STOCHASTIC ZEROTH-ORDER METHOD FOR COMPUTING OPERATOR QUANTITIES

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Key Takeaways

- We introduce a novel stochastic algorithm for computing (several different) matrix quantities.
- Our algorithms steam with zeroth-order methods [6] in terms of using an unbiased estimator for the Riemannian gradient [5].
- Optimal compared to first and zeroth-order methods, since we have the optimal step size, with low cost computation.

Adjoint Mismatch in Inverse Problems

- Let $\mathbb{X}$ and $\mathbb{Y}$ be infinite-dimensional spaces; for linear $\mathcal{A}: \mathbb{X} \to \mathbb{Y}$

$$\mathcal{A}x = y \quad \text{and some noise} \quad y \in \mathbb{Y}.$$

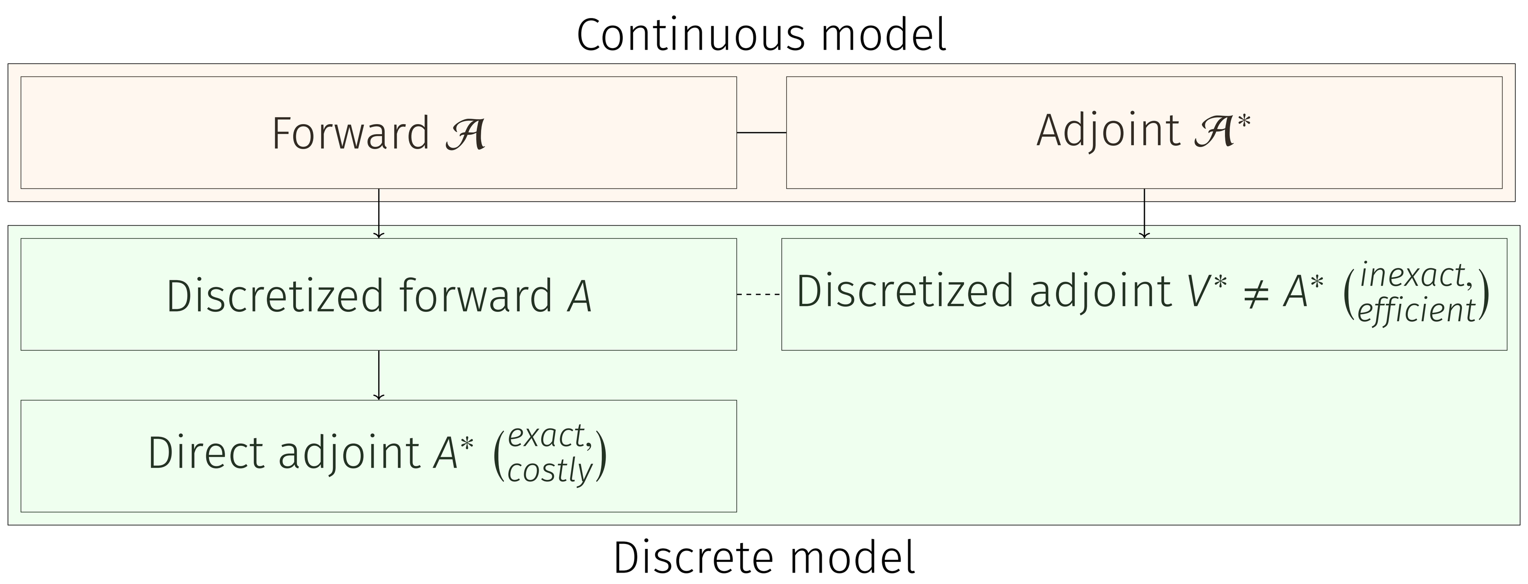
$\rightsquigarrow$ Standard approach

$$\min_{x\in\mathbb{X}} \|\mathcal{A}x - y\|_{\mathbb{Y}}^2 \rightsquigarrow \nabla_x \|\mathcal{A}x - y\|_{\mathbb{Y}}^2 = 0 \rightsquigarrow \mathcal{A}^*\mathcal{A}x = \mathcal{A}^* y.$$

- Minimal norm solution, by More-Penrose pseudo-inverse [1].

