Subspace embedding with random Khatri–Rao products and its application to eigensolvers

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Spectral problems – computationally I

A motivating example

Dirac operator with a radially symmetric potential.

$$D = \begin{bmatrix} 1 + \frac{\gamma}{r} & -\partial_r + \frac{\kappa}{r} \\ \partial_r + \frac{\kappa}{r} & -1 + \frac{\gamma}{r} \end{bmatrix}$$

for $-\sqrt{3}/2 < \gamma < 0$ and $\kappa = j + 1/2$, $j \in \mathbb{Z}$ (ess. s.a. on $C_0^\infty(0,\infty) \otimes C_0^\infty(0,\infty)$).

Essential spectrum is $(-\infty, -1] \cup [1, \infty)$ and the eigenvalues in $(-1, 1)$ are given by the formula

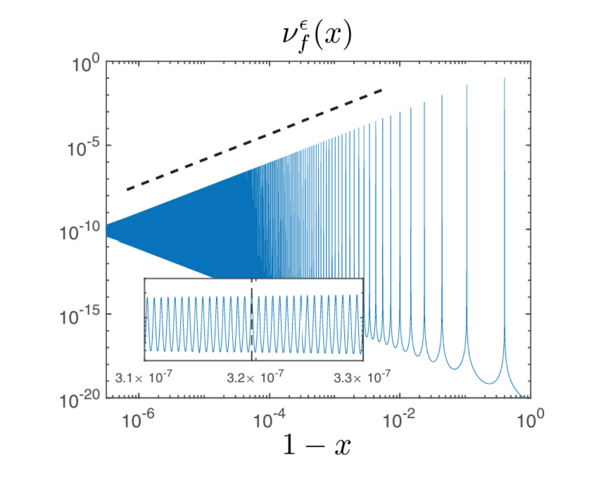
$$\lambda_j(D) = 1 / \sqrt{1 + \frac{\gamma^2}{(j + \sqrt{1 - \gamma^2})^2}}$$

For given $\varepsilon > 0$ and a fixed state vector f plot (intepretable as a smothing convolution)

$$\nu_f^\varepsilon(x) = \varepsilon \, \mathrm{Im} \, \langle (D - (x + \mathrm{i}\varepsilon) I) f, f \rangle \ .$$

Spectral problems – computationally II

Reproduced from Colbrook, Horning and Townsend [CHT21]



Spectral problems – computationally III

Riesz projection

To deal with spectral projections, consider the Ritz integral

$$f \mapsto \Pi_\Gamma f = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (z - A)^{-1} f \, dz \approx \sum_{i=1}^{N} \omega_i (z_i - A)^{-1} f = \pi_N(A) f$$

and store information in π_N. Made practical by

- Ideal computational method by WJ Beyn [Bey12], [BLR14].
- NSA approximation of the Riesz projection in the self-adjoint case: Gopalakrishnan, Grubišić, Ovall [GGO20]

$$f \mapsto \Pi_\Gamma f \approx (\pi_N(A_h) + E_h) f$$

Not the whole story

There is no free lunch!

The process requires many evaluations of the resolvent.

We deal with by

- Spectral mapping gives information on eigenvalues, we need bounds on singular values for oblique spectral projections.
- I will not only be inexact (in evaluating resolvents)
- I will sample them randomly (and try to give definite answers)

Let me be cute

LOCAL MOMENTS AND LOCALIZED STATES

Nobel Lecture, 8 December, 1977

by

PHILIP W. ANDERSON

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Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it. Only now, and through primarily Sir Nevill Mott's efforts, is it beginning to gain general acceptance.

Matrix sketching

Dimension reduction maps

A problem that features a potentially large input matrix $B \in \mathbb{R}^{m\times n}$ is reduced to a smaller one by replacing B with $B\Omega$, where $\Omega \in \mathbb{R}^{n\times \ell}$, $\ell \ll n$, is a random matrix. This idea has been very successfully used as a basis for, e.g., the randomized SVD [HMT11], or in subspace projection methods for large-scale eigenvalue problems, such as FEAST [Pol09].

For further references see:

- [MT20; Mur+23] (randomisation in NLA) Halko Martinson and Tropp [HMT11] (randomised SVD)
- In fact, essentially all iterative methods for large-scale eigenvalue problems, including the power method and the Lanczos algorithm [GV13], make use of random initial guesses, which effectively involves sketching.

