Multilevel quasi-Monte Carlo methods for a random elliptic eigenvalue problem

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Outline

1. The stochastic eigenproblem
2. Approximation strategy
3. Recap on two-grid FE methods for eigenproblems,
   high-dimensional integration and multilevel Monte Carlo methods
4. Two-grid multilevel methods
5. Numerical results

The stochastic eigenproblem

$$\begin{aligned} -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla u(\boldsymbol{x},\boldsymbol{y})) &= \lambda(\boldsymbol{y})u(\boldsymbol{x},\boldsymbol{y}) \quad \text{for } \boldsymbol{x} \in D\,, \\ u(\boldsymbol{x},\boldsymbol{y}) &= 0 \quad \text{for } \boldsymbol{x} \in \partial D\,. \end{aligned}$$

- $\boldsymbol{x} \in D \subset \mathbb{R}^d$ is bounded and convex
- stochastic parameters $\boldsymbol{y} \in [-\frac{1}{2}, \frac{1}{2}]^s$ with $y_j \sim \mathrm{U}(-\frac{1}{2}, \frac{1}{2})$
- s is very large, possibly ∞
- $a_{\min} \leq a(\boldsymbol{x},\boldsymbol{y}) \leq a_{\max}$ for all $\boldsymbol{x}, \boldsymbol{y}$, and

$$a(\boldsymbol{x},\boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{j=1}^{s} y_j a_j(\boldsymbol{x})$$

Quantity of interest:

$$\mathbb{E}_{\boldsymbol{y}}[\lambda(\boldsymbol{y})] = \int_{[-\frac{1}{2},\frac{1}{2}]^s} \lambda(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$$

Related work

1. [G., Graham, Kuo, Scheichl, Sloan 2019] single level QMC analysis for stochastic eigenproblems
2. [Andreev, Schwab 2012] looked at the same eigenproblem using a sparse tensor approximation and proved analyticity of simple eigenpairs
3. [Robbe, Nuyens, Vandewalle 18] Multigrid multilevel MC/QMC methods for elliptic source problems
4. Two-grid FE methods for eigenproblems, e.g., [Xu, Zhou 1999], [Hu, Cheng 2011], [Yang, Bi 2011]
5. QMC for other PDE problems: Dick, Ganesh, Gantner, Graham, Harbrecht, Hermann, Kuo, Le Gia, Nichols, Nuyens, Parkinson, Peters, Robbe, Scheichl, Schwab, Siebenmorgen, Sloan, Ullmann, Vandewalle...

Approximation strategy [G., Graham, Kuo, Scheichl, Sloan, 19]

1. Finite element approximation:

$$\lambda(\boldsymbol{y}) \approx \lambda_h(\boldsymbol{y})$$

   e.g., piecewise linear FE spaces

2. high-dimensional quadrature:

$$\mathbb{E}_{\boldsymbol{y}}\left[\lambda(\boldsymbol{y})\right] \approx \frac{1}{N}\sum_{k=0}^{N-1}\lambda(\boldsymbol{t}_k) := Q_N(\lambda)$$

   e.g., Monte Carlo (MC) or quasi-Monte Carlo (QMC) rules

Combined approximation (single level)

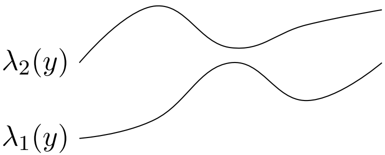
$$\mathbb{E}_{\boldsymbol{y}}[\lambda] \approx Q_N(\lambda_h) = \frac{1}{N}\sum_{k=0}^{N-1}\lambda_h(\boldsymbol{t}_k)$$

What is different from source problems?

1. Eigenvalue problems are nonlinear
2. Two objects of interest: $\lambda(\boldsymbol{y})$ and $u(\boldsymbol{y})$
3. Infinitely many eigenpairs/solutions
4. How to handle multiple eigenvalues?
5. PDE/FE analysis for eigenvalue problems has a different flavour
6. Quasi-Monte Carlo analysis for eigenvalues is more complicated (need to bound derivatives of λ and u with respect to $\boldsymbol{y}$)

Why is simplicity important?

