^0, x^0) & B \\ C^T & 0 \end{pmatrix} \neq 0$$

Claim:

$$f(t^0+\tau, x^0+\Delta x(\tau,\xi)) = 0 \quad \Longleftrightarrow \quad \varphi(\tau,\xi) = 0$$

Bordering option:

$$B = \begin{pmatrix} \delta u \\ \delta v \\ 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 \\ \delta u \\ \delta v \end{pmatrix}$$

Analysing bifurcation equation:
computing *leading terms* of Taylor expansion of $\varphi(\tau, \xi)$ at $(\tau, \xi) = 0 \in \mathbb{R}^2$

Theorem 1 *...*
$\varphi_\tau = 0$, $\varphi_{\xi\tau} \neq 0$, $\varphi_{\tau\tau} \neq 0$ ... codim $= 1$ *singularity*
$\Rightarrow$ *branches*

$$\begin{aligned} \tau &= 0 \\ \xi &= -\frac{1}{2}\frac{\varphi_{\tau\tau}}{\varphi_{\xi\tau}}\tau + O(\tau^2) \end{aligned}$$

$O(\tau^2)$ *link to the solution manifold (1).*

where

$$\begin{aligned} 2\,\varphi_\tau &= (\delta u)^T A'(t^0) v^0 + (u^0)^T A'(t^0)\delta v \\ 2\,\varphi_{\xi\tau} &= (u^0)^T A'(t^0) v^0 - (\delta u)^T A'(t^0)\delta v \\ -\,\varphi_{\tau\tau} &= \frac{1}{2}\Big((\delta u)^T A''(t^0) v^0 + (u^0)^T A''(t^0)\delta u\Big) + \\ & + (\delta u)^T A'(t^0)\Delta v_\tau + (\Delta u_\tau)^T A'(t^0)\delta v \end{aligned}$$

$$\begin{pmatrix} \Delta u_\tau \\ \Delta v_\tau \end{pmatrix} = -\mathcal{M}(t^0, s^0)^+ \begin{pmatrix} A'(t^0) v^0 \\ A'(t^0)^T u^0 \end{pmatrix}$$

while

$$\mathcal{M}(t,s) \equiv \begin{pmatrix} -sI_m & A(t) \\ A^T(t) & -sI_n \end{pmatrix}$$

$I_m \in \mathbb{R}^{m\times m}$, $I_n \in \mathbb{R}^{n\times n}$ ... identities.

Ad: $O(\tau^2)$ link to (1)

$f(t^0+\tau, x^0+\Delta x(\tau,\xi)) = 0,$
$\Delta x(\tau,\xi) = (\Delta s(\tau,\xi), \Delta u(\tau,\xi), \Delta v(\tau,\xi)) \in \mathbb{R}^{1+m+n}$

Expanding $\Delta x(\tau,\xi)$ at $(\tau,\xi)=0$,

$\Delta s_\xi = 0,\ \Delta u_\xi = \frac{1}{2}\delta u,\ \Delta v_\xi = \frac{1}{2}\delta v,$
$\Delta s_\tau = (u^0)^T A'(t^0) v^0,$

$$\begin{pmatrix} \Delta u_\tau \\ \Delta v_\tau \end{pmatrix} = -\mathcal{M}(t^0,s^0)^+ \begin{pmatrix} A'(t^0)v^0 \\ A'(t^0)^T u^0 \end{pmatrix}$$

$\Delta s_{\xi\tau} = \frac{1}{2}\varphi_\tau,$

$$\begin{pmatrix} \Delta u_{\xi\tau} \\ \Delta v_{\xi\tau} \end{pmatrix} = -\frac{1}{2}\mathcal{M}(t^0,s^0)^+ \begin{pmatrix} A'(t^0)\delta v \\ A'(t^0)^T \delta u \end{pmatrix}$$

$\Delta s_{\xi\xi} = \Delta s_{\xi\xi\xi} = \cdots = 0$

The singular point under a perturbation: unfolding

e.g., let

$$A(t) + \varepsilon Z(t) \ \in \mathbb{R}^{m\times n}$$

? $f(t, x\,; \,\varepsilon) = 0$, $x = (s, u, v) \in \mathbb{R}^1 \times \mathbb{R}^m \times \mathbb{R}^n$,

$$f(t, x\,; \,\varepsilon) \equiv \begin{pmatrix} -su + (A(t) + \varepsilon Z(t))\,v \\ (A(t) + \varepsilon Z(t))^T\,u - sv \\ u^T u + v^T v - 2 \end{pmatrix}$$

