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Technische Universität Berlin

Stochastic Zeroth-Order Method for Computing Generalized Rayleigh Quotients

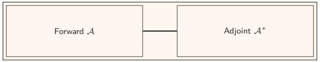
Jonas Bresch | Technical University Berlin | joint work with
Oleh Melnyk, Martin Schoen, Gabriele Steidl

Funded by:
Berlin Mathematical School
BMS

Motivation: Adjoint mismatch

– Let $\mathbb{X}$ and $\mathbb{Y}$ are infinite-dimensional spaces.

Continuous model



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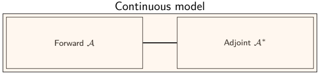

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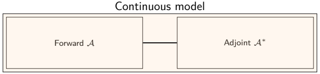

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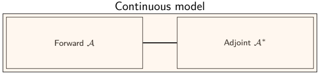

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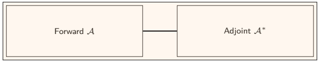

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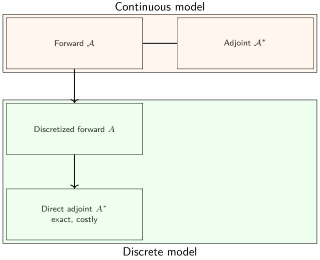

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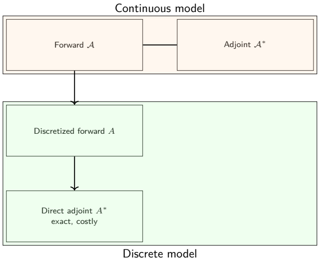

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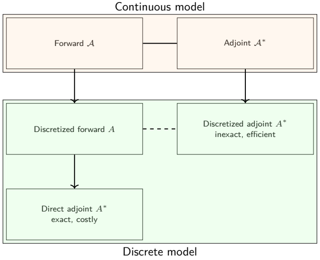
- Instead, $\mathcal{A}^*$ is discretized $\to$ introduces errors $\to$ **adjoint mismatch**[4][5].



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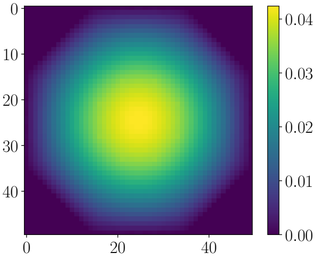
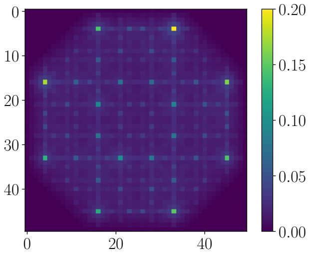
n	α	$\sqrt{\|A_{-\alpha} A_\alpha\|}$	$\|A_\alpha\|$
25	10	0.99999	1.00463
25	30	1.00002	1.05930
25	45	0.99996	1.17387
50	10	1.00080	0.99804
50	30	0.99998	1.05314
50	45	1.00000	1.16840





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- Consider two operators $\mathcal{A}, \mathcal{V} : \mathbb{X} \to \mathbb{Y}$.
- Restrict your self to the setting that $\mathcal{A}$ is your forward model hence $x \mapsto \mathcal{A}x$ for $x \in \mathbb{X}$ is available,
- and $\mathcal{V}$ is your backward model, hence $y \mapsto \mathcal{V}^* y$ for $y \in \mathbb{Y}$ is available.
- For acceleration, replace the true adjoint $V^* \neq A^*$ in the discrete setting $\to$ convergence guarantees are violated.
- The Chambolle–Pock[6], [7] and Primal–Dual Douglas–Rachford[8] algorithm require $\|V\|_2$ and $\|A - V\|_2$ for

$$\min_{x \in \mathbb{X}} f(\mathcal{A}x) + g(x) = \min_{y \in \mathbb{Y}} g^*(-\mathcal{A}^* y) + f^*(y) = \min_{x \in \mathbb{X}} \max_{y \in \mathbb{Y}} g(x) + \langle \mathcal{A}x, y \rangle - f^*(y),$$

  and guaranteed linear convergence.
- For solving $\min_{x \in \mathbb{X}} \|y - \mathcal{A}x\|_{\mathbb{X}}^2 + g(x) + \frac{\kappa}{2}\|x\|_{\mathbb{X}}^2$ the spectral properties of $L = V^* A + \kappa I$[9] is required.
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which **requires both adjoint and inverse**. We refer to eigenvectors of $B^{-1}A^{\mathsf{H}}$ as **generalized eigenvectors** of (A, B).