$\rightsquigarrow$ Discrete forward *and* backward/adjoint model necessary.

- Replace for lower computational cost and availability by a discrete backward model $V^* \neq A^*$.

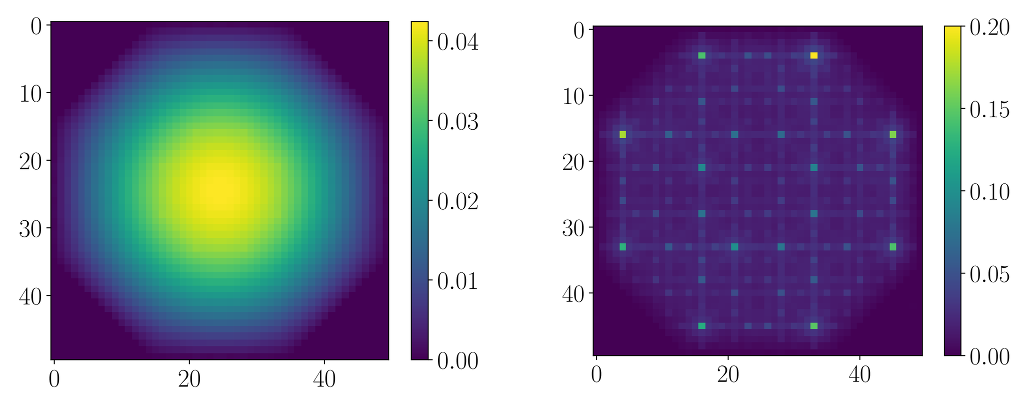


$\rightsquigarrow$ Introduces adjoint mismatch $\rightsquigarrow$ effects convergence of iterative solvers for optimization problems [2, 3], spectral properties.

- Dealing with non-normal $V^*A \rightsquigarrow$ power–schemes may *not converge* or calculate values *far from estimator* [4].

Example: Rotation Operator

n	α	$\sqrt{\|A_{-\alpha}A_\alpha\|}$	$\|A_\alpha\|$
25	10	0.99999	1.00463
25	30	1.00002	1.05930
25	45	0.99996	1.17387
50	10	1.00080	0.99804
50	30	0.99998	1.05314
50	45	1.00000	1.16840



i) power method. ii) our method.

Computing the Extremal Generalized Eigenvalue

- For $A, B \in \mathbb{R}^{d\times d}$ with $B = B^* \succ 0$ consider

$$\mathcal{R}(A, B) = \max_{v\in\mathbb{R}^d\setminus\{0\}} \frac{\langle v, Av\rangle}{\langle v, Bv\rangle} =: r(A, B, v) \qquad (\dagger)$$

- If $B = I_d$, $(\dagger)$ is a problem of finding the largest singular value

$$\langle v, Av\rangle = \langle A^{\mathrm{H}}v, v\rangle \geq 0, \quad v \in \mathbb{R}^d \rightsquigarrow \mathcal{R}(A, I_d) = \max_{v\in\mathbb{S}^{d-1}} \langle v, Av\rangle = \|(A^{\mathrm{H}})^{1/2}\|^2,$$

- If $B \neq I_d$, the maximizer in $(\dagger)$ is the leading eigenvector of $B^{-1}A^{\mathrm{H}}$:

$$\langle v, A^{\mathrm{H}}v\rangle = \langle v, BB^{-1}A^{\mathrm{H}}v\rangle = \lambda\,\langle v, Bv\rangle, \quad \text{with} \quad A^{\mathrm{H}}v = \lambda Bv, \quad v \in \mathbb{R}^d$$

$\rightsquigarrow$ Requires both: adjoint and inverse.