$\lambda_1(\boldsymbol{y})$ is simple *for all* $\boldsymbol{y}$



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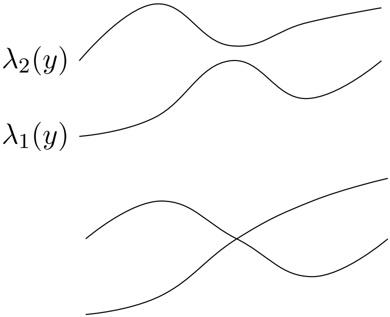

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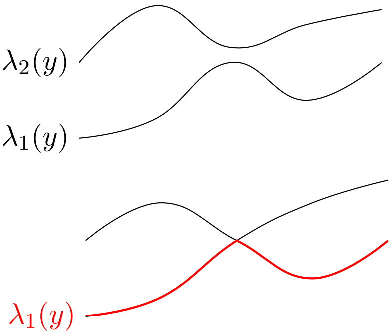

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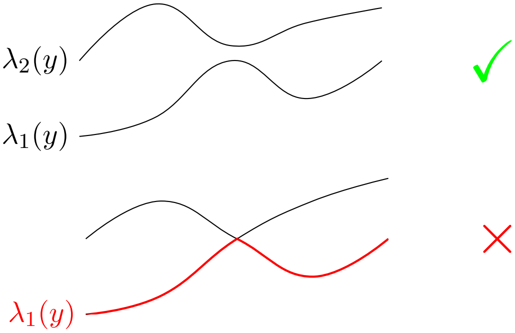

Bounding the spectral gap: $\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y})$

1. Bounds on the stochastic derivatives depend on $1/(\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y}))$.
2. FE error constants also depend on the gap.
3. Convergence of eigensolvers degrade as the gap gets smaller.
4. For $s = \infty$, $[-\frac{1}{2}, \frac{1}{2}]^{\mathbb{N}}$ is not compact

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Lemma (G., Graham, Kuo, Scheichl, Sloan 2019)

For $s = \infty$, assume

$$\sum_{j=1}^{\infty} \|a_j\|_{L^\infty}^p < \infty \quad \text{for } p \in (0, 1),$$

then there exists a $\rho > 0$, independent of $\boldsymbol{y}$, such that

$$\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y}) \geq \rho \quad \text{for all } \boldsymbol{y} \in [-\tfrac{1}{2}, \tfrac{1}{2}]^{\mathbb{N}}.$$

Finite element methods

For $\boldsymbol{y} \in [-\frac{1}{2}, \frac{1}{2}]^{\mathbb{N}}$: find $\lambda(\boldsymbol{y}) \in \mathbb{R}$ and $u(\boldsymbol{y}) \in V := H_0^1$ satisfying, for all $v \in V$,

$$\begin{aligned} \int_D a(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} &= \lambda(\boldsymbol{y}) \int_D u(\boldsymbol{x}, \boldsymbol{y}) v(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \\ \|u(\boldsymbol{y})\|_{L^2} &= 1 \end{aligned}$$

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$$\begin{aligned} \mathcal{A}\big(\boldsymbol{y}; u(\boldsymbol{y}), v\big) &= \lambda(\boldsymbol{y})\big\langle u(\boldsymbol{y}), v\big\rangle \\ \|u(\boldsymbol{y})\|_{L^2} &= 1 \end{aligned}$$

Finite element methods

For $\boldsymbol{y} \in [-\frac{1}{2}, \frac{1}{2}]^s$: find $\lambda_h(\boldsymbol{y}) \in \mathbb{R}$ and $u_h(\boldsymbol{y}) \in V_h$ satisfying

$$\begin{aligned} \mathcal{A}(\boldsymbol{y}; u_h(\boldsymbol{y}), v_h) \;&=\; \lambda_h(\boldsymbol{y})\langle u_h(\boldsymbol{y}), v_h\rangle \quad \text{for all } v_h \in V_h\,, \\ \|u_h(\cdot, \boldsymbol{y})\|_{L^2} \;&=\; 1\,. \end{aligned}$$

e.g., $V_h =$ continuous piecewise linear FE space.

