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An Improved Arc Algorithm for Detecting Definite Hermitian Pencils

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Definite Generalized Eigenproblem

$$Ax = \lambda Bx$$

with A, B Hermitian and B positive definite. Equivalent to

$$Hy \equiv B^{-1/2}AB^{-1/2}y = \lambda y.$$

- All eigenvalues real.
- A and B are simultaneously diagonalizable.

Numerical Solution

- Cholesky–QR.
- Cholesky–Jacobi.

Definite Pair

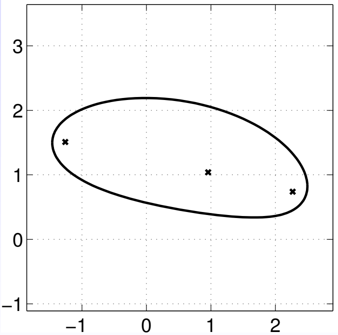
(A, B) is a **definite pair** if

$$\gamma(A, B) := \min_{\substack{z \in \mathbb{C}^n \\ \|z\|_2 = 1}} \sqrt{(z^* A z)^2 + (z^* B z)^2} > 0,$$

where γ is the **Crawford number**.

Equiv: $B(t) = A \sin t + B \cos t$ is pos def, some $t \in \mathbb{R}$.

Field of values of $A + iB$: $\{ z^* A z + i\, z^* B z : z^* z = 1 \}$.



Why Test for Definiteness?

- Theoretical and computational (if "t" known) advantages accrue in $Ax = \lambda Bx$.
- Detect hyperbolicity of quadratic matrix polynomials.
- Allow CG iterations for nonsymmetric saddle point linear systems.

Numerical Methods for Testing Definiteness

Is $A \sin t + B \cos t$ *positive definite for some* $t \in \mathbb{R}$ *?*

- J-orthogonal Jacobi alg (Veselic, 1993).
- Level set alg (H, Tisseur & Van Dooren, 2002).
- Crawford & Moon alg, 1983.
  - PDFIND: Algorithm 646, ACM TOMS, 1986.
  - Received little attention in the literature.
  - Lack of clarity in derivation and statement of alg and explanation of its properties.

Notation

- For a Hermitian pair (A, B) define

$$f(x) = \frac{x^*(A + iB)x}{|x^*(A + iB)x|}, \quad x \in \mathbb{C}^n, \quad x^*(A + iB)x \neq 0.$$

  $f(x)$ lies on the unit circle.

- $\theta[a, b]$ is length of shorter arc on unit circle connecting a and b. When $a = -b$, define $\theta[a, b] = \pi$.

Range of $f(x) = x^*(A + iB)x/|x^*(A + iB)x|$

Lemma 1 (Au-Yeung, 1969)

The range of f is one of the following types.

(i) A closed arc on the unit circle of length $< \pi$ (only possibility for definite(A, B)).

(ii) Two diametrically opposite points on the unit circle.

(iii) Whole unit circle.

(iv) Half circle with or without one or both endpoints.

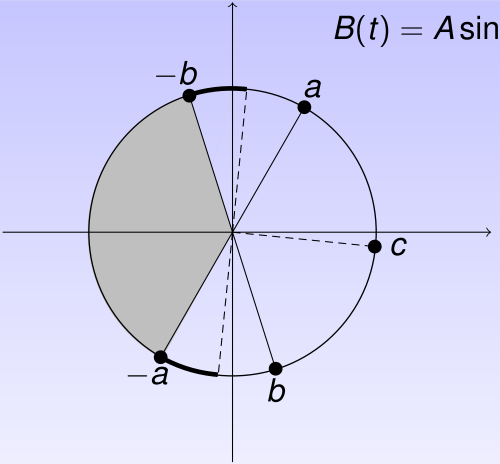
Lemma 2

If $c = e^{it}$ and $B(t) = A \sin t + B \cos t$ is not pos def, then for any x with $x^* B(t) x \le 0$ and $x^*(A + iB)x \neq 0$,