Proposed Method - with Optimal Step Size

1. Set $v^0 = \tilde{v}/\|\tilde{v}\|_B$ with $\tilde{v} \sim \mathcal{N}(0, I_d)$.
2. For the iterate v^k, sample $\tilde{x} \sim \mathcal{N}(0, I_d)$.
3. Project to the tangent space $\mathbb{T}_{v^k}$ and normalize,

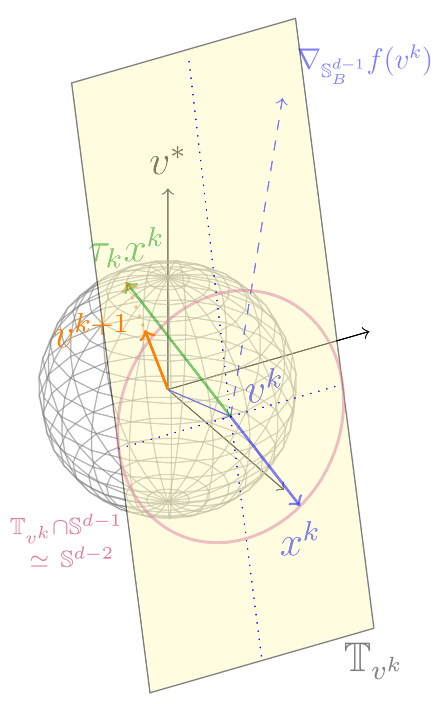
$$x^k := \frac{P_{v^k}\tilde{x}}{\|P_{v^k}\tilde{x}\|}, \quad P_{v^k} := I_d - \frac{(Bv^k)(Bv^k)^{\mathrm{T}}}{\|Bv^k\|^2}. \qquad (\diamond)$$

4. Compute the optimal step size

$$\tau_k := \operatorname*{argmax}_{\tau\in\mathbb{R}} r(A, B, R_{v^k}(\tau x^k)). \qquad (\square)$$

5. Retract $v^k + \tau_k x^k$ onto $\mathbb{S}_B^{d-1}$,

$$v^{k+1} = R_{v^k}(\tau_k x^k) = \frac{v^k + \tau_k x^k}{\|v^k + \tau_k x^k\|_B}. \qquad (\circ)$$



Theorem (Global Convergence, Sublinear Rate [7])

i) If $\dim(G_{\lambda_1}) \geq d-1$, $r(A, B, v^k) = \mathcal{R}(A, B)$ for $k \in \{0, 1\}$.
ii) If $\dim(G_{\lambda_1}) < d-1$, $r(A, B, v^k) \nearrow c \leq \mathcal{R}(A, B)$, and $b_k \to 0$ a.s.,
iii) The sequence $(v^k)_{k\in\mathbb{N}}$ from $(\circ)$ converges to G_{λ_1} a.s.,

$$\operatorname{dist}(G_{\lambda_1}, v^k) \to 0, \qquad r(A, B, v^k) \nearrow \lambda_1 = \mathcal{R}(A, B), \qquad k \to \infty, \text{ a.s.}$$

iv) $\min_{k=0,\dots,n} \mathbb{E}_{x^k,v^k}\left[b_k^2\right] = \min_{k=0,\dots,n} \mathbb{E}_{v^k}\left[\|\operatorname{grad} r(A, B, v^k)\|^2\right] \leq 8\frac{(d-1)\|A\|^2\|B^{-1}\|(1+3\kappa(B))}{(n+1)}.$

Techniques

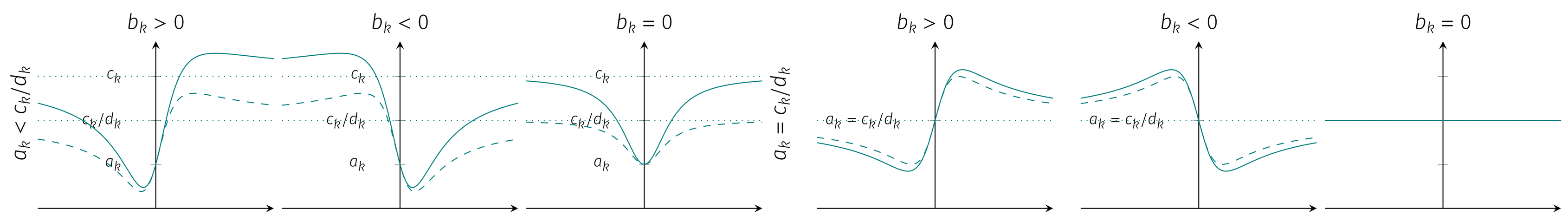
Proposition (Optimal Step Size & Cases, which will Never Occur [7])