FE error:

$$|\lambda(\boldsymbol{y}) - \lambda_h(\boldsymbol{y})| \;\lesssim\; h^2$$

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FE error:

$$|\lambda(\boldsymbol{y}) - \lambda_h(\boldsymbol{y})| \lesssim h^2$$

Generalised matrix eigenproblem:

$$\mathcal{A}(\boldsymbol{y}; u_h(\boldsymbol{y}), v_h) = \lambda_h(\boldsymbol{y}) \langle u_h(\boldsymbol{y}), v_h \rangle$$

$$\Longleftrightarrow$$

$$A_h(\boldsymbol{y}) \boldsymbol{u}_h(\boldsymbol{y}) = \lambda_h(\boldsymbol{y}) B_h \boldsymbol{u}_h(\boldsymbol{y})$$

Quasi-Monte Carlo integration

N-point randomly shifted lattice rule:

$$\int_{[-\frac{1}{2},\frac{1}{2}]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx Q_N f = \frac{1}{N}\sum_{k=0}^{N-1} f\left(\boldsymbol{t}_k\right).$$

- $\boldsymbol{t}_k = \left\{\frac{k\boldsymbol{z}}{N} + \boldsymbol{\Delta}\right\} - \frac{\mathbf{1}}{\mathbf{2}}$,
- $\boldsymbol{z} \in \mathbb{N}^s$ the *generating vector*,
- *random shift* $\boldsymbol{\Delta} \sim \mathrm{U}([0,1]^s)$.
- random shifting $\implies$ unbiased

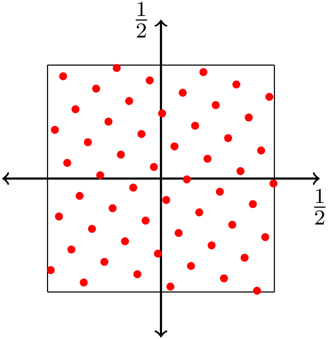

Figure: 2D lattice rule with $N = 55$, $\boldsymbol{z} = (1, 34)$.

The "standard" QMC error analysis

Assumes $f \in \mathcal{W}_{s,\boldsymbol{\gamma}} =:$ s-*dimensional weighted space* [Sloan, Woźniakowski 1998] with:

- weights: $\boldsymbol{\gamma} := \{\gamma_{\mathfrak{v}} > 0 : \mathfrak{v} \subseteq \{1, \ldots, s\}\}$.
- (unanchored) weighted norm

$$\|f\|_{s,\boldsymbol{\gamma}}^2 = \sum_{\mathfrak{v} \subseteq \{1,\ldots,s\}} \frac{1}{\gamma_{\mathfrak{v}}} \int_{[0,1]^{|\mathfrak{v}|}} \left(\int_{[0,1]^{s-|\mathfrak{v}|}} \frac{\partial^{|\mathfrak{v}|}}{\partial \boldsymbol{y}_{\mathfrak{v}}} f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}_{-\mathfrak{v}} \right)^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{v}} \,.$$

CBC error bound

For $f \in \mathcal{W}_{s,\boldsymbol{\gamma}}$, N prime and *good* $\boldsymbol{z}$

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} \left[\left| \int_{[-\frac{1}{2},\frac{1}{2}]^s} f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} - Q_{N,\boldsymbol{\Delta}}(f) \right|^2 \right]} \leq C_{\delta,\boldsymbol{\gamma}} N^{-1+\delta} \|f\|_{s,\boldsymbol{\gamma}}$$

