Krylov methods, determinants and bifurcations in PDEs

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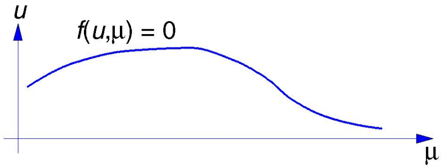
Ddays 2006

$$\frac{dx}{dt} = f(x, \mu), \qquad f : R^m \times R \mapsto R^m,$$

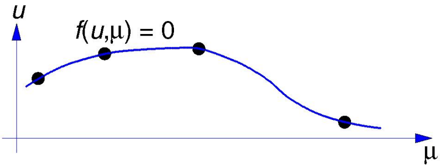
(Branches of) equilibria: $\qquad f(x, \mu) = 0.$

Computation when $m \gg 1$

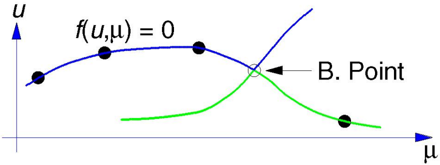
(Discretized PDEs)



$$f(u, \mu) = 0,$$



$$f(u,\mu) = 0,$$

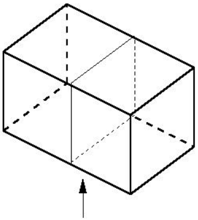


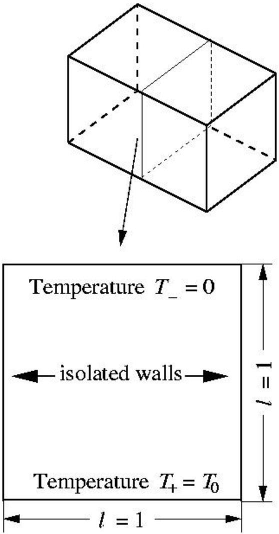
At every computed point, check $\sigma(f_u) \cap \mathbb{R}_+$

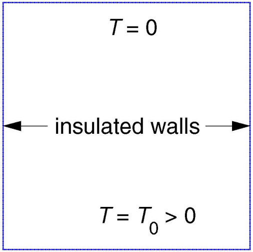
- (m small) by computing $\sigma(f_u)$ (QR iteration), or
- ($m \gg 1$) by computing the right-most part of $\sigma(f_u)$ (IRA) (ARPACK, MATLAB's `eigs`)

Outline

Bénard Convection Problem

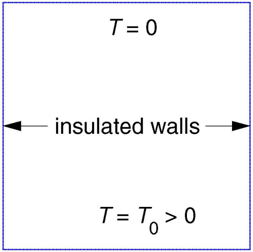



Temperature $T_- = 0$
isolated walls
$l = 1$
Temperature $T_+ = T_0$
$l = 1$



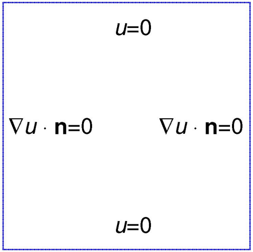
T_0 small:

- linear temperature distribution: $T(y,z) = T_0(1-z)$
- no fluid flow (fuid velocity $\mathbf{v} = 0$)



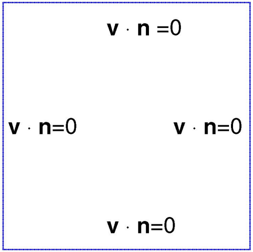
T_0 Large:

- temperature: $T = T_0(1 - z) + u(y, z, t)$
- non zero fuid velocity $\mathbf{v} = \mathbf{v}(y, z, t)$



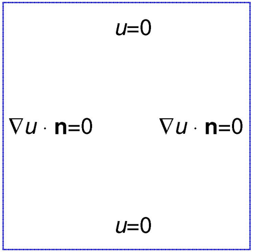
$$u_t + \sqrt{\mu}\mathbf{v}(u) \cdot (\nabla u - \mathbf{e}_3) = \Delta u.$$

$$\mu = Ra, \qquad \mathbf{e}_3 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$



$$u_t + \sqrt{\mu}\mathbf{v}(u)\cdot(\nabla u - \mathbf{e}_3) = \Delta u.$$

$$\left.\begin{aligned} -\nabla p + \mathbf{v} + \sqrt{\mu}u\mathbf{e}_3 &= 0, \\ \nabla\cdot\mathbf{v} &= 0. \end{aligned}\right\}$$



