On the Forsythe conjecture

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joint work with

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George E. Forsythe

Godfather of "Computer Science"

1917–1972

- National Bureau of Standards (1948), Standards Western Automatic Comp.
- Stanford University (1957), founded Computer science department (1965). He hired Gene H. Golub in 1962.
- "*It is generally agreed that he, more than any other man, is responsible for the rapid development of computer science in the world's colleges and universities.*"

  [Donald Knuth]
- 17 Ph.D., e.g. Beresford N. Parlett, Cleve B. Moler, James M. Varah, Richard P. Brent, J. Alan George.

Problem

Problem

A is symmetric and positive definite, b given

Minimize

$$f(x) = \frac{1}{2} x^T A x - x^T b$$

using the **steepest descent** method

input A, b, x_0
for $k = 0, 1, 2, \ldots$ **do**

$$\begin{aligned} g_k &= A x_k - b \\ x_{k+1} &= x_k - \alpha_k \, g_k \end{aligned}$$

end for

Asymptotic behavior of normalized gradients?

Asymptotic behavior

Forsythe and Motzkin conjecture

- Consider the **steepest descent** method and denote

$$v_k \equiv \frac{g_k}{\|g_k\|} .$$

Note that $v_k \perp v_{k+1}$.

- [Forsythe & Motzkin, 1951] conjectured that vectors v_k asymptotically alternate between **two directions**,

$$v_{2k} \to v , \quad v_{2k+1} \to w .$$

- [Akaike 1959]: Proof using methods from probability theory.

  [Forsythe 1968]: Algebraic proof and generalization.

- [Zou & Magoulés, 2022, SIREV]: Still of interest in optimization.

Problem

Forsythe 1968

Minimize

$$f(x) = \frac{1}{2} x^T A x - x^T b$$

using the **s-gradient method**:

input A, b, x_0
for $k = 0, 1, 2, \ldots$ **do**

$$g_k = A x_k - b$$

$$x_{k+1} = \arg\min_{y \in \mathcal{K}_s(A, g_k)} f(x_k + y)$$

end for

This is nothing but restarted CG $\rightarrow$ CG(s).

Asymptotic behavior
and the Forsythe conjecture

- Consider the CG(s) method applied to $Ax = b$, $s > 1$.
- Let x_0 be such that $d(A, g_0) > s$. Then

$$v_k \equiv \frac{g_k}{\|g_k\|}$$

are well defined.

Forsythe's conjecture

Vectors v_k asymptotically alternate between **two directions**,

$$v_{2k} \to v\,, \quad v_{2k+1} \to w\,.$$

- Observation: v_k are the Lanczos vectors and $v_k \perp v_{k+1}$.

Arnoldi projection of v

with respect to A and s

- $A \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$, and $s \geq 1$, we define $w \in \mathbb{R}^n$:

$$w \in \underbrace{A^s v + \mathcal{K}_s(A, v)}_{p(A)v} \quad \text{and} \quad w \perp \mathcal{K}_s(A, v).$$

- $w \neq 0$ is unique if $d(A, v) > s$, denote

$$w = P_s(A; v)\, v\,.$$

- w can be computed using the **Lanczos** algorithm (if A is symmetric) or the **Arnoldi** algorithm.

- Note that $P_s(A; v)$ is independent of scaling of v.

A more general formulation

of the Forsythe conjecture via the Lanczos (Arnoldi) process

- $A \in \mathbb{R}^{n \times n}$ **symmetric**, $v \in \mathbb{R}^n$ with $d(A, v) > s \geq 1$

- **Conjecture**: Consider the algorithm

$w_0 = v$
for $k = 0, 1, 2, \ldots$ **do**

$$\begin{aligned} v_k &= w_k \,/\, \|w_k\| \\ w_{k+1} &= P_s(A; v_k)\, v_k \end{aligned}$$

end for

Then the sequence $\{v_{2k}\}$ has a **single limit** vector.

- The vectors v_k are well defined.