Single level cost & error analysis [G., Graham, Kuo, Scheichl, Sloan, 19]

1. Finite element error & cost: e.g., for piecewise linear FE spaces

$$|\lambda(\boldsymbol{y}) - \lambda_h(\boldsymbol{y})| \lesssim h^2$$
$$\mathrm{cost}(\lambda_h) \eqsim \text{num. iterations} \times h^{-\gamma} \quad \text{for } \gamma > d$$

   (e.g., $\gamma \approx d$ for AMG)

2. Quadrature/sampling error & cost:

$$\sqrt{\mathbb{E}\big[|\mathbb{E}_{\boldsymbol{y}}[\lambda_h] - Q_N(\lambda_h)|^2\big]} \lesssim N^{-\eta}$$
$$\mathrm{cost}(Q_N(\lambda_h)) \eqsim N \times \mathrm{cost}(\lambda_h)$$

   e.g., Monte Carlo ($\eta = \frac{1}{2}$) or quasi-Monte Carlo ($\eta \in [\frac{1}{2}, 1)$)

Total error & cost

RMS error $\lesssim h^2 + N^{-\eta}$

$$\mathrm{cost}(Q_N(\lambda_h)) \eqsim N \times h^{-\gamma}$$

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Total error & cost

RMS error $\lesssim h^2 + N^{-\eta} \lesssim \varepsilon$

$$\mathrm{cost}(Q_N(\lambda_h)) \eqsim N \times h^{-\gamma} \eqsim \varepsilon^{-(1/\eta + \gamma/2)}$$

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Total error & cost

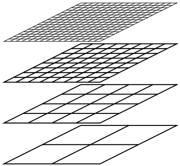
$$\text{RMS error} \lesssim h^2 + N^{-\eta} \lesssim \varepsilon$$

$$\mathrm{cost}(Q_N(\lambda_h)) \eqsim N \times h^{-\gamma} \eqsim \varepsilon^{-(1/\eta+\gamma/2)} = \begin{cases} \varepsilon^{-(2\,+\,\gamma/2)} & \text{MC} \\ \varepsilon^{-(1\,+\,\gamma/2)} & \text{QMC} \end{cases}$$

Multilevel Monte Carlo methods

FE spaces $\{V_\ell\}$ corresponding to $h_0 > h_1 > h_2 > \cdots > 0$.
Then define $\lambda_{-1} \equiv 0$ and

$$\lambda_\ell(\boldsymbol{y}) := \lambda_{h_\ell}(\boldsymbol{y}) \to \lambda(\boldsymbol{y}) \text{ as } \ell \to \infty$$



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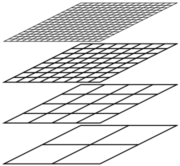


Multilevel estimator:

Finest approximation can be written as a telescoping sum

$$\mathbb{E}_{\boldsymbol{y}}[\lambda_L(\boldsymbol{y})] = \sum_{\ell=0}^{L} \mathbb{E}_{\boldsymbol{y}}[\lambda_\ell(\boldsymbol{y}) - \lambda_{\ell-1}(\boldsymbol{y})]$$

then apply an independent QMC rule on each level

$$\widehat{Q}_L^{\mathrm{ML}}(\lambda) = \sum_{\ell=0}^{L} Q_{N_\ell}(\lambda_\ell - \lambda_{\ell-1}) = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{k=0}^{N_\ell - 1} \lambda_\ell(\boldsymbol{t}_{\ell,k}) - \lambda_{\ell-1}(\boldsymbol{t}_{\ell,k})$$

Multilevel complexity theorem

Theorem (G., Scheichl 2020+)

Suppose that

M1.

$$\sum_{j=1}^{\infty} \left(\|a_j\|_{L^\infty} + \|\nabla a_j\|_{L^\infty} \right)^p < \infty, \qquad \textit{for } p \in (0, 2/3], \quad \textit{and}$$

M2. $\mathrm{cost}\big(Q_\ell(\lambda_\ell - \lambda_{\ell-1})\big) \lesssim N_\ell h_\ell^{-\gamma}$.