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$$u(y, z, \mu) = \sum \tilde{u}_{k,j} \cos(\pi j y) \sin(\pi k z).$$

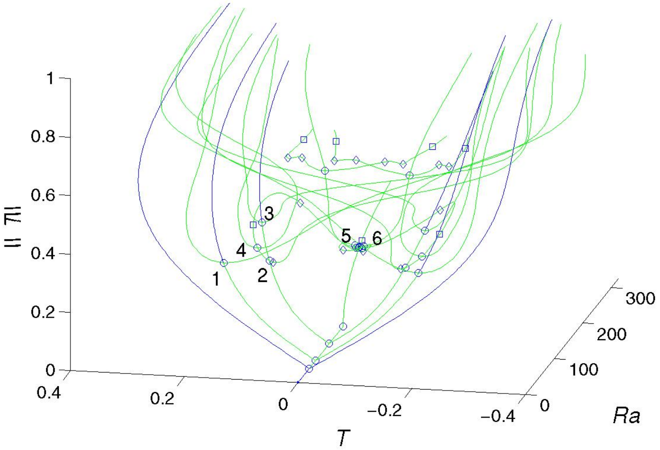
Truncation:

$$0 \leq j \leq N + 1, \qquad 1 \leq k \leq N - 1$$

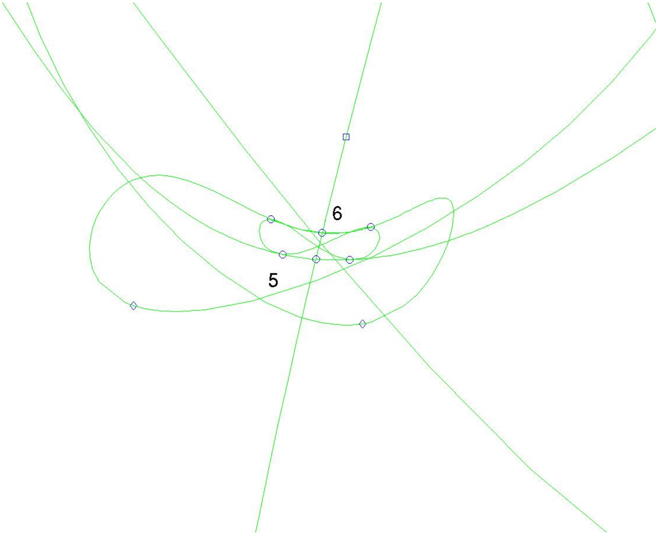
$$N = 24, 48.$$

$$\mathbf{u} = \begin{bmatrix} u \\ \mu \end{bmatrix} \in \mathbb{R}^m,$$

$$m = 576, 2304$$



○: pitchfork/transcritical ◇: saddle-node □: Hopf



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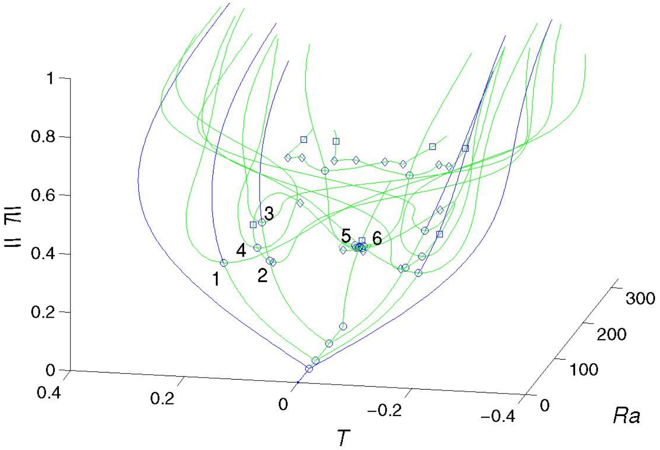