Oblivious subspace embedding I

Oblivious subspace embedding (OSE) property [Sar06]

Given a vector x, a matrix $\Omega \in \mathbb{R}^{n\times\ell}$ satisfies the Johnson-Lindenstrauss (JL) property if up to some prescribed relative tolerance ε:

$$(1-\varepsilon)\|x\|_2 \le \|\Omega^T x\|_2 \le (1+\varepsilon)\|x\|_2.$$

Why is this mathematics

A random matrix $\Omega \in \mathbb{R}^{n\times\ell}$ drawn from a random distribution $\mathcal{D}$ has the (ε, δ, k)-OSE property if,

$$\mathbb{P}\left\{\|(\Omega^T U)^T(\Omega^T U) - I\|_2 > \varepsilon\right\} < \delta, \tag{1}$$

holds for fixed but arbitrary $U \in \mathbb{R}^{n\times k}$ with orthonormal columns.

Small print: **Here, the probability is taken with respect to $\Omega \sim \mathcal{D}$. Random Gaussian matrices $\Omega \in \mathbb{R}^{n\times\ell}$ satisfy the OSE property when $\ell \sim (k + \log(1/\delta))\varepsilon^{-2}$; other classes of random matrices such as SRHT/SRFT are OSE as well but with less favorable requirements for ℓ; see [Woo14; MT20; Mur+23] and the references therein.**

Operator sketching Kressner et al. [PBK24] I

When $H = \sum_{i=1}^{\infty} \lambda_i u_i \otimes u_i$ is a positive Hilbert Schmidt operator on L^2, and K is the covariance operator such that the matrix

$$\hat{K}_{i,j} = \langle K u_i, u_j \rangle$$

is invertible then

$$\mathbb{E}(\|H - H\Omega(\Omega^* H\Omega)^+(H\Omega)^*)\|_{S^1}) \leq (\ldots \frac{k}{p-1} \ldots) \sum_{j=k+1}^{\infty} \lambda_j,$$

where $\Omega : \mathbb{C}^{k+p} \to L^2$ and

$$\Omega e_i \sim \sum_{i=1}^{\infty} \eta_i \sqrt{\sigma_i} \psi_i$$

is the Karhunen-Loeve decomposition defined by the continuous, positive definite function K and $\eta_i \sim N(0,1)$ i.i.d. The expectation is defined as a Bochner vector integral.

Operator sketching Kressner et al. [PBK24] II

A connection with Riesz projections

Given an operator A for which a spectrum mapping theorem holds, apply this for

$$H = \pi_N(A).$$

As the Gaussian process, use $G(0, A^{-2})$.

An explicit representation, after setting $\omega_i = \Omega e_i$

$$H\Omega(\Omega^* H\Omega)^+(H\Omega)^* f = \sum_{i,j=1}^{k+p} H\omega_i(\Omega^* H\Omega)^+_{ij} \langle \omega_i, f \rangle \ .$$

Random Khatri–Rao matrices. I

Let us focus on Kronecker product structured systems

$$A = I \otimes K + K \otimes I + \tilde{V} \otimes \hat{V}, \tag{2}$$

- In applications, it is often beneficial to employ DRMs that exploit the underlying structure of the problem ([Mur+23, Ch. 7])
- Given two matrices, $\tilde{\Omega} \in \mathbb{R}^{\tilde{n} \times \ell}$ with columns $\tilde{\omega}_1, \ldots, \tilde{\omega}_\ell$, and $\hat{\Omega} \in \mathbb{R}^{\hat{n} \times \ell}$ with columns $\hat{\omega}_1, \ldots, \hat{\omega}_\ell$, their Khatri–Rao product is defined as

$$\tilde{\Omega} \odot \hat{\Omega} = \left[\; \tilde{\omega}_1 \otimes \hat{\omega}_1, \quad \tilde{\omega}_2 \otimes \hat{\omega}_2, \quad \ldots, \quad \tilde{\omega}_\ell \otimes \hat{\omega}_\ell \; \right] \in \mathbb{R}^{n \times \ell}, \quad n = \tilde{n} \cdot \hat{n}.$$

- For $A = \sum_{i=1}^{s} \tilde{A}_i \otimes \hat{A}_i$, the computation of $A\Omega$ becomes ([Pal21]):

$$A\Omega = \sum_{i=1}^{s} (\tilde{A}_i \tilde{\Omega}) \otimes (\hat{A}_i \hat{\Omega}).$$

Random Khatri–Rao matrices. II

Our goal

To establish OSE for Khatri–Rao products of random matrices, building on recent work by Ahle et al. [Ahl+20]. The requirement on the number of samples ℓ increases only modestly compared to unstructured random Gaussian matrices; this increase is easily overcome by the improved computational efficiency.