First-Order Riemannian Optimization

Consider the ellipsoid $\mathbb{S}_B^{d-1} := \{v \in \mathbb{R}^d \colon \langle v, Bv \rangle = 1\}$ with $h_{\mathbb{S}_B^{d-1}} = \langle v, Bv \rangle - 1$.

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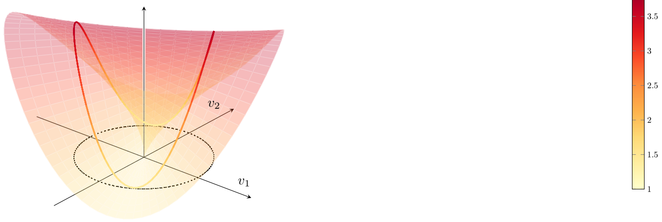

Visualization of the **generalized Rayleigh quotient** $r(A,B,v)$ for $v = (v_1, v_2)^{\mathsf{T}} \in \mathbb{R}^2 \setminus \{0\}$ and

$$A = \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix}.$$

Its values on $\mathbb{S}_B^1$ are highlighted by the solid line. **Left:** $B = I_2$,

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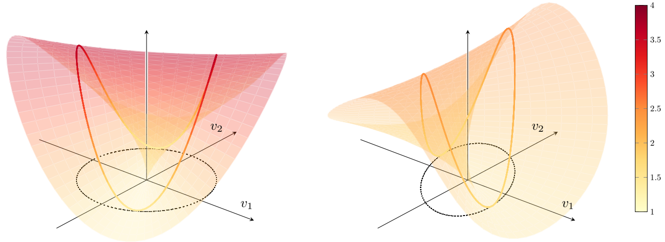

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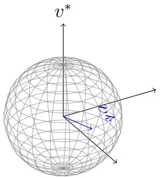

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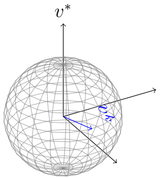

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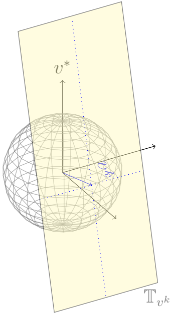

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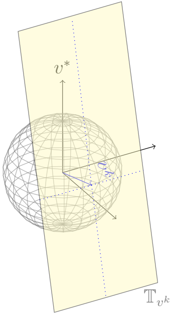

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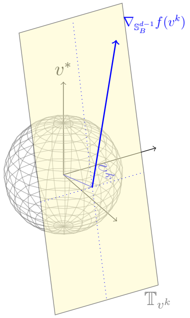

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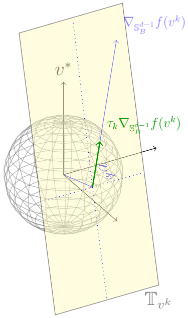

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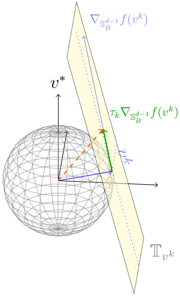

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1. Consider the tangent space $\mathbb{T}_{v^k}$ at v^k for $\mathbb{M} = \mathbb{S}_B^{d-1} = h_{\mathbb{M}}^{-1}(0)$ given by

$$\mathbb{T}_{v^k} := \ker\left(Dh_{\mathbb{S}_B^{d-1}}\right) = \left\{x \in \mathbb{R}^d : \left\langle x, Bv^k \right\rangle = 0\right\} = \operatorname{span}\{Bv^k\}^{\perp}.$$

2. and **orthogonal projection**

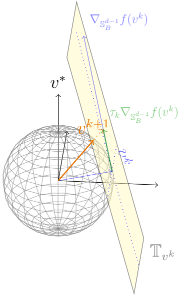
$$P_{v^k} = \left(I_d - \frac{Bv^k (Bv^k)^*}{\|Bv^k\|^2}\right).$$

3. Compute the **Riemannian gradient** as

$$\nabla_{\mathbb{S}_B^{d-1}} f(v^k) = P_{v^k} \nabla f(v^k) \in \mathbb{T}_{v^k}.$$

4. **Rescale** it with **appropriate step size** $\tau_k \in \mathbb{R}$.
5. **Retract**

$$v^{k+1} = R_{v^k}\left(\tau_k \nabla_{\mathbb{S}_B^{d-1}} f(v^k)\right) \quad \text{where} \quad R_{v^k}(\tau_k x^k) := \frac{v^k + \tau_k x^k}{\|v^k + \tau_k x^k\|_B}, \quad x^k \in \mathbb{T}_{v^k}, \quad \tau_k \in \mathbb{R}.$$



[11] Lee, J. M. (2012) – Introduction to Smooth Manifolds,

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For C^1 function[12] on smooth embedded submanifolds, here with $f(v) = \left\langle v, A^{\mathsf{H}} v \right\rangle$, where $v \in \mathbb{R}^d$.