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Cost

- Regular + 1 bif. point computation.
- 21 regular points from 2 to 3.
- $N = 24$ ($m = 576$)

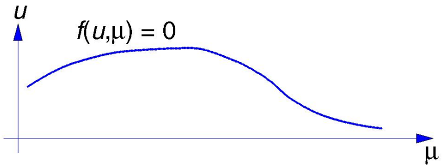
standard:	782 s
iterative:	25 s

Cost (and II)

Regular points
(with and without stability eigen computations)

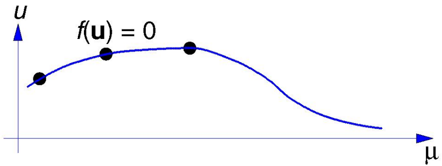
	with	wout	ratio
standard:	667 s	42 s	16.0
iterative:	20 s	0.1 s	200
ratio:	33.4	420	

Keller's pseudo-arclength continuation

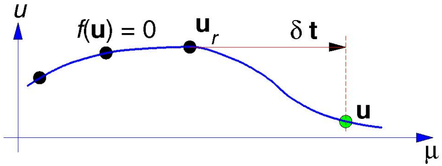


$$f(u, \mu) = 0,$$

Keller's pseudo-arclength continuation



$$\mathbf{u} = \begin{bmatrix} u \\ \mu \end{bmatrix}$$

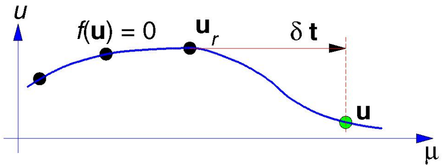


$$\mathbf{u} = \begin{bmatrix} u \\ \mu \end{bmatrix} \quad \text{solution of} \quad F(\mathbf{u}) = \mathbf{0}.$$

$$\text{where} \quad F(\mathbf{u}) = \begin{bmatrix} f(\mathbf{u}) \\ \mathbf{t}^T(\mathbf{u} - \mathbf{u}_r) - \delta \end{bmatrix}$$

$$\text{and} \quad \mathbf{t} = \begin{bmatrix} t \\ \tau \end{bmatrix} \approx \text{ unit tangent.}$$

Keller's pseudo-arclength continuation II



$$F(\mathbf{u}) = \mathbf{0}.$$

Solution by Newton's method: Linear systems $\quad F_{\mathbf{u}}\mathbf{d} = -F.$

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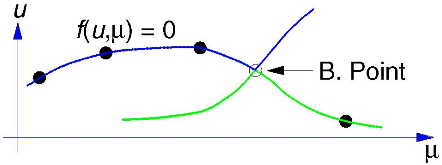

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$\det(F_{\mathbf{u}})$ changes sign at Branching Points.

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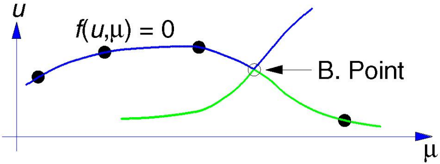

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- Case m small: std. LU decomp. $\Rightarrow$ det available.

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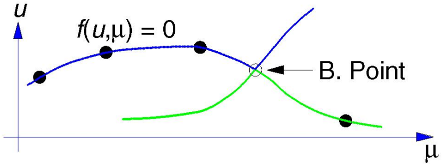

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- Case m large & iterative method: How to compute $\det(F_{\mathbf{u}})$?