Investigate corresponding bifurcation equation
$\varphi(\tau, \xi\,; \,\varepsilon) = 0\,, \quad (\tau, \xi) \in \mathbb{R}^2\,, \varepsilon \in \mathbb{R}$

Bifurcation equation: asymptotic analysis

$$\tau\left(\varphi_{\xi\tau}\,\xi + \frac{1}{2}\varphi_{\tau\tau}\,\tau + \text{h.o.t.}\right) +$$
$$+\ \varepsilon\ \left(\varphi_{\varepsilon} + \varphi_{\xi\varepsilon}\,\xi + \varphi_{\tau\varepsilon}\,\tau + \text{h.o.t.}\right) +$$
$$+\ O(\varepsilon^2) = 0$$

where
$\varphi_\varepsilon = \frac{1}{2}\,\delta u^T\,Z(t^0)\,v^0 + \frac{1}{2}\,(u^0)^T\,Z(t^0)\,\delta v^T$
etc.

$\Longrightarrow$ **structural instability**
compute the *torsion* of the branch

Non-generic point = a singular point of the branch

Case: $s^0 = 0$ ... simple singular value of $A(t^0)$
i.e., $n = m$
$f(t^0, x^0) = 0,\ x^0 = (s^0, u^0, v^0),\ s^0 = 0,$
$\dim \mathrm{Ker}\, f_x(t^0, x^0) \geq 1.$
Let $\dim \mathrm{Ker}\, f_x(t^0, x^0) = 1$
$\Rightarrow$

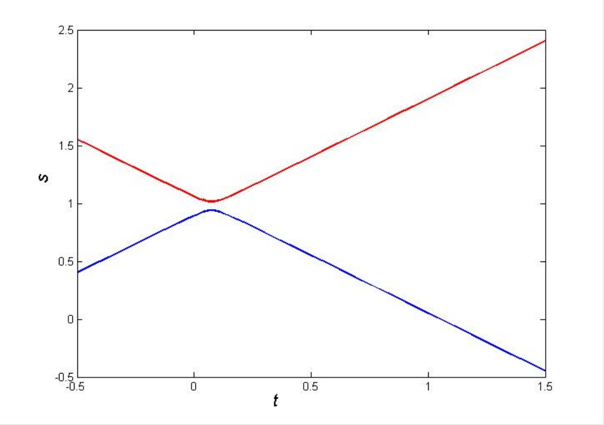
$$\mathrm{Ker}\, f_x(t^0, x^0) = \mathrm{span}\left\{ \begin{pmatrix} 0 \\ u^0 \\ v^0 \end{pmatrix} \right\},\ \|\delta u\| = \|\delta v\| = 1$$

Analysis (dimensional reduction, bifurcation equation, unfolding)
$\Longrightarrow$ **structural stability**

Ad **Example 1** resume:

$$A(t) = \left[\begin{array}{cc} 1-t & 0 \\ 0 & 1+t \end{array} \right] + \varepsilon \left[\begin{array}{cc} 1/2 & 1 \\ -1/4 & 0 \end{array} \right]$$

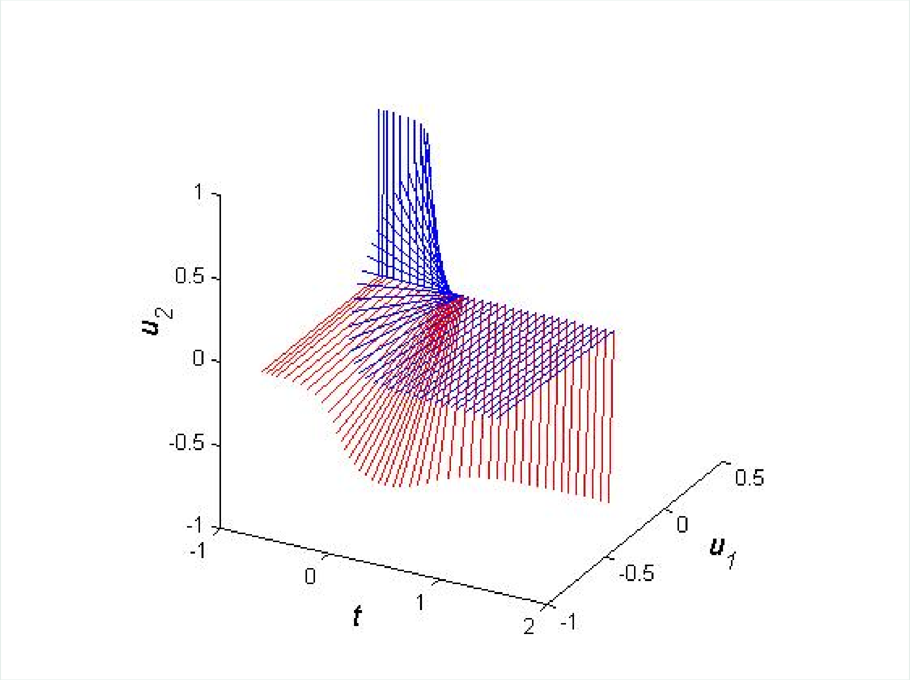
ASVD: $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \leq t \leq 1.5$.