Theorem (Sublinear Convergence Rate – Critical Points[13])

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4. **Optional:** Use multiple directions to **improve** the **variance**

$$\widehat{\mathrm{grad}}_m f(v^k) := \frac{1}{m} \sum_{i=1}^{m} \frac{f(R_{v^k}(\mu_k x^{k,i})) - f(v^k)}{\mu_k} x^{k,i}, \quad \text{where} \quad x^{k,i} := P_{v^k} \tilde{x}^i, \quad \tilde{x}^i \overset{\text{iid.}}{\sim} \mathcal{N}(0, I_d), \quad i \in \{1, \dots, m\}$$

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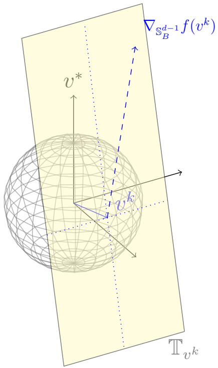

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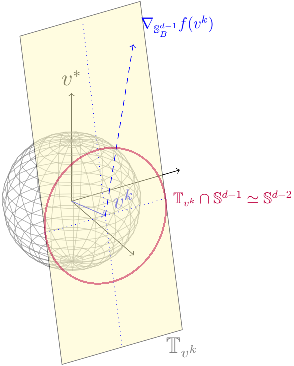

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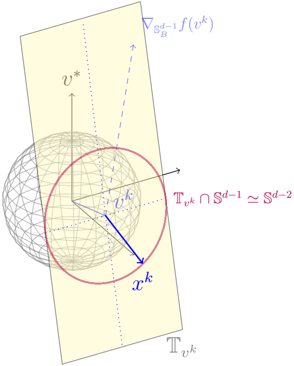

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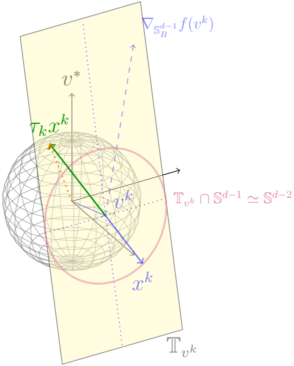
$$\tau_k := \operatorname*{argmax}_{\tau \in \mathbb{R}} f(R_{v^k}(\tau x^k))$$



Proposed Method

Are we able to compute "the optimal" step size τ_k?

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 a random direction $\tilde{x} \sim \mathcal{N}(0, I_d)$.
3. Project to the tangent space and normalize,

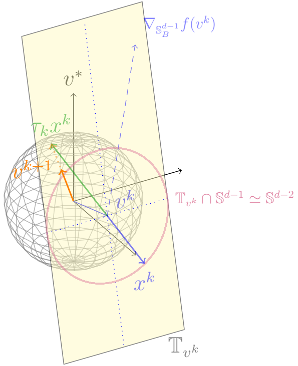
$$x^k := P_{v^k}\tilde{x}/\|P_{v^k}\tilde{x}\|.$$

4. Compute the optimal step size

$$\tau_k := \underset{\tau \in \mathbb{R}}{\operatorname{argmax}}\, f(R_{v^k}(\tau x^k))$$

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

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



Optimal Stepsize τ_k – Solving a Quadratic Subproblem, a sub-generalized Rayleigh Problem

Theorem (On the Optimal Step Size & Cases, which will Never Arise, a.s.)

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If $b_k \neq 0$, *then*

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

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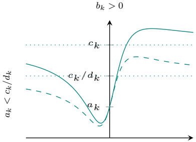

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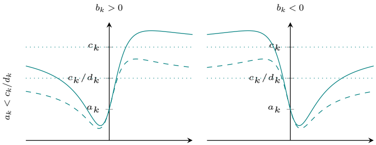

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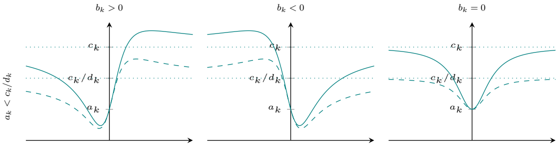

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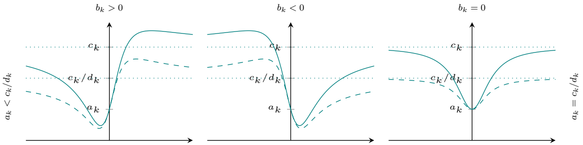