Our result

Given an integer $k \geq 1$, real numbers $\varepsilon \in (0,1]$, $\delta \in (0,1/2)$, and $n = \tilde{n}\hat{n}$, consider $\Omega = \frac{1}{\sqrt{\ell}}(\tilde{\Omega} \odot \hat{\Omega}) \in \mathbb{R}^{n \times \ell}$ for independent Gaussian random matrices $\tilde{\Omega} \in \mathbb{R}^{\tilde{n} \times \ell}$ and $\hat{\Omega} \in \mathbb{R}^{\hat{n} \times \ell}$. Then Ω has the (ε, δ, k)-OSE property, provided that

$$\ell \geq C \cdot \left(k^{3/2}\varepsilon^{-2} + k\log(1/\delta)\varepsilon^{-2} + k^{1/2}\log^2(1/\delta)\varepsilon^{-1}\right), \quad C = (2000e^4)^2. \quad (3)$$

- We went from k for Gaussian matrices to $k^{3/2}$ with nastier constants.

Eigenvalue solvers with random Khatri–Rao matrices. I

Let

$$A = I \otimes K + K \otimes I + \tilde{V} \otimes \hat{V},$$

and use a circular contour with the trapezoidal rule to obtain

$$\Pi_\Gamma \Omega = \frac{1}{2\pi i} \int_\Gamma (zI - A)^{-1} \Omega \, \mathrm{d}z \approx \frac{1}{2\pi i} \sum_{i=1}^{q} w_i (z_i I - A)^{-1} \Omega. \tag{4}$$

Contour integration methods [Pol09; TP14; SS03; Asa+09; Bey12] reduce the computing the eigenvalues of the matrix A that lie inside a contour $\Gamma \subseteq \mathbb{C}$ reduces to approximating the integral of the resolvent applied to a (random) matrix Ω by using a quadrature formula.

Eigenvalue solvers with random Khatri–Rao matrices. II

Approximating the range

The range of the computed matrix on the right-hand side approximately spans the corresponding invariant subspace. Assume that Ω is a Khatri–Rao product of two matrices. Then evaluating

$$(zI - A)(\tilde{\omega} \otimes \hat{\omega}) = (zI \otimes I - I \otimes K - K \otimes I - \tilde{V} \otimes \hat{V})^{-1}(\tilde{\omega} \otimes \hat{\omega}),$$

can be rewritten as solving a sequence of Sylvester equations with rank-one right hand side,

$$\left(I \otimes \left(\frac{z}{2}I - K\right) + \left(\frac{z}{2}I - K\right) \otimes I - \tilde{V} \otimes \hat{V}\right) x = \tilde{\omega} \otimes \hat{\omega}.$$

which can be done much more efficiently.

Eigenvalue solvers with random Khatri–Rao matrices. III

CAVEAT - other spectral transformation also yield operator equations

The LOBPCG (Locally Optimally Block Preconditioned Conjugate Gradient) method [Kny01] for computing extreme eigenvalues of a large symmetric positive definitive matrix can also be implemented so that it exploits an initial iteration with a Khatri–Rao product structure. We show that this is possible by keeping the subsequent iterations in a low-rank factored form, and by limiting the rank of the iterates via truncation. Experimentally, we observe that this does not hamper convergence and leads to an efficient algorithm.

Efficient implementation I

We consider a two-dimensional Schrödinger equation

$$\begin{aligned} -\Delta u(x,y) + V(x,y)\cdot u(x,y) &= \lambda u(x,y), && (x,y)\in D=[a,b]\times[a,b],\\ u(x,y) &= 0, && (x,y)\in\partial D, \end{aligned}$$

where $V(x,y)$ is a given potential.