Krylov Methods for $Ax = b$

- Krylov space $\mathcal{V}_k = \mathrm{span}(\mathbf{v}_1, A\mathbf{v}_1 \ldots, A^{k-1}\mathbf{v}_1)$.
- Arnoldi vectors $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$, *orthonormal* basis of $\mathcal{V}_k$
- matrix. $V_k = [\mathbf{v}_1, \ldots, \mathbf{v}_k]$
- Arnoldi decompostion of A ($m \times m$ matrix)

$$AV_k = V_k H_k + \epsilon[0, \ldots, 0, \mathbf{v}_{k+1}], \qquad k \ll m \quad \text{(hopefully)}$$

$H_k \quad k \times k$, (only $\mathbf{v} \mapsto A\mathbf{v}$ required)

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- GMRES (Saad & Schultz (1986)) for $A\mathbf{x} = \mathbf{b}$: $\quad \mathbf{v}_1 = \mathbf{b}/\left\|\mathbf{b}\right\|$

$$\begin{bmatrix} H_k \\ \epsilon e_k^T \end{bmatrix} y = \left\|\mathbf{b}\right\| e_1, \qquad \text{and} \quad \mathbf{x} \approx \mathbf{x}_k = V_k y.$$

$$(e_1, \ldots, e_k, \text{coordinate vectors in } \mathbb{R}^k)$$

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- Newton's method for $F(\mathbf{u}) = 0 \quad \Rightarrow \quad F_{\mathbf{u}}\mathbf{d} = -F$

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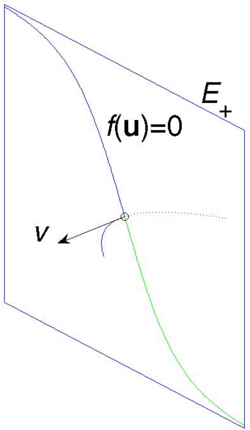
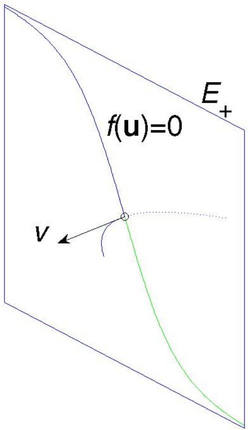
IDEA: $\mathrm{sign}(\det(F_{\mathbf{u}})) \approx \mathrm{sign}(\det(H_k))\mathrm{sign}(\det(\mathcal{P}))$?

Need to be Careful with Symmetries



$$E_+ = \mathrm{Ker}(S - I), \qquad (S \text{ symmetry,})$$

Need to be Careful with Symmetries



$$E_+ = \mathrm{Ker}(S - I), \qquad F_{\mathbf{u}}\mathbf{v} = 0, \qquad \mathbf{v} \notin E_+$$

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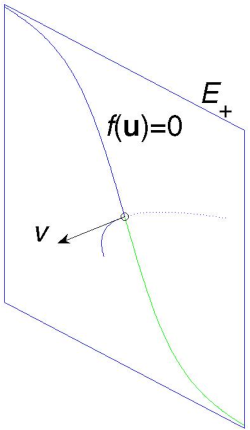

$$E_+ = \mathrm{Ker}(S - I), \qquad \mathcal{P}^{-1} F_{\mathbf{u}} E_+ \subset E_+$$

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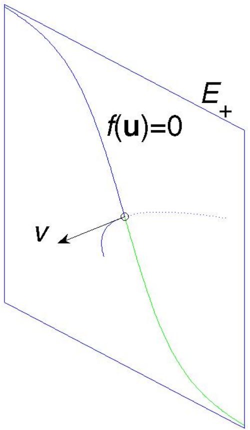
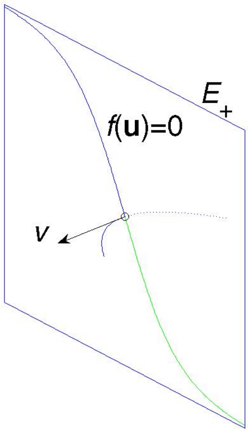


$$E_+ = \mathrm{Ker}(S - I), \qquad \mathbf{v}_1 \in E_+ \quad \Rightarrow \quad H_k \quad \text{of} \quad \mathcal{P}^{-1} F_{\mathbf{u}}|_{E_+}$$



$E_+ = \mathrm{Ker}(S - I)$, $\det(F_{\mathbf{u}|_{E_+}})$ does not change sing at B.P.