$\theta[f(x), c] \ge \pi/2.$

Pictorial Explanation

$$B(t) = A \sin t + B \cos t$$



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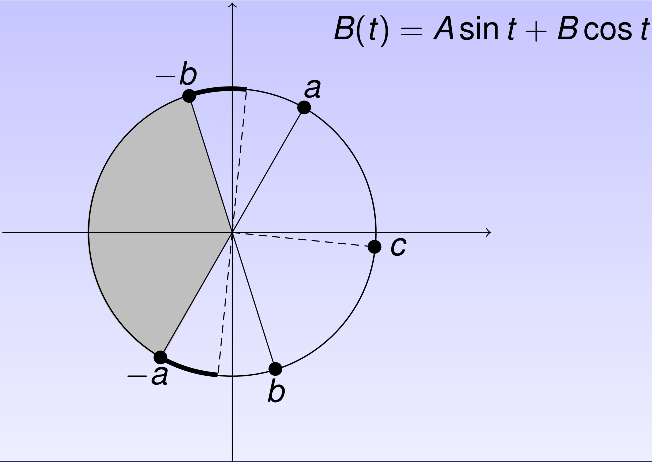

Lemma

On the kth step, $\theta[a_k, b_k] \geq \pi(1 - 2^{-k})$, regardless of whether the pair (A, B) is definite or not.

Improved Arc Algorithm

Starting phase: determine (A, B) indef. or starting arc $[a, b]$.
Main loop: $\theta = \theta[a, b]$

1 $c = ae^{i\theta/2} = \sin t + i \cos t$
2 if $B(t) > 0$, quit **(pair definite)**, end
3 Find unit norm vector x s.t. $x^* B(t) x \leq 0$.
4 if $x^*(A + iB)x = 0$, quit **(pair is indefinite)**, end
5 $d = f(x)$
6 $\theta = \theta/2 + \theta[c, f(x)]$
7 if $\theta \geq \pi -$ tol
8   quit **(pair is indefinite)**, end
9 elseif $\theta[a, d] < \theta[b, d]$
10   $a = d$, goto line 1
11 else
12   $b = d$, goto line 1
13 end

The Improvements

- New starting phase; no assumption on definiteness of (A, B). Handles (I, I).
- Tests whether $f(x)$ defined before computing it.
- Introduced tolerance tol.
- Midpoint computed stably. Original formula $c = (a+b)/|a+b|$ is unstable!
- Allow for non-expansion of arc due to rounding errors.
- …

Stability of Determination

- Determination of definiteness on lines 2, 4, is **numerically stable**: correct decision for $(A + \Delta A, B + \Delta B)$ with

$$\| [\, \Delta A \quad \Delta B \,] \|_2 \le c_n u \| [\, A \quad B \,] \|_2,$$

  c_n a constant, u the unit roundoff.

- $\gamma(A, B)$: distance from (A, B) to nearest indefinite pair. $\theta[\widetilde{\alpha}, \widetilde{\beta}]$: length of range($f$).

$$\frac{\gamma(A, B)}{\| [\, A \quad B \,] \|_2} \le \frac{1}{\sqrt{2}} (\pi - \theta[\widetilde{\alpha}, \widetilde{\beta}]),$$

  Wrong determination of indefiniteness on line 8 only when (A, B) close to an indefinite pair.

Testing Definiteness, Negative Curvature (1)

- Is $C = B(t) = A \sin t + B \cos t > 0$?
- If not, compute $x \neq 0$ s.t. $x^* C x \leq 0$.

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At step k of Cholesky,

$$P^T C P = \begin{bmatrix} R_{11}^* \\ R_{12}^* \end{bmatrix} \overset{\qquad k \qquad\quad n-k}{\begin{bmatrix} R_{11} & R_{12} \end{bmatrix}} + \begin{matrix} k \\ n-k \end{matrix} \overset{\;\; k \qquad n-k}{\begin{bmatrix} 0 & 0 \\ 0 & S_k \end{bmatrix}}.$$

If $s_{11}^{(k)} \leq 0$, $x = P \begin{bmatrix} R_{11}^{-1} R_{12} \\ -I \end{bmatrix} e_1$ satisfies $x^* C x \leq 0$.

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- $P = I$.
- Complete pivoting.
- "Early exit" complete pivoting.

Testing Definiteness, Negative Curvature (2)

Better for $C = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, with $|s_{pq}| := \max_{i,j} |s_{ij}|$:

$$y = \begin{cases} e_p, & p = q, \\ \frac{1}{\sqrt{2}}(e_p - \mathrm{sign}(s_{pq})e_q), & p \neq q. \end{cases}$$

Lemma

If $\lambda_{\min}(S) \leq 0$ and $s_{ii} \leq 0$ for all i then y satisfies $y^*Sy \leq \lambda_{\min}(S)/(n-k)$.

- Hard to predict which choice of x minimizes # iterations.