Symmetric matrices

Norms of w_k

It holds that

$$w_{k+1} \;=\; P_s(A; v_k)\, v_k$$

and

$$\|w_{k+1}\| \;=\; \min_{p \in \mathcal{M}_s} \|p(A) v_k\| \;\leq\; \min_{p \in \mathcal{M}_s} \|p(A)\|\,.$$

Theorem

It holds that

$$\|w_k\| \;\leq\; \|w_{k+1}\| \qquad k = 0, 1, 2, \ldots$$

with equality iff $v_k = v_{k+2}$.

Consequence:

$$\|w_k\| \;\longrightarrow\; \tau \quad \text{as} \quad k \to \infty\,.$$

Distance between v_{k+2} and v_k

$$
\begin{aligned}
1 - \frac{1}{2}\|v_{k+2} - v_k\|^2 &= \langle v_{k+2}, v_k \rangle = \frac{1}{\|w_{k+2}\|}\langle w_{k+2}, v_k \rangle \\
&= \frac{1}{\|w_{k+2}\|}\langle P_s(A; v_{k+1})\, v_{k+1}, v_k \rangle \\
&= \frac{1}{\|w_{k+2}\|}\langle v_{k+1}, P_s(A; v_{k+1})\, v_k \rangle \\
&= \frac{1}{\|w_{k+2}\|}\langle v_{k+1}, A^s\, v_k \rangle \\
&= \frac{1}{\|w_{k+2}\|}\langle v_{k+1}, \underbrace{P_s(A; v_k)\, v_k}_{w_{k+1}} \rangle \\
&= \frac{\|w_{k+1}\|}{\|w_{k+2}\|} \;\to\; 1
\end{aligned}
$$

A short summary

$A \in \mathbb{R}^{n\times n}$ **symmetric**, $v \in \mathbb{R}^n$ with $d(A,v) > s \geq 1$

$w_0 = v$
for $k = 0, 1, 2, \ldots$ **do**

$$\begin{aligned} v_k &= w_k \,/\, \|w_k\| \\ w_{k+1} &= P_s(A; v_k)\, v_k \end{aligned}$$

end for

We know that

$$\|w_k\| \;\leq\; \|w_{k+1}\|\,, \qquad \|w_k\| \;\to\; \tau\,,$$

and

$$\|\, v_{k+2} - v_k \,\| \to 0\,.$$

Bolzano-Weierstraß $\to$ $\{v_{2k}\}$ has a convergent subsequence.

Example

- The property

$$\| v_{k+2} - v_k \| \to 0$$

is **not sufficient** for the existence of a **single** limit vector.

- Complex points

$$\mu_k \ = \ e^{\mathbf{i}\omega_k} \, , \qquad \omega_k \ = \ \sum_{j=1}^{k} \frac{\pi}{j}$$

satisfy $| \mu_k - \mu_{k+1} | \to 0$, but $\{\mu_k\}$ does not converge.

- It may be **difficult** to find a counterexample **numerically**.

The set of limit vectors

- Let Σ^A be the set of unit norm vectors such that $d(A, v) > s$.
- Define the **transformation** $T_A : \Sigma^A \to \Sigma^A$

$$v \mapsto T_A(v) \equiv \frac{P_s(A; v)\, v}{\|P_s(A; v)\, v\|}$$

so that

$$v_{k+2} = T_A(T_A(v_k))\,.$$

- $T_A \circ T_A : \Sigma^A \to \Sigma^A$ is well defined and **continuous**.

Theorem

The set Σ_*^A of limit vectors of the sequence $\{v_{2k}\}$ satisfies:

(1) Σ_*^A is a **closed** and **connected** set in $\mathbb{R}^n$.

(2) $\Sigma_*^A \subseteq \Sigma^A$, and each $v_* \in \Sigma_*^A$ satisfies $v_* = T_A(T_A(v_*))$.

