Subspace acceleration for the Crawford number computation

An eigenvalue optimization approach

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Abstract

In this work, we revisit eigenvalue optimization problems depending on one parameter, with a particular focus on their application to Crawford number computation. The Crawford number of a matrix A is defined as the distance between zero and the numerical range of A:

$$\gamma(A) = \min\{\,|z|\colon z \in \mathcal{F}(A)\,\}, \qquad \mathcal{F}(A) = \{\,v^*Av\colon v \in \mathbb{C}^n, \|v\|_2 = 1\,\}.$$

Our approach is based on an eigenvalue optimization characterization of the Crawford number.

- We establish local convergence of order $1+\sqrt{2} \approx 2.4$ for an existing subspace method applied to such eigenvalue optimization problems.
- We show that the relevant part of the objective eigenvalue function is strongly concave. This enables us to develop a subspace method that only uses three-dimensional subspaces but still achieves global convergence and a local convergence that is at least quadratic.

Eigenvalue optimization & subspace acceleration

Consider the univariate eigenvalue optimization problem over a closed interval $\Omega \subset \mathbb{R}$

$$\max_{\theta\in\Omega} \varphi(\theta) \quad \text{with} \quad \varphi(\theta) = \lambda_{\min}(H(\theta)), \tag{1}$$

where $H(\theta) \in \mathbb{C}^{n\times n}$ is Hermitian and real analytic for $\theta \in \Omega$.

Given an orthonormal basis $V \in \mathbb{C}^{n\times k}$ of a k-dimensional subspace of $\mathbb{C}^n$, the subspace acceleration techniques discussed, e.g., in [4, 5], proceed by considering the reduced objective function

$$\varphi(\theta; V) = \lambda_{\min}(V^*H(\theta)V).$$

Typically $k \ll n$ and it can therefore be expected that computing the maximum of $\varphi(\theta; V)$ on Ω is cheaper than solving (1).

Using the subspace spanned by eigenvectors from previous iteration to build the reduced objective function that determines the next iterate, we obtain the basic subspace Algorithm 1.

Algorithm 1. Subspace method for univariate eigenvalue optimization

Input: Real analytic Hermitian matrix-valued function $H(\theta)$, initial guess θ_0, tolerance $\mathsf{tol} > 0$.
Output: Approximation solution $\theta_{k+1}, \varphi_{k+1}$ of eigenvalue optimization problem (1).

1: Compute $\lambda_0 = \lambda_{\min}(H(\theta_0))$ and corresponding normalized eigenvector v_0.
2: Initialize $V_0 = v_0$.
3: **for** $k = 0, 1, \ldots, n-1$ **do**
4: Solve $\theta_{k+1} = \arg\max_{\theta\in\Omega} \lambda_{\min}(V_k^*H(\theta)V_k)$ and set $\varphi_{k+1} = \lambda_{\min}(V_k^*H(\theta_{k+1})V_k)$.
5: *Stopping criteria*: **if** $\varphi_{k+1} - \lambda_k < \mathsf{tol}\cdot|\varphi_{k+1}|$ **then** terminate.
6: Compute the smallest eigenvalue λ_{k+1} with normalized eigenvector v_{k+1} of $H(\theta_{k+1})$.
7: *Subspace update*: $V_{k+1} = \mathrm{orth}([V_k, v_{k+1}])$.
8: **end for**

Crawford number computation via EigOpt

We exploit the well-known eigenvalue optimization characterization [2] of the Crawford number:

$$\gamma(A) = \max\left\{ \max_{\theta\in[0,2\pi]} \lambda_{\min}(S\cos\theta + K\sin\theta), \quad 0 \right\},$$

where $S = (A + A^*)/2$ and $K = (A - A^*)/2\imath$. To obtain $\gamma(A)$, we maximize the objective function

$$\varphi(\theta) = \lambda_{\min}(H(\theta)) \quad \text{with} \quad H(\theta) = S\cos\theta + K\sin\theta. \tag{2}$$

Assuming the Crawford number $\gamma(A) > 0$, we have $\varphi(\theta)$ satisfy the following properties.