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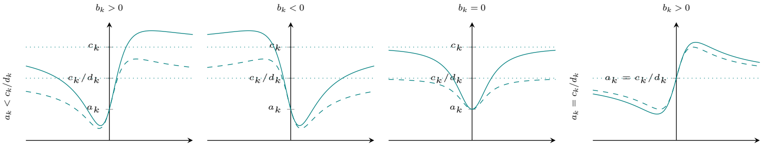

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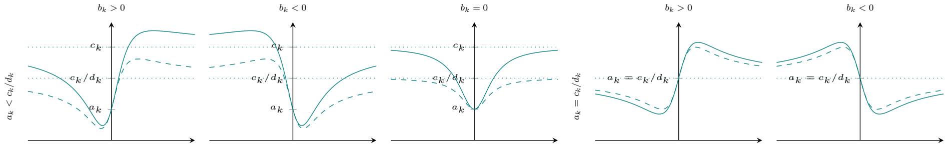

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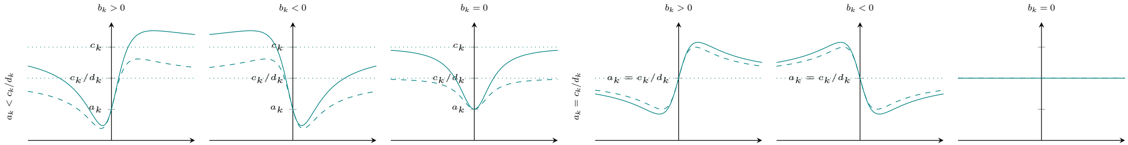

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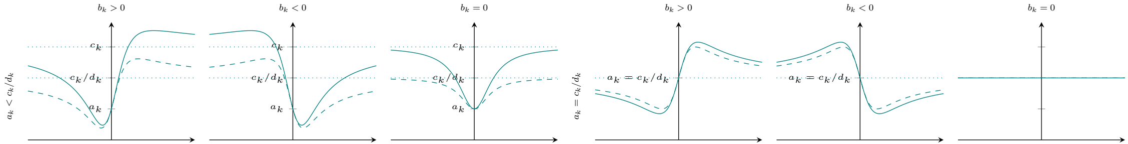

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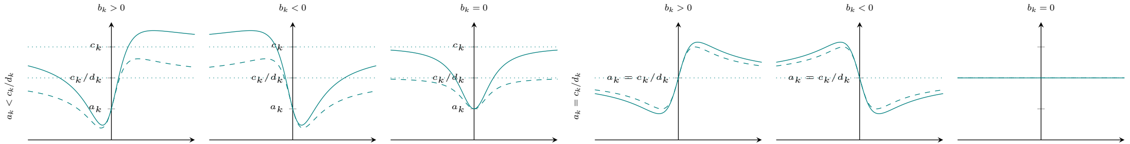

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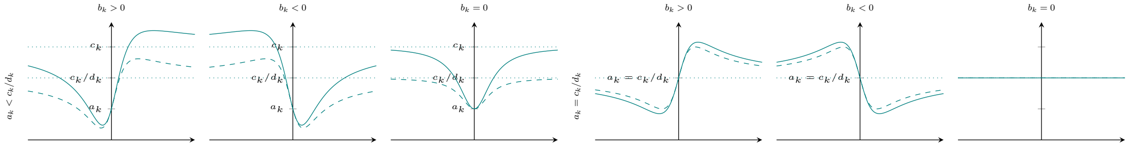

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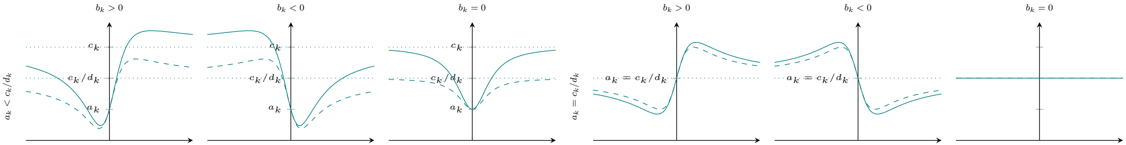

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$$\operatorname{spec}(B^{-1}A^{\mathsf{H}}) := \{\lambda \in \mathbb{R} \mid \exists v \in \mathbb{S}_B^{d-1}, A^{\mathsf{H}} v = \lambda B v\} = \{\lambda_1, \ldots, \lambda_d\}, \quad \lambda_1 \geq \ldots \geq \lambda_d.$$

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Let $v^k \in \mathbb{S}_B^{d-1}$ *and* $x^k = P_{v^k}\tilde{x}/\|P_{v^k}\tilde{x}\| \in \mathbb{T}_{v^k} \cap \mathbb{S}^{d-1}$, $\tilde{x} \sim \mathcal{N}(0, I_d)$. *Then,* v^k *is a generalized eigenvector of* (A^{H}, B) *if and only if* $b_k := \langle x^k, A^{\mathsf{H}} v^k \rangle = 0$ *a.s. if and only if* $\nabla_{\mathbb{S}_B^{d-1}} f(v^k) = 0$ *(then, stop the algorithm).*