Degree of limit vectors v_*

$A \in \mathbb{R}^{n\times n}$ **symmetric**, $v \in \mathbb{R}^n$ with $d(A,v) > s \geq 1$

$w_0 = v$
for $k = 0, 1, 2, \ldots$ **do**

$$v_{k+1} = T_A(v_k)$$

end for

Theorem

Each limit vector v_* of $\{v_{2k}\}$ satisfies

$$s < d(A, v_*) \leq 2s\,.$$

Proof based on $v_* = T_A(T_A(v_*))$.

The case $s = 1$

Without loss of generality A is diagonal

- $\forall$ limit vector v_* of $\{v_{2k}\}$ we have $d(A, v_*) = 2$,

  $$v_* \; = \; \alpha\, e_i + \beta\, e_j$$

  for some canonical basis vectors e_i and e_j, $\alpha\beta \neq 0$, and

  $$\tau = \left\| A v_* - \left({v_*}^T A v_* \right) v_* \right\|$$

  giving

  $$\tau^2 = \alpha^2 \left(1 - \alpha^2\right) (\lambda_i - \lambda_j)^2. \qquad (*)$$

- **Finitely many** combinations of distinct $i, j \in \{1, 2, \ldots, n\}$, for each such combination **finitely many** values of α satisfying $(*)$.

- Σ_*^A is **connected** $\Rightarrow$ there is just **one** limit vector.

The same approach

does not work for $s = 2$

- $\tau = \|P_s(A; v)v\|$ gives

$$\tau^2 = v^T A^4 v + \frac{\left(v^T A^3 v\right)^2 - \left(v^T A^2 v\right)^3}{\left(v^T A v\right)^2 - v^T A^2 v}.$$

- $d(A, v_*) = 3$ or $d(A, v_*) = 4$:

$$v_* \ = \ \alpha\, e_i + \beta\, e_j + \gamma\, e_\ell$$

  $\alpha^2 + \beta^2 + \gamma^2 = 1.$

- **One** nonlinear equation with **two** degrees of freedom.

- **Infinitely many** solutions.

The case $s = 2$

$$\|w_{k+1}\|\, v_{k+1} \;=\; w_{k+1} \;=\; P_s(A; v_k) v_k$$

so that

$$\underbrace{\|w_{k+1}\|\,\|w_{k+2}}_{\to \tau^2}\|\, v_{k+2} = \underbrace{P_s(A; v_{k+1}) P_s(A; v_k)}_{Q_{2s}(A; v_k)}\, v_k$$

and each limit vector v_* of $\{v_{2k}\}$ satisfies

$$\tau^2\, v_* \;=\; Q_{2s}(A; v_*) v_* \,,$$

where v_* has either 3 or 4 nonzero components.

The case $s = 2$

and results of [Zhuk and Bondarenko, 1983]

- If v_* has 4 nonzero components with indexes $i_1, \ldots, i_4$, then

$$\tau^2 = Q_{2s}(\lambda_{i_j}; v_*), \qquad j = 1, \ldots, 4.$$

4 interpolation conditions $\rightarrow$ Q_{2s} is determined **uniquely**.

- If v_* has 3 nonzero components and if A is positive definite, then Q_{2s} is again **unique**. [Zhuk and Bondarenko, 1983]

- Finitely many combinations of sets of $i_j \in \{1, 2, \ldots, n\} \Rightarrow$ **finitely many** polynomials Q_{2s} that correspond to v_*'s.

- Quoting [Zabolotskaya, 1979] they use as a proven fact that the convergence of the coefficients of Q_{2s} implies the existence of a **single limit vector** v_*.

- We consider the case $s = 2$ to be still open.