Testing Definiteness, Negative Curvature (3)

Error in computing $x = P \begin{bmatrix} R_{11}^{-1} R_{12} \\ -I \end{bmatrix} e_1$ is proportional to

$\mathrm{cond}(R_{11}) = \| \, |R_{11}^{-1}||R_{11}| \, \|_\infty$.

- With no pivoting (Crawford & Moon), no bound on $\mathrm{cond}(R_{11})$.
- With complete pivoting, $\mathrm{cond}(R_{11}) \le 2^k - 1$.

- Inaccurate DNC direction x can cause arc not to expand, or even shrink.
- Allowed to continue, the alg “restarts”.

Experiment 1

10×10 indefinite pair from Crawford (1986).

Chol : Cholesky without pivoting,

Chol(cp) : Cholesky with complete pivoting,

eig : take as DNC $x_{\min}$ in $(x_{\min}, \lambda_{\min})$.

	iters	curvatures $x^*B(t)x/\|x^*(A+iB)x\|$
PDFIND	8	-1.8e-16, 1.3e-17, -1.9e-1, -3.3e-16, -1.6e-16, -1.6e-16, -3.1e-3, -2.5e-1
Chol	6	2.7e-17, -3.8e-1, -6.1e-16, -3.6e-2, -6.3e-3, -4.9e-1
Chol(cp)	2	-9.9e-1, -4.6e-1
eig	2	-9.7e-1, -1.9e-1

Experiment 2

Definite pair (A_n, B_n):
$A_n \geq 0$, singular; B_n singular, indefinite.

Number of iterations:

	PDFIND	Chol	Chol(cp)	eig
$n = 64$, tol $= nu$	21	38	2	5
$n = 64$, tol $= 0$	21	43	> 100	18
$n = 80$, tol $= nu$	21	38	2	4
$n = 80$, tol $= 0$	21	43	8	>100

- (A_n, B_n) within distance $u \approx 10^{-16}$ of being indefinite.
- Algs determine pair is indefinite.
- Tolerance tol plays a key role.

Application 1: Testing for Hyperbolicity

Hermitian $Q(\lambda) = \lambda^2 A + \lambda B + C$ with $A > 0$ is **hyperbolic** if

$$(x^* Bx)^2 > 4(x^* Ax)(x^* Cx) \quad \text{for all nonzero vectors } x.$$

Equivalently $Q(\mu) < 0$ some $\mu \in \mathbb{R}$ **or**

$$(\mathcal{A}, \mathcal{B}) = \left(\begin{bmatrix} -C & 0 \\ 0 & A \end{bmatrix}, - \begin{bmatrix} B & A \\ A & 0 \end{bmatrix} \right) \quad \text{is definite.}$$

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For $s \neq 0$, ($s = \sin t$, $c = \cos t$)

$$s\mathcal{A} + c\mathcal{B} = \begin{bmatrix} I & -\frac{c}{s} I \\ 0 & I \end{bmatrix} \begin{bmatrix} -sC - cB - \frac{c^2}{s} A & 0 \\ 0 & sA \end{bmatrix} \begin{bmatrix} I & 0 \\ -\frac{c}{s} I & I \end{bmatrix}$$

$\Rightarrow$ $s\mathcal{A} + c\mathcal{B}$ is congruent to $s\,\mathrm{diag}(-Q(c/s), A)$.

Experiment 3

$Q_\beta(\lambda)$: `nlevp('spring',100,1,10*ones(100,1))` scaled to yield ill-conditioned congruences.

Chol-cong: use congruence, midpoint: $c = ae^{i\theta/2}$,

Chol-cong*: use congruence, midpoint: $c = (a + b)/|a + b|$.

Key: 1 = definite, 0 = indefinite, -1 = failure, (# iters).

β	Chol-cong	Chol-cong*	PDFIND
0.51965	1 (1)	0 (5)	0 (7)
0.51966	1 (1)	0 (5)	−1 (7)
0.51967	1 (1)	1 (6)	0 (7)
0.51969	1 (1)	0 (5)	−1 (7)
0.51970	1 (1)	0 (6)	−1 (7)
0.51971	1 (1)	0 (5)	1 (3)

Application 2: Saddle Point Problems

Involve matrices of the form

$$\mathcal{A} = \begin{bmatrix} A & B \\ B & -C \end{bmatrix},$$

where $A = A^T \in \mathbb{R}^{n \times n}$, $A > 0$ and $C = C^T \in \mathbb{R}^{m \times m}$, $C \geq 0$.