- Using finite elements to discretize this equation would lead to a generalized eigenvalue problem $Ax = \lambda Bx$ with matrices A and $B \neq I$ both represented as short sums of Kronecker products.
- For simplicity, we use a finite differences discretization that yields $B = I$ and leads to a standard eigenvalue problem $Av = \lambda v$ with

$$A = -(I\otimes T + T\otimes I) + \operatorname{diag}(V(x_i, y_j)) \in \mathbb{R}^{\hat{n}\tilde{n}\times\hat{n}\tilde{n}}. \tag{5}$$

Here $T = \operatorname{tridiag}(1,-2,1)/h^2$, $x_i = a + hi$, $y_j = a + hj$, and $h = (b-a)/(\tilde{n}+1)$ where $\tilde{n} = \hat{n}$ is the number of discretization points for each coordinate.

Efficient implementation II

Note

In order to obtain Kronecker structure for the last term in (5), the potentially needs to represented or approximated as a sum of separable functions. In particular, if the potential has the form $V(x,y) = f(x) + f(y) \pm g(x)g(y)$, then

$$A = I \otimes K + K \otimes I + \tilde{V} \otimes \hat{V}, \qquad (6)$$

where $K = -T + \mathrm{diag}(f(x_i))$, $\tilde{V} = \pm\,\mathrm{diag}(g(x_i))$, $\hat{V} = \mathrm{diag}(g(x_i))$.

Operator equations solvers I

For large $A = I \otimes K + K \otimes I + \tilde{V} \otimes \hat{V}$, it will be beneficial to exploit the Kronecker structure and rewrite

$$\left(I \otimes \left(\frac{z}{2} I - K\right) + \left(\frac{z}{2} I - K\right) \otimes I - \tilde{V} \otimes \hat{V}\right) x = \tilde{\omega} \otimes \hat{\omega}. \tag{7}$$

as a matrix equation.

Convention

For this purpose, we let vec : $\mathbb{R}^{\hat{n} \times \tilde{n}} \to \mathbb{R}^{\hat{n}\tilde{n}}$ denote vectorization, which stacks the columns of a matrix into a long vector. The inverse of vec is denoted by mat : $\mathbb{R}^{\hat{n}\tilde{n}} \to \mathbb{R}^{\hat{n} \times \tilde{n}}$.

Letting $X = \mathrm{mat}(x)$ and using that $\mathrm{mat}(\tilde{\omega} \otimes \hat{\omega}) = \hat{\omega}\tilde{\omega}^T$, we obtain a multiterm Sylvester equation of the form

$$\left(\frac{z}{2} I - K\right) X + X \left(\frac{z}{2} I - K\right) - \hat{V} X \tilde{V} = \hat{\omega}\tilde{\omega}^T. \tag{8}$$

Operator equations solvers II

Solution method

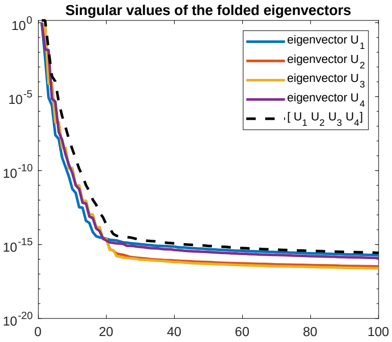
To solve (8), we have adapted the preconditioned low-rank BiCGstab (biconjugate gradient stabilized method) algorithm from [BB13] to multiterm Sylvester equations. The preconditioner consists of applying a few iterations of the ADI method (implemented as described in [Kür16]) to the Sylvester matrix equation

$$\left(\frac{z}{2}I - K\right)X + X\left(\frac{z}{2}I - K\right) = \hat{P}\tilde{P}^*,$$

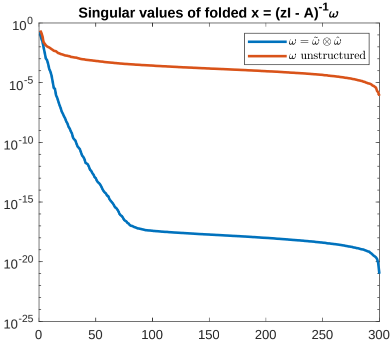
for the low-rank right-hand sides appearing in the course of BiCGstab.

Explicit Numerical Content

Some results I



(a) Singular value decay of matricized eigenvectors belonging to 4 smallest eigenvalues.



(b) Singular value decay of solution to multiterm Sylvester equation (7) for different right-hand sides ω.

Figure: Properties of the eigenvalue problem arising from a discretized Schrödinger equation with potential $V(x, y) = (x^2 + y^2 - xy)/2$.