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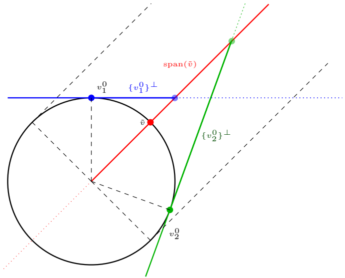

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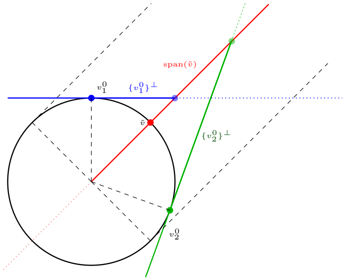

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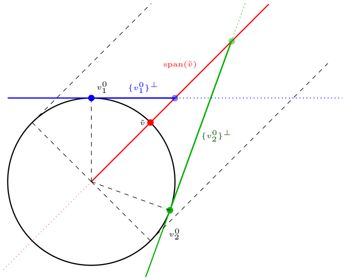

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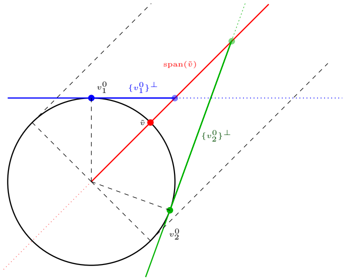

Convergence Towards the Leading Eigenspace

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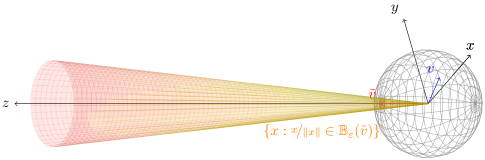

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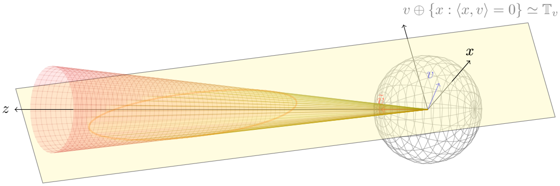

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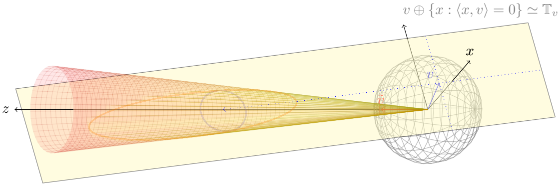

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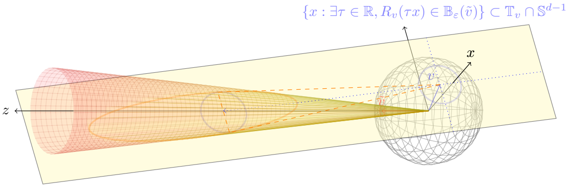


Convergence Towards the Leading Eigenspace

Theorem ($|b_k| \to 0$, Convergence, Sublinear Rate)

i) *If* $\dim(G_{\lambda_1}) < d-1$, $r(A,B,v^k)$ *converges, strictly increasing, and* $b_k \to 0$ *a.s.*

ii) *There exists a random variable* λ *with values in* $\operatorname{spec}(B^{-1}A^{\mathrm{H}})$ *such that* $\operatorname{dist}(G_\lambda, v^k) \to 0$, *a.s.*

iii) *The sequence* $(v^k)_{k\in\mathbb{N}}$ *generated by the construction converges to* G_{λ_1} *a.s., i.e. it holds*

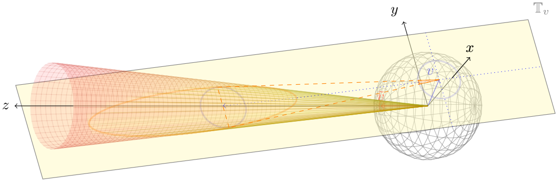
$$\operatorname{dist}(G_{\lambda_1}, v^k) \to 0, \qquad r(A,B,v^k) \nearrow \lambda_1, \quad k \to \infty, \text{ a.s.}$$

iv) *It holds* $$\min_{k=0,\dots,n} \mathbb{E}_{x^k,v^k}\left[b_k^2\right] = \min_{k=0,\dots,n} \mathbb{E}_{v^k}\left[\left\|\nabla_{\mathbb{S}_B^{d-1}} f(v^k)\right\|^2\right] \le 8\frac{(d-1)\|A\|^2\|B^{-1}\|(1+3\kappa(B))}{(n+1)}.$$

Proof:
1) never stops a.s.,
2) converges to a critical point,
3) must be the global maximum.