$$t \longrightarrow s_1(t), s_2(t)$$

the case: $\varepsilon = 0.1$.

Ad **Example 1** resume:



$$t \longrightarrow U_1(t),\ U_2(t)$$

twist, *torsion* of the branches

Non-generic point = a singular point of the branch

Case: $s^0 = 0$ ... nonsimple singular value of $A(t^0)$
i.e., $m > n$
$f(t^0, x^0) = 0$, $x^0 = (s^0, u^0, v^0)$, $s^0 = 0$,
$\dim \mathrm{Ker}\, f_x(t^0, x^0) \geq 2$.

$\Longrightarrow$ **structural instability**

Example 2:

$$A(t) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & 1 \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix} \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix}$$

ASVD: $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \le t \le 1.5$.

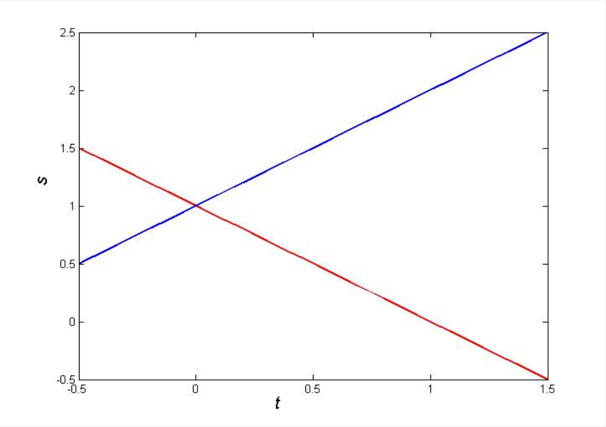
e.g.

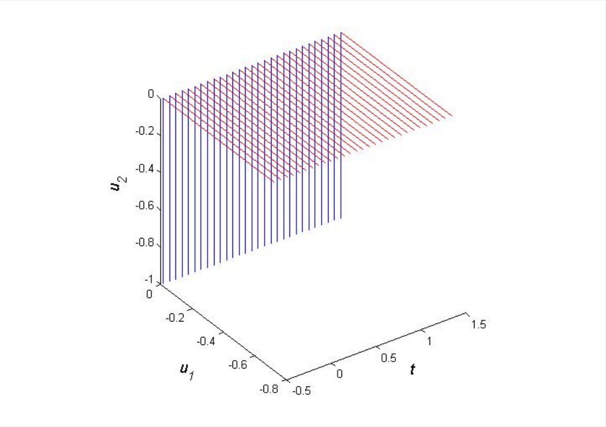
$$U(t) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -1 \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}, V(t) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, s_1(t) = 1-t\,, s_2(t) = 1+t\,.$$

$\Rightarrow$ branches

$$\begin{aligned} t &\longmapsto \left(s_1(t); \frac{\sqrt{2}}{2}; 0; \frac{\sqrt{2}}{2}; 1; 0\right) \\ t &\longmapsto (s_2(t); 0; -1; 0; 0; -1) \end{aligned}$$

Example 2 continued:





$t \longrightarrow s_1(t), s_2(t)$ $\qquad$ $t \longrightarrow U_1(t), U_2(t)$

Non-generic points on the path ($\equiv$ branch):