- **Strong concavity**: φ is strongly concave on the open set $\{\theta : \varphi(\theta) > 0\}$.
- **Bracketing**: Let θ_ℓ, θ_u be such that $\theta_\ell < \theta_u < \theta_\ell + 2\pi$. If $v(\theta_\ell), v(\theta_u) \in \mathcal{V}$ with $v(\theta)$ to be the eigenvector of $\lambda_{\min}(H(\theta))$, then $\arg\max_{\theta\in[\theta_\ell,\theta_\ell+2\pi]} \varphi(\theta; V) \in (\theta_\ell, \theta_u)$ iff $\arg\max_{\theta\in[\theta_\ell,\theta_\ell+2\pi]} \varphi(\theta) \in (\theta_\ell, \theta_u)$.

Full subspace method

Apply Algorithm 1 to $\varphi(\theta) = \lambda_{\min}(S\cos\theta + K\sin\theta)$. The reduced φ function takes the form

$$\varphi(\theta; V_k) = \lambda_{\min}(V_k^*H(\theta)V_k) = \lambda_{\min}(S_k\cos\theta + K_k\sin\theta),$$

where $S_k = V_k^*SV_k = (A_k + A_k^*)/2$ and $K_k = V_k^*KV_k = (A_k - A_k^*)/2\imath$, with $A_k = V_k^*AV_k$. So the reduced problem in line 4 of Algorithm 1 amounts to computing the Crawford number of A_k:

$$\gamma(A_k) = \max\left\{ \max_{\theta\in[0,2\pi]} \varphi(\theta; V_k),\ 0 \right\} \tag{3}$$

Since A_k is expected to be a small matrix, the computation of $\gamma(A_k)$, together with the optimal value θ_{k+1} , is not expensive and can be performed by many linearly convergent algorithms; see, e.g., [3, 6].

Theorem 1. *Let $\gamma(A) > 0$, and $\varphi(\theta_*) = \lambda_{\min}(H(\theta_*)) = \max_{\theta\in[0,2\pi]} \lambda_{\min}(H(\theta))$ is a simple eigenvalue. The full subspace method is globally convergent with local R-convergence rate*

$$\sigma = 1 + \sqrt{2} \approx 2.4142. \tag{4}$$

In other words, there is a sequence $(\varepsilon_k)_{k=0}^\infty$ such that $|\theta_k - \theta_*| \le \varepsilon_k$ and $\lim_{k\to\infty} |\varepsilon_k|/|\varepsilon_{k-1}|^\sigma < \infty$.

Three-vector version

The bracketing property allows us to develop a variant of the subspace method that only uses 3 vectors to generate the projection subspace but still enjoys favorable convergence properties.

Algorithm 2. 3-vector subspace method

Input: Matrix $A \in \mathbb{C}^{n\times n}$, initial guess $\theta_0 \in (0, 2\pi)$, tolerance $\mathsf{tol} > 0$.
Output: Approximation of Crawford number $\gamma(A)$.

1: Initialize: $\ell_0 = 0$, $u_0 = 2\pi$, and $V_0 = \mathrm{orth}([v(\ell_0), v(\theta_0), v(u_0)])$.
2: **for** $k = 0, 1, 2, \ldots$ **do**
3: $\theta_{k+1} = \arg\max_{[0,2\pi]} \lambda_{\min}(V_k^*H(\theta)V_k)$ with $\varphi_{k+1} = \lambda_{\min}(V_k^*H(\theta_{k+1})V_k)$.
4: **if** $\varphi_{k+1} \le 0$, **then** return $\gamma(A) = 0$.
5: *Stopping criteria*: **if** $k > 0$ **and** $\lambda_k - \varphi_{k+1} < \mathsf{tol}\cdot\varphi_{k+1}$, **then** return $\gamma = \varphi_{k+1}$.
6: *Interval update*:
if $\theta_{k+1} \in [\ell_k, \theta_k]$, **then** $(\ell_{k+1}, u_{k+1}) = (\ell_k, \theta_k)$, **otherwise** $(\ell_{k+1}, u_{k+1}) = (\theta_k, u_k)$.
7: Compute smallest eigenvalue λ_{k+1} and corresponding eigenvector $v(\theta_{k+1})$ of $H(\theta_{k+1})$.
8: *Subspace update:* $V_{k+1} = \mathrm{orth}([v(\ell_{k+1}), v(\theta_{k+1}), v(u_{k+1})])$
9: **end for**