Lemma (Uniform Bound → Borel–Cantelli)

For any $\varepsilon > 0, \tilde{v} \in \mathbb{S}_B^{d-1}$ *with*
$D_v := \{x \in \mathbb{T}_v : \exists \tau \in \mathbb{R}, R_v(\tau x) \in \mathbb{B}_\varepsilon(\tilde{v})\}$
is $\inf_{v\in\mathbb{S}_B^{d-1}} \sigma_{Bv}(D_v) > c$ *unif. bounded.*



Connection to Zeroth-Order Methods & Acceleration

Proposition (Estimating the Riemannian Gradient, Variance Reduction)

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1. **Sample** multiple $x^{k,i} \in \mathbb{T}_{v^k} \cap \mathbb{S}^{d-1}$ by $P_{v^k} x^i$ where $x^i \overset{\text{iid.}}{\sim} \mathcal{N}(0, I_d)$,

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Restrictions & Extensions

– **Operator norm** [15] via $f = \|A \cdot\|^2$ for $A \in \mathbb{F}^{m\times d}$, i.e. singular values of A

[15] Bresch, J. et al. (2024) – Matrix-free stochastic calculation of operator norms without using adjoints, **SIAM J. Matrix Anal. Appl.**
[16] Bresch, J. (2025) – Geometry-Aware Ansätze in Image Processing and Stochastic Calculations of Matrix Quantities, **Dissertation**
[17] Bresch, J. et al. (2025) – Computing adjoint mismatch of linear maps, **arXiv:2503.21361**

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- **Operator norm** [15] via $f = \|A\cdot\|^2$ for $A \in \mathbb{F}^{m\times d}$, i.e. singular values of A
- **Generalized operator norm** [16] via $f = \|A\cdot\|^2/\|B\cdot\|^2$ for $A \in \mathbb{F}^{m\times d}$ and $B \in \mathbb{F}^{\ell\times d}$ where $\ell \gg d$ (necessary), i.e. singular values of $(B^*B)^{-1}A^*A$, with unconstrained sampling approach, i.e. $x^k \sim \mathcal{U}(\mathbb{S}^{d-1})$,
$$a_k := \left\|Av^k\right\|^2, b_k := \left\langle Av^k, Ax^k\right\rangle, c_k := \left\|Ax^k\right\|^2, d_k := \left\|Bv^k\right\|^2, e_k := \left\langle Bv^k, Bx^k\right\rangle, f_k := \left\|Bx^k\right\|^2,$$
such that
$$\tau_k = \operatorname*{argmax}_{\tau\in\mathbb{R}} \frac{a_k+2b_k\tau+c_k\tau^2}{d_k+2e_k\tau+f_k\tau^2} = -\frac{\beta_k}{2\gamma_k} + \operatorname{sign}\left(\frac{\alpha_k}{\gamma_k}\right)\left(\frac{\beta_k^2}{4\gamma_k^2} - \frac{\alpha_k}{\gamma_k}\right)^{1/2}, \qquad \text{where} \quad \begin{cases} \alpha_k &:= b_k d_k - a_k e_k, \\ \beta_k &:= c_k d_k - a_k f_k, \\ \gamma_k &:= c_k e_k - b_k f_k, \end{cases}$$

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- **Adjoint mismatch** [17] via $f = \left\langle \cdot^1, (A-V)\,\cdot^2\right\rangle = \left\langle \cdot^1, A\,\cdot^2\right\rangle - \left\langle V^*\cdot^1, \cdot^2\right\rangle$, where $v \mapsto Av$ and only $u \mapsto V^*u$ are available,
$$a_k := \langle u^k, Av^k\rangle - \langle V^*u^k, v^k\rangle, \qquad b_k := \langle w^k, Av^k\rangle - \langle V^*w^k, v^k\rangle, \qquad e_k := a_kb_k + c_kd_k,$$
$$c_k := \langle u^k, Ax^k\rangle - \langle V^*u^k, x^k\rangle, \qquad d_k := \langle w^k, Ax^k\rangle - \langle V^*w^k, x^k\rangle, \qquad f_k := a_k^2 + c_k^2 - b_k^2 - d_k^2$$
and two iterates v^k, u^k and two optimal step sizes (ξ_k, τ_k) (depending on each other).
$$(\tau_k, \xi_k) = \operatorname*{argmax}_{\tau,\xi\in\mathbb{R}} \frac{\langle u^k+\tau w^k, (A-V)(v^k+\xi x^k)\rangle^2}{\left\|u^k+\tau w^k\right\|^2\cdot\left\|v^k+\xi x^k\right\|^2} = \left(-\operatorname{sign}(e_k)\left(\frac{f_k}{2|e_k|} - \left(\frac{f_k^2}{4e_k^2}+1\right)^{1/2}\right), \frac{c_k+\tau_kd_k}{a_k+\tau_kb_k}\right).$$