$\mathcal{A}$ is **indefinite**: n positive e'vals and $\text{rank}(C + BA^{-1}B^T)$ negative e'vals.

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$\mathcal{A}$ is **indefinite**: n positive e'vals and rank$(C + BA^{-1}B^T)$ negative e'vals.

Theorem (Liesen & Parlett, 2008)

If the symmetric pair $(\mathcal{A}, \mathcal{J})$ with $\mathcal{J} = \begin{bmatrix} I_n & 0 \\ 0 & -I_m \end{bmatrix}$ is definite then there exists a well-defined CG method for solving linear systems with $\mathcal{J}\mathcal{A}$.

Experiment 4

$$\mathcal{A} = \begin{bmatrix} A & B \\ B & -C \end{bmatrix}$$ from Stokes problem (IFISS).

$$\mathcal{A}(\alpha) = \begin{bmatrix} \alpha^2 A & \alpha B^T \\ \alpha B & -C \end{bmatrix} = \begin{bmatrix} \alpha I_n & 0 \\ 0 & -I_m \end{bmatrix} \begin{bmatrix} A & B^T \\ B & C \end{bmatrix} \begin{bmatrix} \alpha I_n & 0 \\ 0 & -I_m \end{bmatrix}.$$

Definiteness test and DNC computed with attempted sparse Cholesky ($n = 578$, $m = 256$).

α	definite	iters	stage at which Cholesky terminates							
0.1	no	5	579	56	56	57	57			
0.5	no	8	579	75	111	161	230	580	264	581
1.0	yes	5	579	82	129	200	834			
5.0	yes	2	579	834						

Sparse Cholesky often terminates at stage $k \ll n + m = 834$.

Application 3: Crawford Number

$$\gamma(A,B) = \min_{\substack{x\in\mathbb{C}^n \\ \|x\|_2=1}} |d(x)|, \quad d(x) = x^*(A+iB)x$$

$$= \max(0, \max_{-\pi\le\theta\le\pi} g(\theta)), \quad g(\theta) = \lambda_{\min}(A\cos\theta + B\sin\theta).$$

- Arc alg provides upper bound for free: $\gamma(A,B) \le \min\{d(x) : x \text{ is DNC}\}$.
- Arc alg returns t s.t. $B(t) > 0$. Then $\gamma(A,B) \ge \lambda_{\min}(B(t))$.

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$$= \max(0, \max_{-\pi\le\theta\le\pi} g(\theta)), \quad g(\theta) = \lambda_{\min}(A\cos\theta + B\sin\theta).$$

- Arc alg provides upper bound for free: $\gamma(A,B) \le \min\{d(x) : x \text{ is DNC}\}$.
- Arc alg returns t s.t. $B(t) > 0$. Then $\gamma(A,B) \ge \lambda_{\min}(B(t))$.
- Exploit definiteness of $B(t)$ to determine $t_1 \le t_2$ s.t. $B(\theta) > 0$ for all $\theta \in (t_1, t_2)$. Then $\gamma(A,B) = -\min_{t_1<\theta<t_2} -g(\theta)$ is a quasiconvex minimization problem.

Experiment 5

Four 25×25 definite pairs from Crawford (1986).

$\gamma(A, B) = \lambda_{\min}(B(t_{\mathrm{opt}}))$.
(γ_ℓ, γ_u): lower and upper bounds from arc alg.
(t_1, t_2): interval of definiteness.

k	$\gamma(A_k, B_k)$	t_{opt}	(γ_ℓ, γ_u)	(t_1, t_2)
1	1.4	0.79	(1.4,1.4)	(0.32,1.3)
2	6.0	-0.79	(5.5,8.1)	(-1.3,-0.54)
3	7e-9	1.6e-8	(4.7e-9,5.9e-2)	(0, 1.9e-7)
4	1.0	1.5e-8	(0.71,1.0)	(-4.7e-1, 1.6)

- (γ_ℓ, γ_u) provides good estimate of $\gamma(A, B)$.
- Length of (t_1, t_2) much smaller than 2π.

Concluding Remarks on Arc Algorithm

- **Fuller understanding** of its behaviour — in particular for indefinite pairs.
- Crucial to the efficiency & reliability of alg are: **initialization**, **termination**, and computation of **angles** & **directions of negative curvature**.
- **Remarkably efficient** in general (a few partial Cholesky factorizations). *Alg often doesn't need to determine* range(f) *accurately.*
- Recommend to use Cholesky w/complete pivoting for small dense problems and sparse Cholesky for large sparse problems.

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