MANCHESTER 1824

The University of Manchester

An Improved Arc Algorithm for Detecting Definite Hermitian Pencils

Nick Higham
School of Mathematics
The University of Manchester

higham@ma.man.ac.uk
http://www.ma.man.ac.uk/~higham/

Joint work with Chun-Hua Guo and Françoise Tisseur

MOPNET, Cardiff, March 2009

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

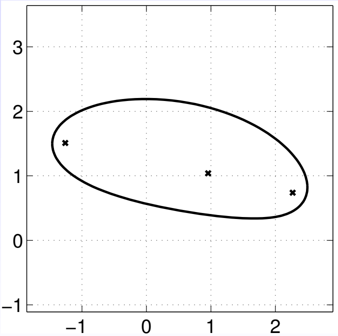
(A, B) is a **definite pair** if

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

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.

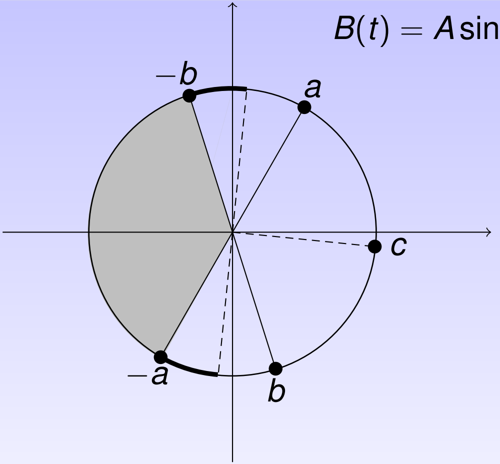
(iii) Whole unit circle.

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

Lemma 2

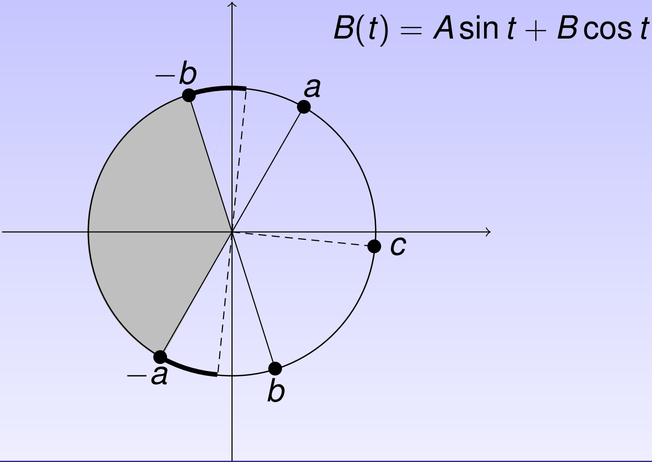
If $c = e^{it}$ and $B(t) = A \sin t + B \cos t$ is not pos def, then for any x with $x^* B(t) x \le 0$ and $x^*(A+iB)x \ne 0$, $\theta[f(x), c] \ge \pi/2$.

Pictorial Explanation



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

Pictorial Explanation



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. $x^* B(t) x \le 0$.
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 $\theta \ge \pi - \mathrm{tol}$
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. $x^* C x \leq 0$.

Testing Definiteness, Negative Curvature (1)

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

At step k of Cholesky,

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

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

Testing Definiteness, Negative Curvature (1)

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

At step k of Cholesky,

$$P^T C P = \begin{bmatrix} R_{11}^* \\ R_{12}^* \end{bmatrix} \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \begin{bmatrix} R_{11} & R_{12} \end{bmatrix} \end{array} + \begin{array}{c} \\ k \\ n-k \end{array} \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & S_k \end{bmatrix} \end{array}.$$

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

- $P = I$.
- 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 $y^* S y \leq \lambda_{\min}(S)/(n-k)$.

- 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 $x^*B(t)x/\lvert x^*(A+iB)x\rvert$
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**

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

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**

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

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 $\operatorname{rank}(C + BA^{-1}B^T)$ negative e'vals.

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.

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
  $\gamma(A,B) \ge \lambda_{\min}(B(t))$.

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 $\gamma(A,B) \ge \lambda_{\min}(B(t))$.
- 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).

$\gamma(A, B) = \lambda_{\min}(B(t_{\text{opt}}))$.
(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* $\mathrm{range}(f)$ *accurately.*
- Recommend to use Cholesky w/complete pivoting for small dense problems and sparse Cholesky for large sparse problems.

Bibliography I

Yik-Hoi Au-Yeung.
A theorem on a mapping from a sphere to the circle and the simultaneous diagonalization of two Hermitian matrices.
Proc. Amer. Math. Soc., 20:545–548, 1969.

Yik-Hoi Au-Yeung.
Some theorems on the real pencil and simultaneous diagonalization of two Hermitian bilinear functions.
Proc. Amer. Math. Soc., 23:246–253, 1969.

Timo Betcke, Nicholas J. Higham, Volker Mehrmann, Christian Schröder, and Françoise Tisseur.
NLEVP: A collection of nonlinear eigenvalue problems.
http://www.mims.manchester.ac.uk/research/numerical-analysis/nlevp.html.

Bibliography II

Charles R. Crawford.
ALGORITHM 646 PDFIND: A routine to find a positive definite linear combination of two real symmetric matrices.
ACM Trans. Math. Software, 12(3):278–282, 1986.

Charles R. Crawford and Yiu Sang Moon.
Finding a positive definite linear combination of two Hermitian matrices.
Linear Algebra Appl., 51:37–48, 1983.

Chun-Hua Guo, Nicholas J. Higham, and Françoise Tisseur.
An improved arc algorithm for detecting definite Hermitian pairs.
MIMS EPrint 2008.115, Manchester Institute for Mathematical Sciences, The University of Manchester, UK, November 2008.

Bibliography III

- Chun-Hua Guo, Nicholas J. Higham, and Françoise Tisseur.
  Detecting and solving hyperbolic quadratic eigenvalue problems.
  SIAM J. Matrix Anal. Appl., 30(4):1593–1613, 2009.

- Chun-Hua Guo and Peter Lancaster.
  Algorithms for hyperbolic quadratic eigenvalue problems.
  Math. Comp., 74(252):1777–1791, 2005.

- Jörg Liesen and Beresford N. Parlett.
  On nonsymmetric saddle point matrices that allow conjugate gradient iterations.
  Numer. Math., 108(4):605–624, 2008.

David J. Silvester, Howard C. Elman, and Alison Ramage.
Incompressible flow and iterative solver software (IFISS) version 2.2.
http://www.maths.manchester.ac.uk/~djs/ifiss/.