Some results II

$\tilde{n} = \hat{n}$	1000	2000	3000	worst $\|Ax - \lambda x\|$	worst $\|\lambda_i - \lambda_i\|$	memory
sparse direct	8.35s	46.47s	138.59s	$1 \cdot 10^{-7}$	$6 \cdot 10^{-10}$	27.9 GB
BiCGstab tol=10^{-6}	5.86s	12.81s	19.59s	$7 \cdot 10^{-3}$	$1 \cdot 10^{-8}$	400 MB
BiCGstab tol=10^{-10}	15.85s	30.97s	56.58s	$6 \cdot 10^{-7}$	$6 \cdot 10^{-10}$	400 MB

Mathieu potential I

Lyonell's example

For the last example, we let V be a Gaussian perturbation of the Mathieu potential, thanks to Lyonell Boulton and Michael Levitin [BL07]:

$$V(x,y) = \cos(x) + \cos(y) - 6\exp\left(-x^2 - y^2\right), \text{ for } (x,y) \in [-25, 25]^2.$$

Target: we would like to compute the single eigenvalue of A that lies in the middle of the spectrum between two clusters of eigenvalues.

Particularities

- To illustrate this, we first discretize the domain using only 100 points on each axis, solve the smaller eigenvalue problem, and plot the 100 smallest eigenvalues of A as purple crosses in Figure 2. Our objective is to find the eigenvalue closest to -0.2.
- As a spectral transformation, we work with the positive definite matrix $\tilde{A} = (A + 0.2I)^2$, so that the desired eigenvalue is on the edge of the spectrum.

Mathieu potential II

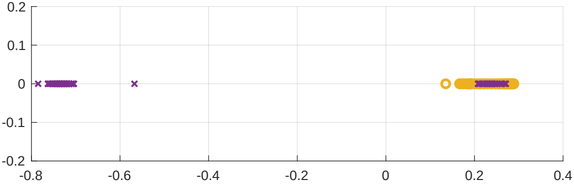


Figure: Yellow circles mark the 100 smallest eigenvalues of $\tilde{A}$. The smallest one corresponds to the desired eigenvalue of A, 100 smallest eigenvalues of A and $(A + 0.2I)^2$ where A is the eigenvalues problem from Example **??** with 100 discretization points.

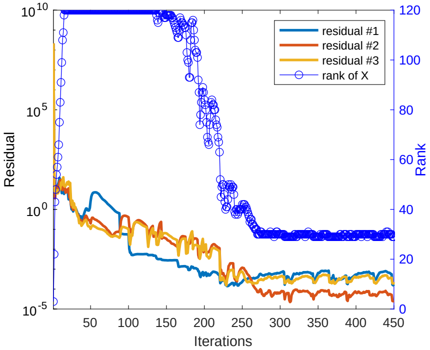
Returning to the original problem where the discretization uses 3000 points on each axis, resulting in a matrix A of size $3000^2 \times 3000^2$, we apply LOBPCG Algorithm to $\tilde{A} = (A + 0.2I)^2$ with $k = 1$ and block size $\ell = 3$.
The preconditioner used in LOBPCG Algorithm is then set to $M = I \otimes K^2 + K^2 \otimes I$. In this example, to obtain an accurate approximation we needed to take a higher maximal rank $r_{max} = 120$ and 12 ADI iterations in the Sylvester solver.

Mathieu potential III

Results

This example turns out to be less favorable for LOBPCG Algorithm compared to the other two examples above. More iterations are required, likely due to the use of a lower-quality preconditioner. However, one can still obtain satisfactory residuals and accurate eigenvalue approximations.
The entire computation takes 915.43 seconds (i.e., 2.03s per iteration on average).

Mathieu potential IV



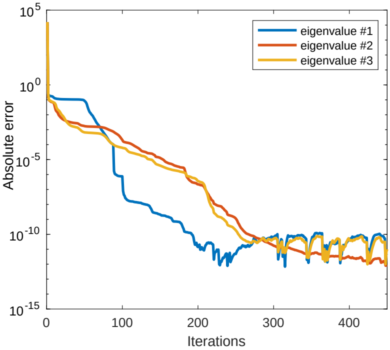


Figure: Residual with respect to $\tilde{A}$ and absolute errors of the computed eigenvalues when LOBPCG with low-rank truncation is applied.

Some final remarks

- Works (empirically) for complex valued potentials
- More abstractly, for sectorial operators
- Nonlinear eigenvalue problems when applied on the nonlinear resolvent
- CAVEAT: we need singular value estimates, but eigenvalue estimates are mo accessible through spectral mapping.

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