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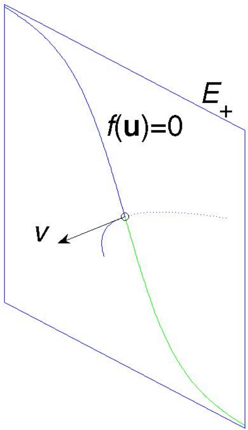

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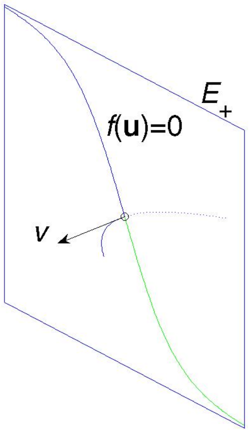
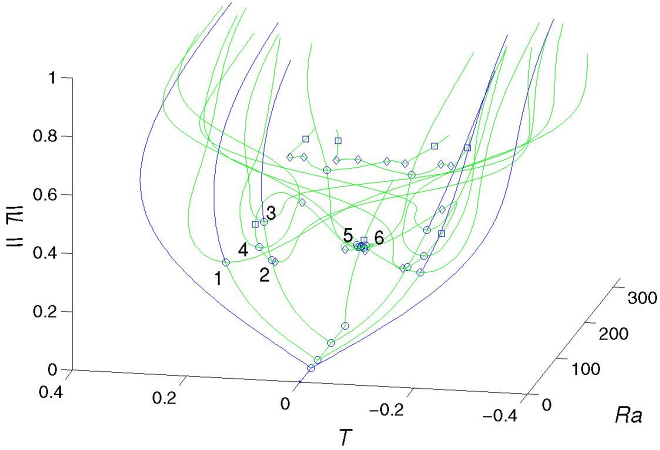
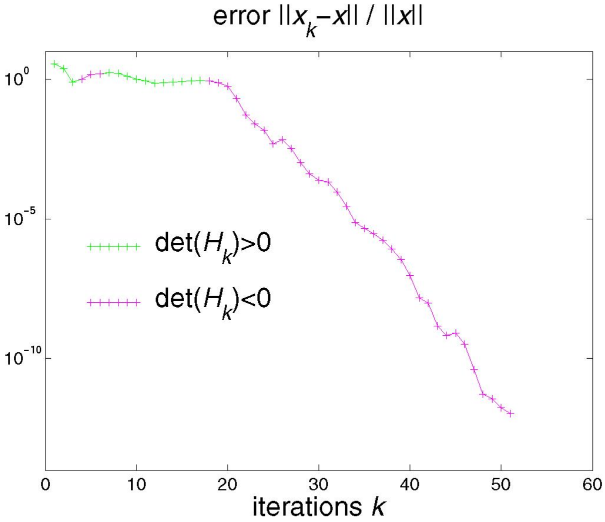


$E_+ = \mathrm{Ker}(S - I), \qquad \mathbf{v}_1 = (\mathbf{b} - A\mathbf{x}_0)/\left\|\mathbf{b} - A\mathbf{x}_0\right\|, \qquad \mathbf{x}_0 \text{ random}$



$$TOL = 5 \times 10^{-4}, \quad 5 \times 10^{-6}, \quad 5 \times 10^{-8},$$

Typical Results



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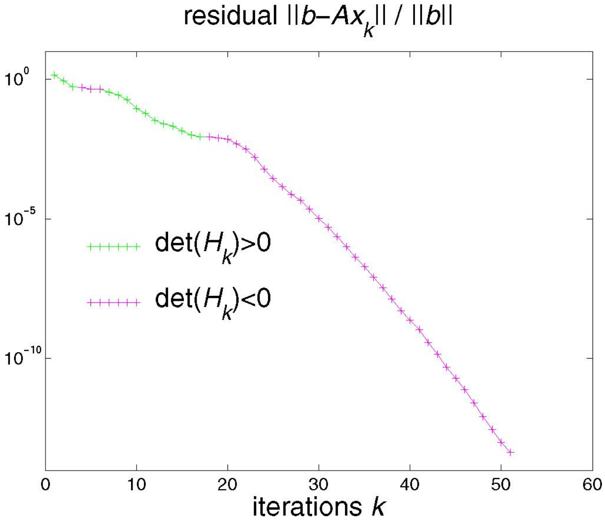