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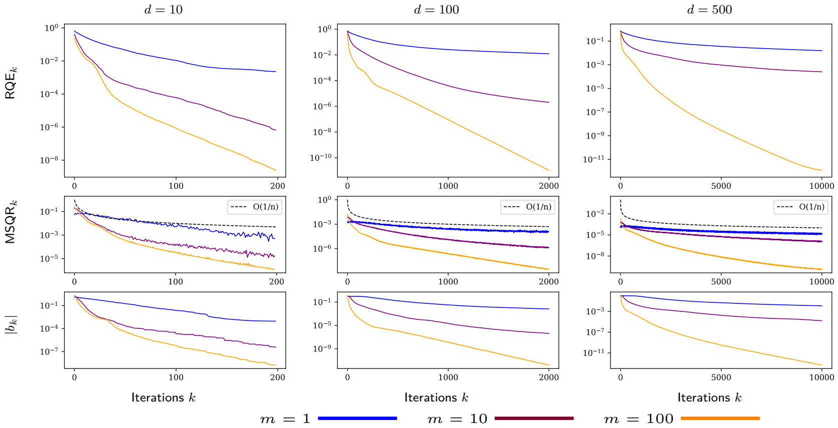
Numerical Simulations – Proof of Concept



Relative quotient error

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

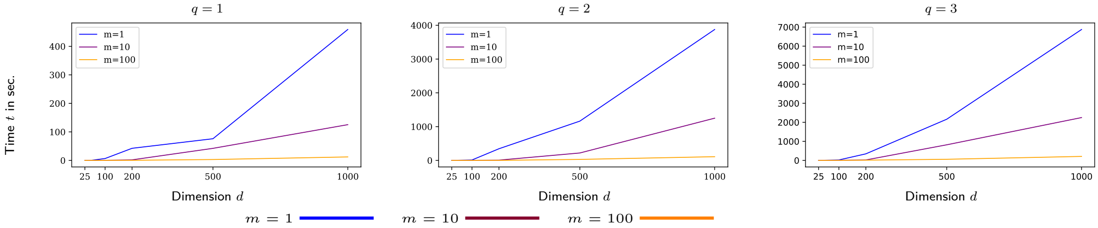
Minimal squared residual in the eigenvector equation

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

Comparison for different sizes $d \in \{10, 100, 500\}$ and samples $m \in \{1, 10, 100\}$.
Here A and $\tilde{B}$ are Gaußian and

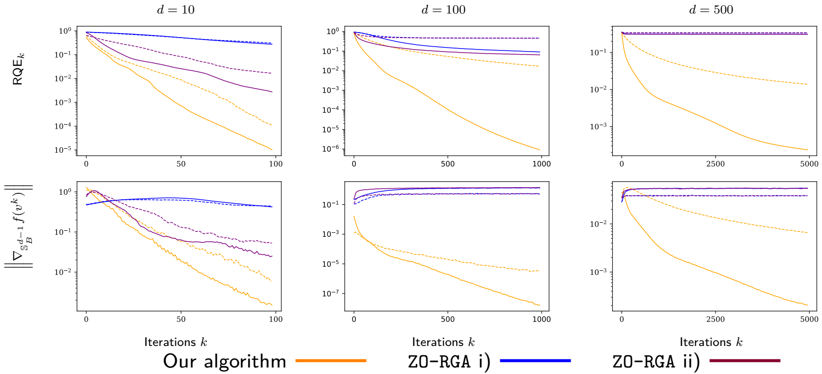
$$B = (\tilde{B} + d \cdot I_d)^{\mathsf{T}} (\tilde{B} + d \cdot I_d).$$

Numerical Simulations – Time, Sampling, and Dimension Trial



Runtime of our algorithm for $m \in \{1, 10, 100\}$ for the matrices with $\kappa(B) \approx 10^q$ for varying dimension d. The methods are stopped whenever RQE $< 10^{-2}$ or after $100 \cdot d$ iterations.
Here A is Gaussian, $B = Q\,\mathrm{diag}(\lambda)Q^\mathsf{T}$ with Q random unitary and $\lambda_j \sim 10^{\mathsf{Unif}([1,q])}$.

Numerical Simulations – Comparison for Zeroth-Order Riemannian Gradient Methods



Comparison of **our algorithm** with the **two variants** of `ZO-RGA`[18] for $m = 100$ and $d \in \{10, 100, 500\}$.