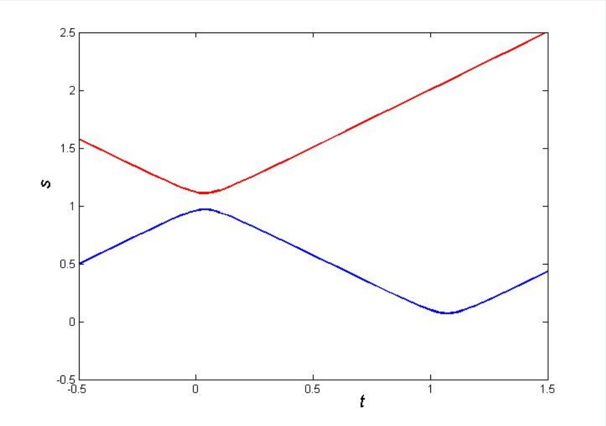
at $t = 0$: $s_1(0)$, $s_2(0)$ ... nonsimple (multiple) singular value of $A(0)$

at $t = 1$: $s_1(1)$ ... zero singular value of $A(1)$: nonsimple

Example 2 continued:

$$A(t) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & 1 \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix} \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} + \varepsilon \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 1 & 1 \end{bmatrix}$$

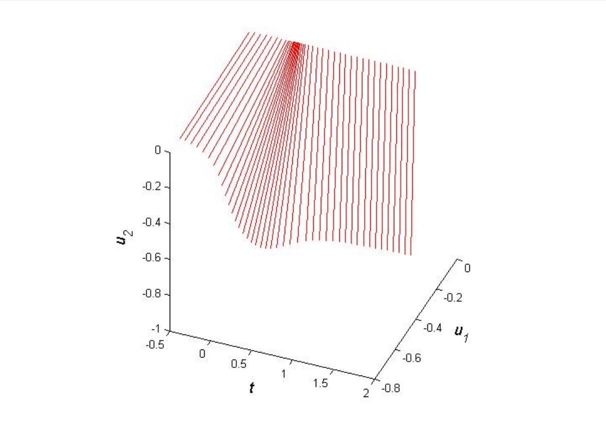
ASVD: $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \le t \le 1.5$.



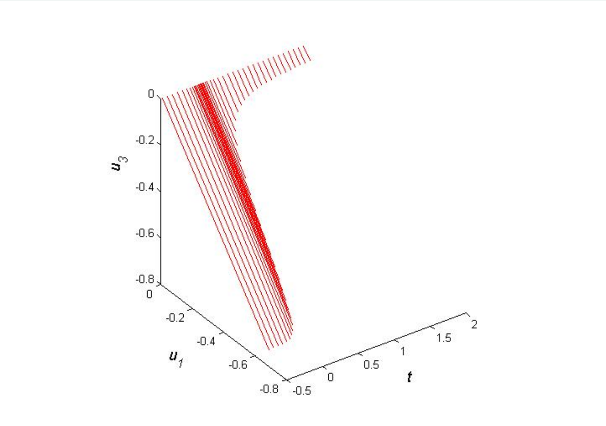
$$t \longrightarrow s_1(t), s_2(t)$$

the case: $\varepsilon = 0.1$.

Example 2 continued:

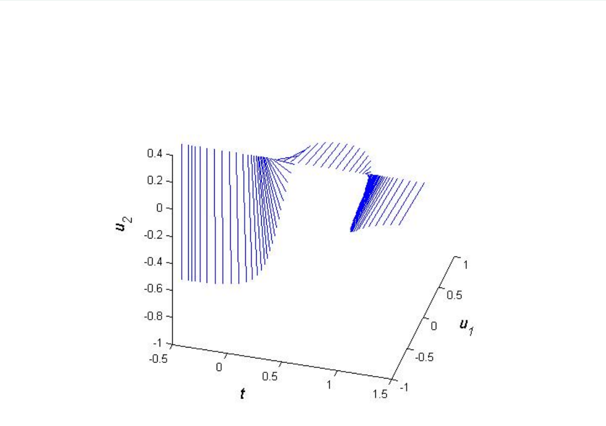


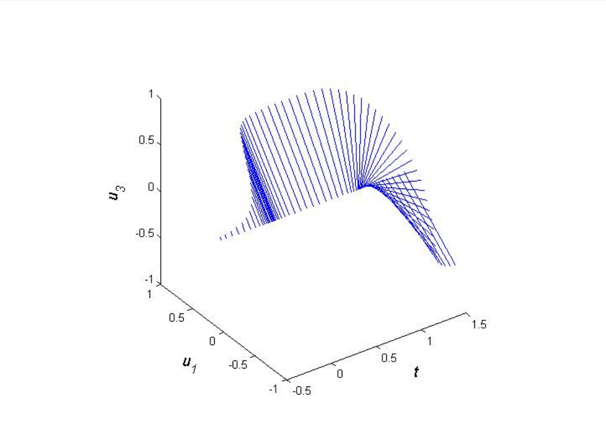
$$t \longrightarrow U_1(t)$$



$$t \longrightarrow U_1(t)$$

Example 2 continued:





$t \longrightarrow U_2(t)$ $\qquad$ $t \longrightarrow U_2(t)$

Conclusions

- **ASVD** versus a pathfollowing the simple singular values
- The pathfollowing of the simple nonzero singular value
  ... an efficient tool to compute pseudospectra
- The pathfollowing may get stuck at isolated points $\equiv$ **singular points**
  $\exists$ a link to the **non-generic points** of **ASVD**
- Singular points can be
  - investigated by reducing the problem to **bifurcation equation**
  - approximated by computing leading terms of bifurcation equation
- An unfolding of the bifurcation equation
  $\Longrightarrow$ an analysis of the **structural stability**

Supplement:

- **Computing ASVD**
  - all singular values
  - a bunch selected singular values
  - just one singular value

- **Simple singular value**

- **Pseudospectra**: motivation

Ad:

- **Computing ASVD**
  - all singular values

- An incremental technique using the classical SVD, of order $O(\tau^2)$ ... see Bunse-Gerstner, Byers, Mehrmann, Nichols, Numer. Math. 60 (1991)

- solving ODE: A Cauchy problem for $x' = H(t,x)$, $H : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$, $N = n + n^2 + m^2$ ... see Wright, Numer. Math. 63 (1992)

The comparison: The ODE integration lacks the precision ... see Mehrmann, Rath, Electronic Transactions on Numerical Analysis 1 (1993)

Ad:

- **Computing ASVD**
  - a bunch selected singular values

ASVD ... for large sparse matrices?

Apply

the pathfollowing of an implicitly defined curve

Janovská, Janovský, Tanabe, Proceedings of ENUMATH 2005,
Springer Verlag (2006), 911–918

- Consider *branches* of singular values $s_i(t) \in \mathbb{R}$ and corresponding left/right singular vectors $U_i(t) \in \mathbb{R}^m$, $V_i(t) \in \mathbb{R}^n$:

$$\begin{aligned} A(t)V_i(t) &= s_i(t)U_i(t)\,, \\ A(t)^T U_i(t) &= s_i(t)V_i(t)\,, \\ U_i(t)^T U_i(t) &= V_i(t)^T V_i(t) = 1 \end{aligned}$$

  for $t \in [a, b]$.

- Add the natural orthogonality conditions $U_i(t)^T U_j(t) = V_i(t)^T V_j(t) = 0$, $i \neq j$, $t \in [a, b]$.

- Consider just p, $p \leq n$, selected singular values $S(t) = (s_1(t), \ldots, s_p(t)) \in \mathbb{R}^p$, and the corresponding left/right singular vectors $U(t) = [U_1(t), \ldots, U_p(t)] \in \mathbb{R}^{m \times p}$, $V(t) = [V_1(t), \ldots, V_p(t)] \in \mathbb{R}^{n \times p}$ as smooth functions of $t \in [a, b]$.

In the operator setting,

$$F : \mathbb{R} \times \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \rightarrow \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p} \times \mathbb{R}^{p\times p} \times \mathbb{R}^{p\times p}$$

i.e.,

$$F : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^M \,, \qquad N = p(1+n+m)\,, \qquad M = p(m+n+2p)\,,$$

where

$$\begin{aligned} F(t,X) &\equiv \Big(A(t)V - U\boldsymbol{\Sigma}, A^T(t)U - V\boldsymbol{\Sigma}, U^TU - I, V^TV - I\Big)\,, \\ X &\equiv (S,U,V) \in \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p}\,, \qquad \boldsymbol{\Sigma} \equiv \mathrm{diag}(S) \end{aligned}$$

$$F(t,X) = 0$$

... a system of *overdetermined nonlinear equations*

Computing the curve $F(t, X) = 0$

via a **predictor-corrector** pathfollowing algorithm

In particular, *tangent continuation* is applied

Deuflhart, Hohmann,
Numerical Analysis in Modern Scientific Computing, 2003.