Then, for $\varepsilon > 0$*, with* $h_\ell = 2^{-\ell}$ *one can choose* L *and* $\{N_\ell\}$ *such that*

$$\sqrt{\mathbb{E}\big[|\mathbb{E}_{\boldsymbol{y}}[\lambda] - \widehat{Q}_L^{\mathrm{ML}}(\lambda)|^2\big]} \lesssim \varepsilon\,,$$

and for $\delta > 0$

$$\mathrm{cost}(\widehat{Q}_L^{\mathrm{ML}}(\lambda)) \lesssim \begin{cases} \varepsilon^{-(1+\delta)} & \gamma < 2, \\ \varepsilon^{-(1+\delta)}|\log(\varepsilon^{-1})|^2 & \gamma = 2, \\ \varepsilon^{-\gamma/2} & \gamma > 2. \end{cases}$$

A key lemma — Bounding the stochastic derivatives

Lemma (G., Scheichl 2020+)

Suppose that $s = \infty$ *and*

$$\sum_{j=1}^{\infty} \big(\|a_j\|_{L^\infty} + \|\nabla a_j\|_{L^\infty} \big)^p < \infty, \qquad \textit{for } p \in (0, 2/3],$$

then for $\mathfrak{u} \subset \mathbb{N}$ and all $\boldsymbol{y} \in [-\frac{1}{2}, \frac{1}{2}]^s$

$$\left| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_\mathfrak{u}} \lambda(\boldsymbol{y}) \right| \lesssim \prod_{j \in \mathfrak{u}} \frac{1}{\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y})} \|a_j\|_{L^\infty},$$

$$\left\| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_\mathfrak{u}} u(\boldsymbol{y}) \right\|_V \lesssim \prod_{j \in \mathfrak{u}} \frac{1}{\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y})} \|a_j\|_{L^\infty},$$

$$\left\| \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_\mathfrak{u}} \Delta_{\boldsymbol{x}} u(\boldsymbol{y}) \right\|_V \lesssim \prod_{j \in \mathfrak{u}} \frac{1}{\lambda_2(\boldsymbol{y}) - \lambda_1(\boldsymbol{y})} \|a_j\|_{W^{1,\infty}}.$$

Two-grid FE methods for eigenproblems

(Accelerated) two-grid method [Hu & Cheng 2011]

Given $H > h$:

1. Find $\lambda_H(\boldsymbol{y}) \in \mathbb{R}$ and $u_H(\boldsymbol{y}) \in V_H$ such that

$$\begin{aligned} \mathcal{A}(\boldsymbol{y}; u_H(\boldsymbol{y}), v_H) &= \lambda_H(\boldsymbol{y})\langle u_H(\boldsymbol{y}), v_H\rangle \quad \text{for all } v_H \in V_H, \\ \|u_H(\boldsymbol{y})\|_{L^2} &= 1\,. \end{aligned}$$

2. Find $u^h \in V_h$ such that

$$\mathcal{A}(\boldsymbol{y}; u^h(\boldsymbol{y}), v_h) - \lambda_H(\boldsymbol{y})\langle u^h(\boldsymbol{y}), v_h\rangle = \langle u_H(\boldsymbol{y}), v_h\rangle \quad \text{for all } v_h \in V_h.$$

3. $\lambda^h(\boldsymbol{y}) = \dfrac{\mathcal{A}(\boldsymbol{y}; u^h(\boldsymbol{y}), u^h(\boldsymbol{y}))}{\langle u^h(\boldsymbol{y}), u^h(\boldsymbol{y})\rangle}$