Theorem 2. *Let $\gamma(A) > 0$. Then the iterates $\theta_1, \theta_2, \theta_3, \ldots$ produced by Algorithm 2 are globally convergent to θ_*. The convergence is locally at least quadratic, provided that $\lambda_{\min}(H(\theta_*))$ is a simple eigenvalue. Moreover, if the sequence is also locally alternating around θ_*, i.e.,*

$$(\theta_{k+1} - \theta_*)(\theta_k - \theta_*) < 0, \quad \textit{for all} \quad k > p,$$

with some $p \in \mathbb{N}$, then the local convergence order is improved to $\sigma \approx 2.26953$.

Numerical experiments

Example 1. Our convergence results implies for k sufficiently large that

$$|e_k| \approx c|e_{k-1}|^\sigma \quad \Longrightarrow \quad \ln e_k \approx \sigma \ln e_{k-1} + \ln c \quad \text{with} \quad e_k = |\theta_k - \theta_*|.$$

We demonstrate the locally converge order with the testing matrix $A = G\cdot\exp(\pi\imath/3) - (4+2\imath)\cdot I_n$, where $G = \mathrm{Grcar}$ matrix of size $n = 120$. To verify the slope σ, we perform the computation with 620 decimal digits using the Advanpix MP toolbox. (Available from `www.advanpix.com`.)

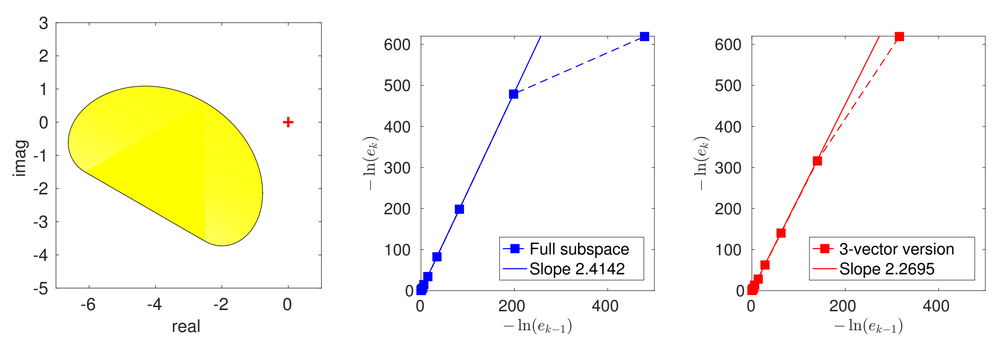

Figure 1: Left: numerical range plot; Middle and Right: observed convergence order.

Example 2. Crawford number computation problem arising from the study of coercivity constants of boundary integral operator in acoustic scattering [1]. We compare the performance of the subspace algorithm with Uhlig's Algorithm [6], a popular algorithm to compute the Crawford number.

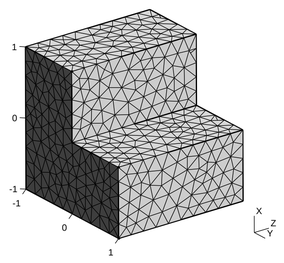

Figure 2: L-shaped obstacle in acoustic scattering, discretized with mesh size 0.2.

Table 1: Results for discretized operators with mesh size 0.02 and $n = 396\,162$.

wave number k	memory A^k	Crawford number $\gamma(A^k)$		its.	timing (h)
2	46 GB	Alg. 1	1.556145884392413e-01	5	2.5
		Uhlig's	1.556145884392416e-01	11	4.4
10	54 GB	Alg. 1	1.880394259192281e-01	7	6.1
		Uhlig's	1.880394259192323e-01	30	29.9
20	60 GB	Alg. 1	1.777716873410842e-01	8	8.1
		Uhlig's	1.777716873410810e-01	24	24.9

Conclusions

- We have analyzed the convergence of the subspace method for univariate eigenvalue optimization. The obtained convergence order improves upon existing results, and it appears to be tight.
- For the Crawford number, we have established novel strongly concavity properties of the objective function. This has resulted in a three-dimensional subspace method that is proven to enjoy favorable convergence properties.

References

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