Let $v^k \in \mathbb{S}_B^{d-1}$, $x^k \in \mathbb{T}_{v^k} \cap \mathbb{S}^{d-1}$, then $r(A, B, R_{v^k}(\tau x^k)) = \frac{a_k + b_k\tau + c_k\tau^2}{1 + d_k\tau^2}$ with

$$a_k := \langle v^k, Av^k\rangle, \; b_k := \langle x^k, Av^k\rangle + \langle v^k, Ax^k\rangle, \; c_k := \langle x^k, Ax^k\rangle, \; d_k := \langle x^k, Bx^k\rangle. \qquad (\bowtie)$$

If $b_k \neq 0$, then

$$\tau_k = \operatorname{sgn}(b_k)\left(\frac{c_k - a_k d_k}{|b_k| d_k} + \sqrt{\frac{(c_k - a_k d_k)^2}{(b_k d_k)^2} + \frac{1}{d_k}}\right) \in \mathbb{R}\setminus\{0\}.$$



Lemma (Never Accruing Cases [7, 8])

Let $v^k \in \mathbb{S}_B^{d-1}$ and x^k as in $(\diamond)$.

$$v^k \in G_\lambda \quad \Leftrightarrow \quad b_k := \langle x^k, A^{\mathrm{H}}v^k\rangle = 0 \text{ a.s.} \quad \Leftrightarrow \quad \operatorname{grad} r(A, B, v^k) = 0.$$

- *Generalized eigenspaces* of (A, B), i.e. $B^{-1}A^{\mathrm{H}}$:

$$G_\lambda := \{v \in \mathbb{R}^d \setminus \{0\} : A^{\mathrm{H}}v = \lambda Bv\} = \{v \in \mathbb{R}^d \setminus \{0\} : B^{-1}A^{\mathrm{H}}v = \lambda v\},$$

- with *generalized eigenvalues* of (A, B), i.e. $\operatorname{spec}(B^{-1/2}A^{\mathrm{H}}B^{-1/2})$:

$$\{\lambda \in \mathbb{R} \mid \exists v \in \mathbb{S}_B^{d-1}, A^{\mathrm{H}}v = \lambda Bv\} = \{\lambda_1, \dots, \lambda_d\}, \quad \lambda_1 \geq \dots \geq \lambda_d.$$

i) $r(A, B, v^{k+1}) - r(A, B, v^k) = a_{k+1} - a_k = \frac{1}{2}\tau_k b_k > 0$, a.s.
ii) If $\dim(G_\lambda) < d-1$, then [7, 8]
$\rightsquigarrow$ v^{k+1} is not a generalized eigenvector, a.s., if v^k is neither one.
$\rightsquigarrow$ v^k is not a generalized eigenvector, a.s, for $(v^k)_{k\in\mathbb{N}}$

Proposition (Borel–Cantelli & Bounded Sampling Probabilty [7])