Nonsymmetric matrices

Worst-case GMRES

and the cross equality

- For a given s, there exists a unit norm vector b such that

$$\| r \| \;=\; \min_{p \in \pi_s} \| p(A) b \| \;=\; \max_{\|v\|=1} \min_{p \in \pi_s} \| p(A) v \| \,.$$

Theorem [Zavorin '02; Faber, Liesen, T. '13]

If b is a worst-case GMRES initial vector for A and s, then

$$b \xrightarrow{\text{GMRES}(A,b,s)} r \xrightarrow{\text{GMRES}(A^T,r,s)} \| r \|^2 \, b \,.$$

- We say that b satisfies the **cross equality** for A and s if

$$b \xrightarrow{\text{GMRES}(A,b,s)} r \xrightarrow{\text{GMRES}(A^T,r,s)} z \in \text{span}\{b\}.$$

GMRES Cross iteration algorithm

and the Forsythe conjecture [Faber, Liesen, T., 2013]

Given A, s, and b, it seems that b_k **converge** to a vector satisfying the **cross equality** for A and s:

$b_0 = b$

for $k = 1, 2, \ldots$ **do**

$$\begin{aligned} r_k &= \mathrm{GMRES}(A,\, b_{k-1},\, s) \\ c_k &= r_k / \|r_k\| \\ z_k &= \mathrm{GMRES}(A^T,\, c_k,\, s) \\ b_k &= z_k / \|z_k\| \end{aligned}$$

end for

$$\|r_k\| \leq \|z_k\| \leq \|r_{k+1}\| \leq \|z_{k+1}\|$$

The algorithm does **not** find a **worst-case** initial vector in general.

Arnoldi Cross iteration algorithm

and generalization of the Forsythe conjecture for nonsymmetric matrices

Given $A \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$ such that $d(A, v) > s \geq 1$

$w_0 = v$

for $k = 0, 1, 2, \ldots$ **do**

$$\begin{aligned} v_k &= w_k \,/\, \|w_k\| \\ w_{k+1} &= P_s(B; v_k)\, v_k \end{aligned}$$

end for

where $B = A$ (for k even), $B = A^T$ (for k odd).

Conjecture

The subsequence $\{v_{2k}\}$ has a **single limit** vector.

Results [Faber, Liesen, T., 2023]

for nonsymmetric matrices

$$\|w_k\| \;\leq\; \|w_{k+1}\| \quad \text{and} \quad \|\, v_{k+2} - v_k \,\| \to 0\,.$$

$$T_A(v) \;\equiv\; \frac{P_s(A;v)\,v}{\|P_s(A;v)\,v\|}$$

Theorem

The set Σ_*^A of limit vectors of the sequence $\{v_{2k}\}$ satisfies:

(1) Σ_*^A is a **closed** and **connected** set in $\mathbb{R}^n$.

(2) $\Sigma_*^A \subseteq \Sigma^A$, and each $v_* \in \Sigma_*^A$ satisfies $v_* = T_{A^T}(T_A(v_*))$.

It holds that $s \;<\; d(A, v_*)$, but it **does not** hold in general that

$$d(A, v_*) \;\leq\; 2s\,.$$

Orthogonal matrices

Arnoldi Cross Iteration

for orthogonal matrices and $s = 1$

Given $A \in \mathbb{R}^{n\times n}$ **orthogonal**, $v \in \mathbb{R}^n$ such that $d(A, v) > s = 1$

$w_0 = v$
for $k = 0, 1, 2, \ldots$ **do**

$$\begin{aligned} v_k &= w_k \,/\, \|w_k\| \\ \alpha_k &= v_k^T A v_k \\ w_{k+1} &= (B - \alpha_k I) v_k \end{aligned}$$

end for

where $B = A$ (for k even), $B = A^T$ (for k odd).

$$\|w_{k+1}\|^2 = 1 - \alpha_k^2 \quad \Rightarrow \quad |\alpha_k| \geq |\alpha_{k+1}|\,.$$

Without loss of generality

A is block diagonal

$A \in \mathbb{R}^{n\times n}$ can be orthogonally block-diagonalized $A = U\,G\,U^T$ with U **orthogonal** and

$$G = \begin{bmatrix} G_1 & & & & & \\ & \ddots & & & & \\ & & G_m & & & \\ & & & [\pm 1] & & \\ & & & & \ddots & \\ & & & & & [\pm 1] \end{bmatrix}$$

where

$$G_j = \begin{bmatrix} c_j & s_j \\ -s_j & c_j \end{bmatrix}$$

with $c_j^2 + s_j^2 = 1$ and $s_j \neq 0$.