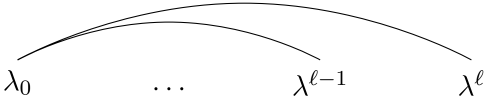
Two-grid FE error:

$$|\lambda(\boldsymbol{y}) - \lambda^h(\boldsymbol{y})| \lesssim H^8 + h^2\,,$$

so taking $H \eqsim h^{1/4}$ we obtain the optimal rate of h^2

Two-grid multilevel method

Key idea: two-grid update on level ℓ



Two-grid multilevel estimator

$$\widehat{Q}_L^{\mathrm{TG}}(\lambda) = \sum_{\ell=0}^{L} Q_{N_\ell}(\lambda^\ell - \lambda^{\ell-1}) = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{k=0}^{N_\ell - 1} \lambda^\ell(\boldsymbol{t}_{\ell,k}) - \lambda^{\ell-1}(\boldsymbol{t}_{\ell,k})$$

$\lambda^{-1} = 0$, $\lambda^0 = \lambda_{h_0}$ and $\lambda^\ell = \lambda^{h_\ell}$ (two-grid update using (λ_{h_0}, u_{h_0}))

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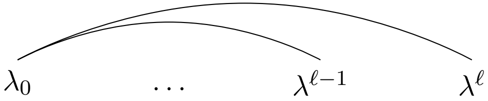

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Things to note:

1. require $h_0 < h_\ell^{1/4}$, e.g., $h_0 = 1/8$ then $h_\ell \leq 1/4096$
2. order of cost is the same, but it will be reduced by a constant factor corresponding to the number of iterations of eigensolver

Numerical results

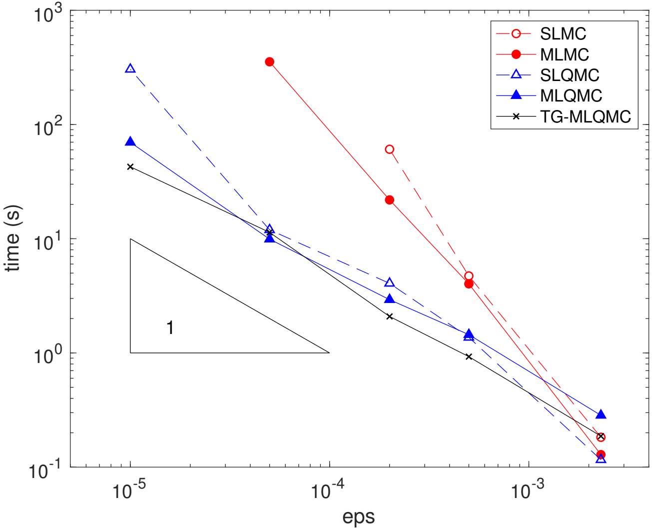
$$-\nabla \cdot \big(a(x,\boldsymbol{y})u(x,\boldsymbol{y})\big) \;=\; \lambda(\boldsymbol{y})u(x,\boldsymbol{y}) \quad \text{for } x \in (0,1)$$

with

$$a(x,\boldsymbol{y}) \;=\; 1 + \sum_{j=1}^{s} \frac{y_j}{1+(j\pi)^2}\sin(j\pi x)$$

- $s = 32$
- $N_\ell = 2^{n_\ell}$, and we use an embedded lattice rule
- $h_\ell = 2^{-\ell}$
- error tolerances: $10^{-2} \geq \varepsilon \geq 10^{-5}$

Cost vs. error



Summary

1. Designed a combined multilevel QMC + two-grid FE method to approximate the expectation of the minimal eigenvalue.
2. Numerical results show speedup compared to single level strategy & QMC speedup over MC
3. Similar results hold for linear functionals of the eigenfunction u_1.

Extensions & future work

1. $s = \infty$ and hierarchy of truncation dimensions $\{s_\ell\}$
2. higher-order QMC rules & FE methods
3. log-normal coefficient (then $y_j \sim \mathcal{N}(0,1)$)
4. non-symmetric eigenvalue problems, e.g., convection-diffusion.

Main references

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Thanks for listening!