Experiment: homotopy

$$A(t) = t\,A2 + (1-t)\,A1\,, \quad t \in [0,1]$$

where

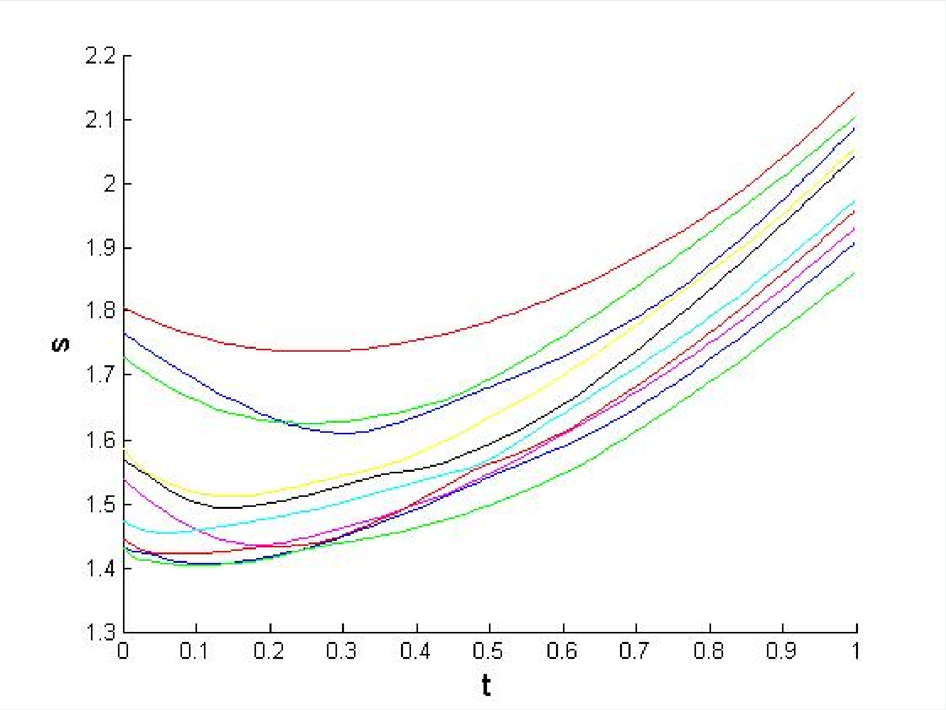
$$A1 \equiv \texttt{well1033.mtx}\,, \quad A2 \equiv \texttt{illc1033.mtx}$$

see ... `http://math.nist.gov/MatrixMarket/`

$A1, A2 \in \mathbb{R}^{1033\times 320}$, sparse, well/ill-conditioned

Initialization: at $t = 0$,
the 10 largest singular values, left/right singular vectors of A
computed via `svds` ... see MATLAB Function Reference

Parameter t vs. the 10 largest singular values s:



Recall

Branching scenario at non-generic points:

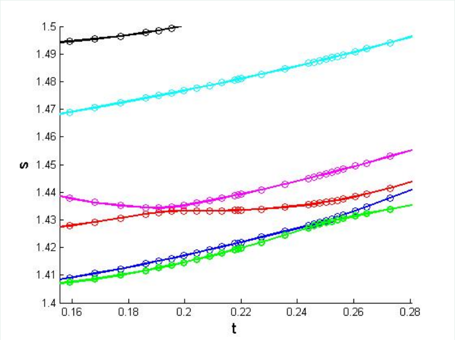
... the branches $t \longmapsto s_i(t)$ of singular values, $i = 1, \ldots, p$, may intersect at isolated points only, namely, at the points where

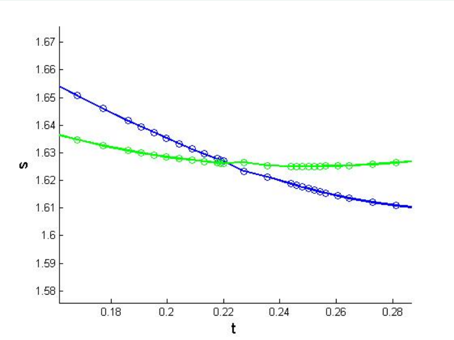
$$s_i(t) = s_j(t) \quad \text{or} \quad s_i(t) = -s_j(t)$$

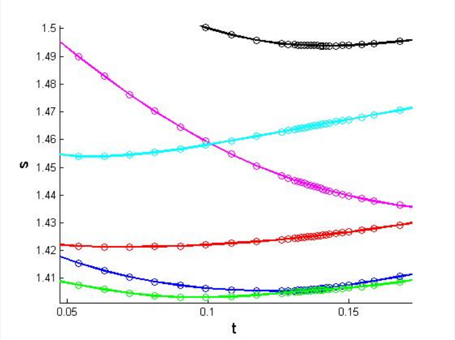
for $i \neq j$

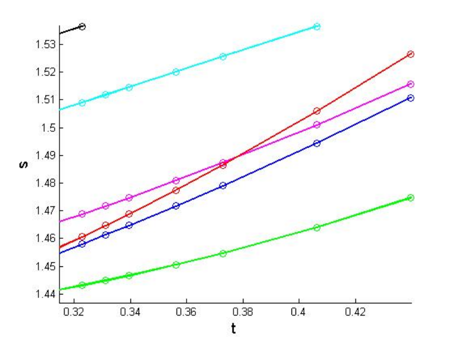
Bunse-Gerstner, Byers, Mehrmann and Nichols: Numer.Math. 60 (1991)
Wright: Numer.Math. 60 (1992)