Convergence

for orthogonal matrices and $s = 1$

For simplicity

$$A = \begin{bmatrix} G_1 & & & \\ & G_2 & & \\ & & \ddots & \\ & & & G_m \end{bmatrix}, \quad v_k = \begin{bmatrix} v_k^{(1)} \\ v_k^{(2)} \\ \vdots \\ v_k^{(m)} \end{bmatrix}, \quad v_k^{(j)} \in \mathbb{R}^2 .$$

Lemma [Faber, Liesen, T., 2023]

Let $0 < c_1 < \cdots < c_m$ and $d(A, v) > 1$ and $v^{(1)} \neq 0$.

For k sufficiently large there exists $0 < \varrho < 1$ such that

$$\| v_{2k+2}^{(j)} \| \leq \varrho \| v_{2k}^{(j)} \|, \quad j = 2, \ldots, m ,$$

and

$$\| v_{2k+2}^{(1)} - v_{2k}^{(1)} \| \leq \varrho^k .$$

Convergence result

Orthogonal matrices, $s = 1$

Theorem [Faber, Liesen, T., 2023]

Let $0 < c_1 < \cdots < c_m$ and $d(A, v) > 1$ and $v^{(1)} \neq 0$.

Then the sequence $\{v_{2k}\}$ converges to a **single limit vector**.

Proof. Using the previous

$$\|v_{2k+2} - v_{2k}\|^2 \;=\; \sum_{j=1}^{m} \|v_{2k+2}^{(j)} - v_{2k}^{(j)}\|^2 \;\leq\; 3\,\varrho^{2k}$$

which implies

$$\sum_{k=0}^{\infty} \|\, v_{2k+2} - v_{2k} \,\| < \infty\,.$$

Connection to worst-case Arnoldi problem

Orthogonal matrices, $s = 1$

$$\max_{\|v\|=1} \min_{\alpha\in\mathbb{R}} \|Av - \alpha v\|^2 = \max_{\|v\|=1} \|Av - \langle v, Av\rangle v\|^2$$
$$= 1 - \min_{\|v\|=1} \langle v, Av\rangle^2$$

and the optimal α_* is given by

$$\alpha_* = \min_{\|v\|=1} |\langle v, Av\rangle| = \min_{z\in F(A)} |z| = c_1 .$$

We can prove that α_k in the Cross Iteration algorithm satisfy

$$\lim_{k\to\infty} \alpha_k = c_1 .$$

Hence, Cross Iteration algorithm finds a **worst-case vector**.

Conclusions

- We revised Forsythe's results and **generalized** them for symmetric and nonsymmetric matrices.

- **Conjecture** for symmetric and nonsymmetric matrices.

- For $s = 1$, we proved the existence of a **single limit** vector of the sequence $\{v_{2k}\}$ for symmetric and orthogonal matrices.

- We proved several new results about the limiting behavior of the sequence $\{v_{2k}\}$, but the conjecture still **remains open**.

Related papers

V. Faber, J. Liesen and P. Tichý, [On the Forsythe conjecture, submitted to SIMAX, 2022: https://arxiv.org/abs/2209.14579.]

- M. Afanasjew, M. Eiermann, O. G. Ernst, and S. Güttel, [A generalization of the steepest descent method for matrix functions, Electron. Trans. Numer. Anal., 28 (2007/08), pp. 206-222.]
- V. Faber, J. Liesen and P. Tichý, [Properties of worst-case GMRES, SIAM J. Matrix Anal. Appl., 34 (2013), pp. 1500-1519.]
- G. E. Forsythe, [On the asymptotic directions of the s-dimensional optimum gradient method, Numer. Math., 11 (1968), pp. 57-76.]
- P. F. Zhuk and L. N. Bondarenko, [A conjecture of G. E. Forsythe, Mat. Sb. (N.S.), 121(163) (1983), pp. 435-453.]

Thank you for your attention!