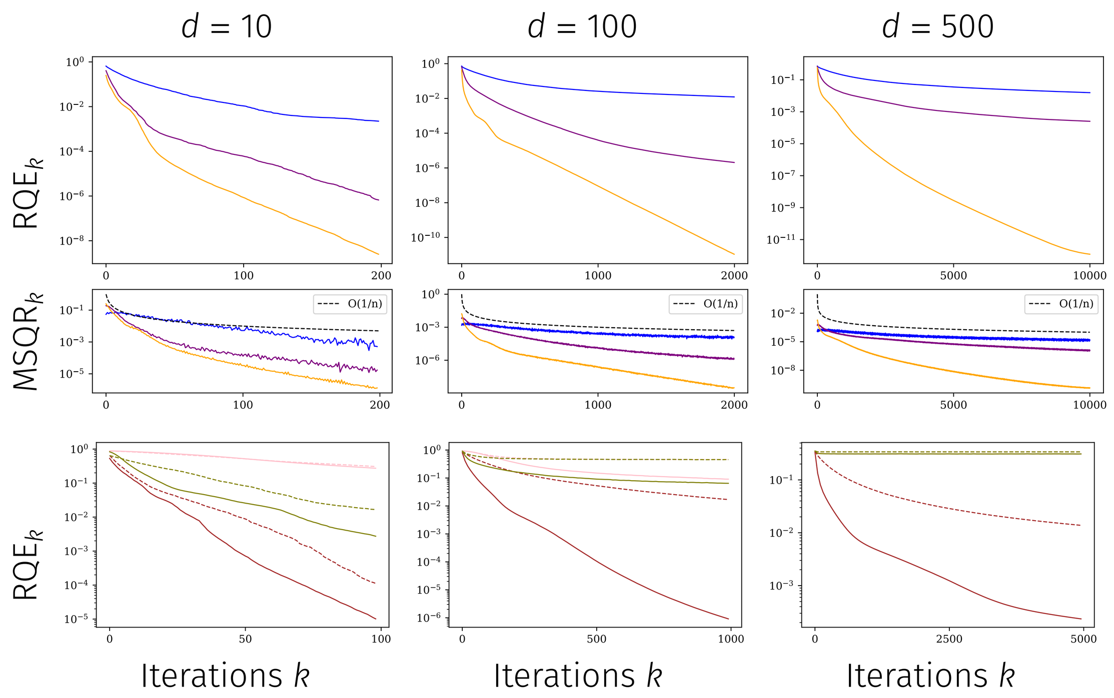
Let $\tilde{v}, v^k \in \mathbb{S}_B^{d-1}$, x^k as in $(\diamond)$, b_k as in $(\bowtie)$, and $\varepsilon > 0$.

- $\mathbb{E}_{x^k|v^k}[b_k x^k] = \frac{2}{d}\operatorname{grad} r(A, B, v^k)$, where

$$\operatorname{grad} r(A, B, v^k) = P_{v^k}\nabla\langle v^k, Av^k\rangle = 2\left(I_d - \frac{(Bv^k)(Bv^k)^{\mathrm{T}}}{\|Bv^k\|^2}\right)A^{\mathrm{H}}v^k.$$

- $\mathbb{P}_{x^k|v^k}(x^k \in \{x \in \mathbb{T}_{v^k} \cap \mathbb{S}^{d-1} \mid \exists \tau \in \mathbb{R}, R_{v^k}(\tau x) \in \mathbb{B}_\varepsilon(\tilde{v})\}) > p_{\varepsilon,d,B}.$

Numerical Experiments



Relative quotient error

$$\mathrm{RQE}_k := \frac{\mathcal{R}(A,B) - f(v^k)}{\mathcal{R}(A,B)}.$$

Minimal squared residual

$$\mathrm{MSQR}_k := \min_{n\leq k} \left\|A^{\mathrm{H}}v^n - \langle v^n, A^{\mathrm{H}}v^n\rangle Bv^n\right\|^2.$$

$m = 1$ — $m = 10$ — $m = 100$ —
A and $\tilde{B}$ are Gaußian and

$$B = (\tilde{B} + d\cdot I_d)^{\mathrm{T}}(\tilde{B} + d\cdot I_d).$$

Our — ZO-RGA i) — ZO-RGA ii) [6] —
$m = 10$ - - - - $m = 100$ —
$\tilde{A}$, $\tilde{B}$ are Gaußian, and

$$A = \tilde{A}^{\mathrm{T}}\tilde{A}, \quad B = \tilde{B}^{\mathrm{T}}\tilde{B}.$$

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