Zooms:


s
t
1.4
1.41
1.42
1.43
1.44
1.45
1.46
1.47
1.48
1.49
1.5
0.16
0.18
0.2
0.22
0.24
0.26
0.28


s
t
1.58
1.59
1.6
1.61
1.62
1.63
1.64
1.65
1.66
1.67
0.18
0.2
0.22
0.24
0.26
0.28


s
t
1.41
1.42
1.43
1.44
1.45
1.46
1.47
1.48
1.49
1.5
0.05
0.1
0.15


s
t
1.44
1.45
1.46
1.47
1.48
1.49
1.5
1.51
1.52
1.53
0.32
0.34
0.36
0.38
0.4
0.42

Find path: $(t, X(t))$, $t \in [a, b]$,
$X(t) = (S(t), U(t), V(t)) \in \mathbb{R}^p \times \mathbb{R}^{m\times p} \times \mathbb{R}^{n\times p}$

Implementation of the algorithm

- Initialization: $(S(a), U(a), V(a))$ ... via `svd`, `svds`

  Assumption: $S(a) = (s_1(a), \ldots, s_p(a))$, $s_i(a)$ are simple for $i = 1, \ldots, p$.

  $\Longrightarrow$ a local existence of the branch

- **Non-generic points** on the path
  at such t: $s_i(t)$ ... nonsimple singular value

  In practice, the continuation may get stuck.

- **Remedies:** Extrapolation strategies
  - "Early Warning" of such values of t
  - "Jump Over" singular point

Ad:

- **Computing ASVD**
  - just one singular value

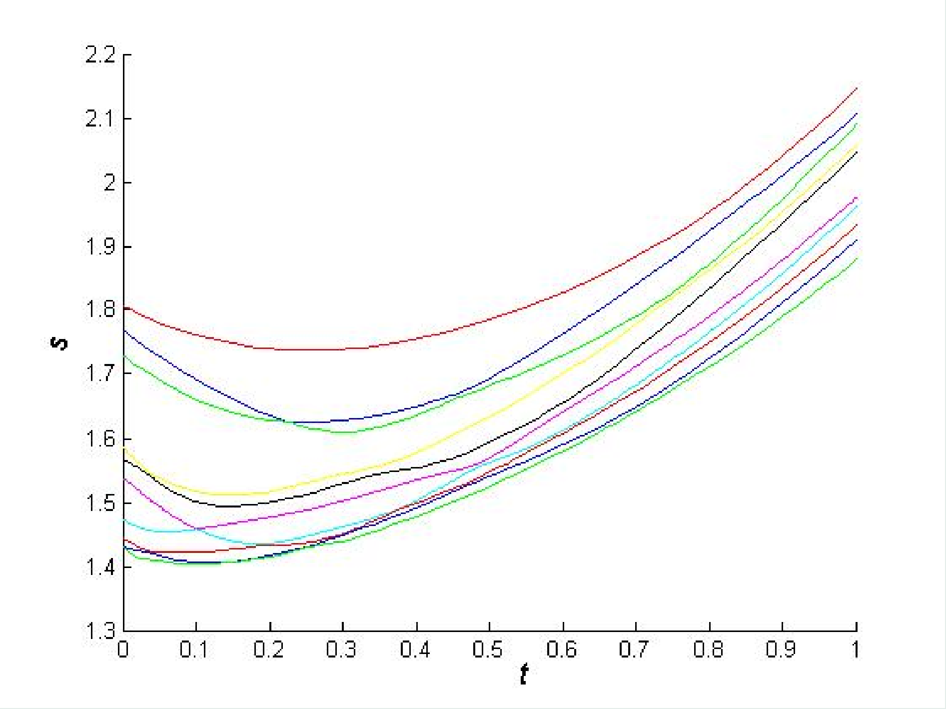
Experiment: homotopy

$$A(t) = t\,A2 + (1-t)\,A1\,, \quad t \in [0,1]$$
$$A1 \equiv \texttt{well1033.mtx}\,, \quad A2 \equiv \texttt{illc1033.mtx}$$