$m = \infty$:
$$f(u,\mu) = \Delta u + R(u,\mu),$$

$$\Delta^{-1} f_u = I + \Delta^{-1} R_u, \qquad \Delta^{-1} R_u \text{ compact.}$$

$$\mathcal{P}^{-1} F_{\mathbf{u}} = I + T, \qquad T \text{ compact.}$$

Singular values of T

(Nevanlinna (1993), I. Moret (1997), Eiermann & Ernst (2000), . . .)

$m < \infty$

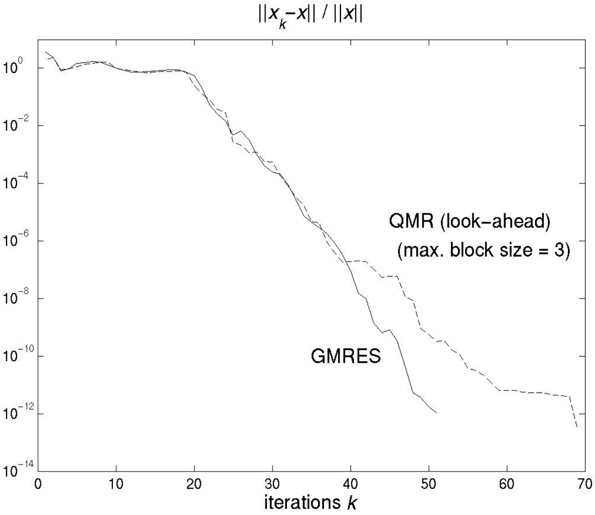
$$\mathcal{P}^{-1} F_{\mathbf{u}}^{(m)} \underset{m\to\infty}{\longrightarrow} I + T,$$

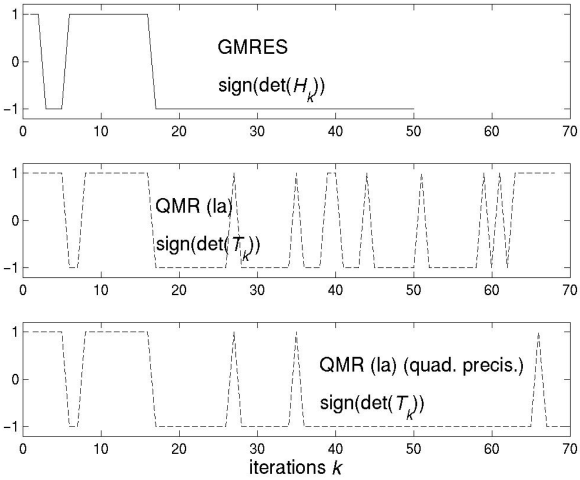
Other (Krylov) Methods

- BICG (Lanczos (1952))
- CGS (Sonneveld (1989))
- QMR (Freund & Nachtigal (1991))
  (non-orthogonal basis)
- BiCGSTAB (van der Vorst (1992))
- (*) QMR with look ahead (Freund & Nachtigal (1994))
  (Robustness improved)

- GMRES (Saad & Schultz (1986))

$$V_k^T V_k = I \quad \Rightarrow \quad \text{theory.}$$


||x_k−x|| / ||x||
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
0
10
20
30
40
50
60
70
iterations k
QMR (look−ahead)
(max. block size = 3)
GMRES


GMRES
sign(det(H_k))
QMR (la)
sign(det(T_k))
QMR (la) (quad. precis.)
sign(det(T_k))
iterations k

Conclusions

- Eigenvalues
  - Exorbitant computational cost with iterative Lin. Alg.
  - Test functions partial solution
- GMRES method
  - Allows computation of $\mathrm{sign}(\det)$
  - Robust
  - Theory
- Other Krylov methods (for non symmetric matrices)
  - Neither robust nor theory-backed
  - More work needed