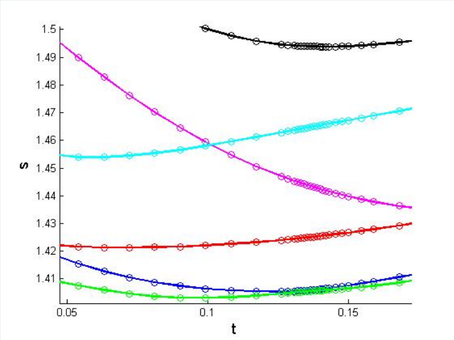
... continued

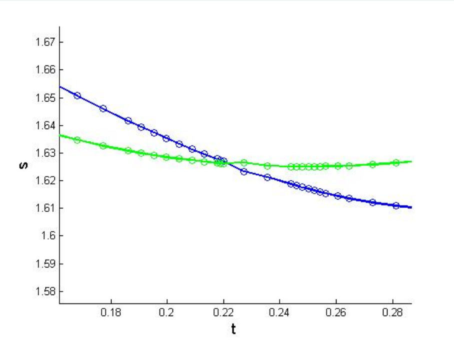
Corrected figures

Parameter t vs. the 10 largest singular values s, **revised**

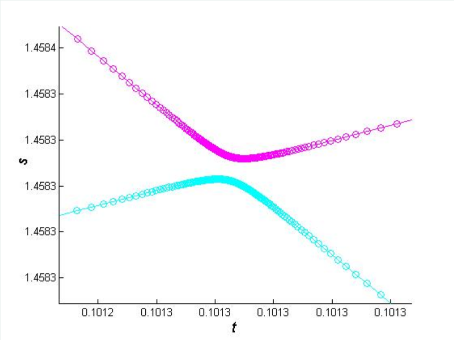


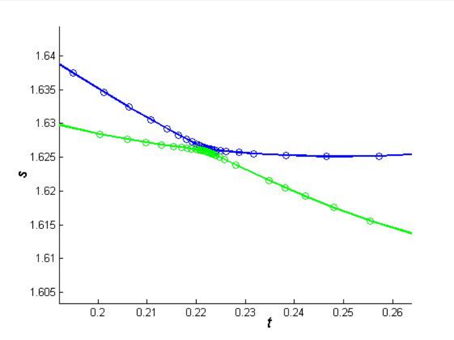
Zooms: former version





Zooms: revised





Ad:

- **Simple singular value**

Definition 1 *We say that* $s \in \mathbb{R}$ *is a* **singular value** *of the matrix* A *if there exist* $u \in \mathbb{R}^m$ *and* $v \in \mathbb{R}^n$ *such that*

$$Av - su = 0\,, \quad A^T u - sv = 0\,, \quad \|u\| = \|v\| = 1\,. \tag{3}$$

The vectors v *and* u *are called*
the right and the left singular vectors of the matrix A*.*

Definition 2 $s \in \mathbb{R}$ *is a* **simple singular value** *of the matrix* A *if there exist* $u \in \mathbb{R}^m$ *and* $v \in \mathbb{R}^n$ *such that*

$$(s, u, v)\,, \quad (s, -u, -v)\,, \quad (-s, -u, v)\,, \quad (-s, u, -v)$$

are, for the given s*, the only solutions to (3).*
A singular value s *which is not a simple singular value*
is called **nonsimple (multiple) singular value***.*

Lemma 1 A triplet $\mathbf{s \neq 0}$, $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ satisfies (1) if and only if

$$A^T A v = s^2 v\,, \quad u = \frac{1}{s} A v\,, \quad \|v\| = 1\,, \quad s \neq 0\,.$$

Note that a nonzero simple singular value s can be identified with a nonzero simple eigenvalue s^2 of the matrix $A^T A$.

Lemma 2 $\mathbf{s = 0}$ is a simple singular value of A if and only if $m = n$ and $\dim \mathrm{Ker} A = 1$.

Let us remark that if $m > n$ then the problem

$$Av = 0\,, \quad A^T u = 0\,, \quad \|u\| = \|v\| = 1\,,$$

has infinitely many solutions.

Ad:

- **Pseudospectra**: motivation

Pseudospectra

$A \in \mathbb{R}^{n \times n}$ ... **nonsymmetric**: small perturbations can move the eigenvalues dramatically

Effects:

- transient growth for A^k (discrete time stability)
- transient growth for $exp(t * A)$ (continuous time stability)
- ill-conditioned eigenvalue computations
- convergence of matrix iterations

Remedies?
Computing pseudospectra: early warning