Comparison of

- $m = 10$ (dashed lines)
- $m = 100$ (solid lines).

Here $\tilde{A}$, $\tilde{B}$ are Gaußian, and

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

[18] Li, J., Balasubramanian, K., and Ma, S. (2023) – Stochastic zeroth-order Riemannian derivative estimation and optimization, **Math. Oper. Res.**

Conclusion & Outlook

- We proposed an adjoint-free method for finding the maximum of generalized Rayleigh quotient.
- It stems from zeroth-order methods, but gives a better performance due to optimal step size selection.
- We derived sublinear convergence guarantees to the set of maximizers.

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Thanks for your attention!

Stochastic Zeroth-Order Method for Computing Generalized Rayleigh Quotients,
JB, Oleh Melnyk, Martin Schoen, Gabriele Steidl

Included Publications

[1] Bresch, J. et al. Matrix-free stochastic calculation of operator norms without using adjoints. In: **SIAM J. Matrix Anal. Appl.** (2024). arXiv:2410.08297, accepted in SIAM J. Matrix Anal. Appl. (February, 2026). DOI: 10.48550/arXiv.2410.08297.

[2] Bresch, J. et al. Computing adjoint mismatch of linear maps. In: **arXiv:2503.21361** (2025). arXiv:2503.21361, advanced state of review in J. Comput. Appl. Math. (February, 2026). DOI: 10.48550/arXiv.2503.21361.

[3] Bresch, J. et al. Stochastic zeroth-order method for computing the generalized Rayleigh quotient. In: **arXiv:2512.05520** (2025). arXiv:2512.05520, submitted to Linear Algebra Appl., November. DOI: 10.48550/arXiv.2512.05520.

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Motivation: Adjoint Mismatch

- **Inverse problems:** $\mathcal{A}x = y$
- might **not solvable**, instead
  $\min_{x\in\mathbb{X}} \|\mathcal{A}x - y\|_{\curvearrowright}$ where $\mathcal{A} : \mathbb{X} \to \mathbb{Y}$
- **Normal equation:** $\mathcal{A}^*\mathcal{A}x = \mathcal{A}^*y$

$\to$ pseudo inverse $\mathcal{A}^\dagger$, noncontinuous

- discretization $A \in \mathbb{R}^{m\times d}$

$\to$ exact adjoint A^* may be **expensive** or **unavailable**

- Replacing A^* by a discretized adjoint V^* $\to$ **adjoint mismatch**
- **Affects** convergence $\|V\|, \|A - V\|$

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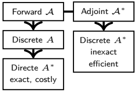

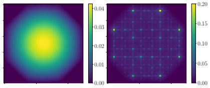

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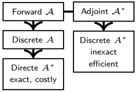

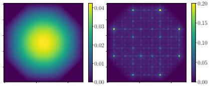

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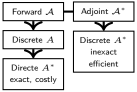

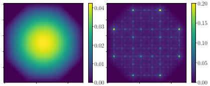

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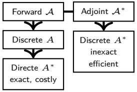

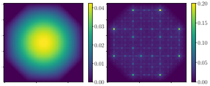

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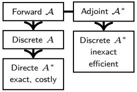

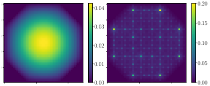

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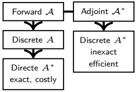

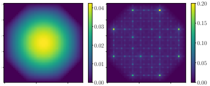

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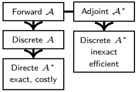

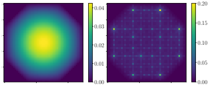

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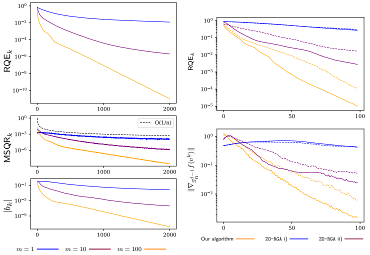

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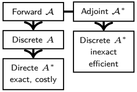
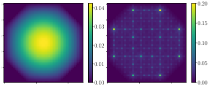
- VV^* unavailable for estimating
- V^*A nonnormal → not convergent





Extensions, Restrictions of $\mathcal{R}(A, B)$

- Operator norms $\|A\|$, $\|A/B\|$
- Adjoint mismatch $\|A - V\|$

Optimization Target

- Maximize the **generalized Rayleigh quotient** $\mathcal{R}(A,B) = \max_{v\neq 0} \frac{\langle v, Av\rangle}{\langle v, Bv\rangle}$
- $A \in \mathbb{R}^{d\times d}$, B Hermitian pos. def.
  $\langle v, Av\rangle = 1/2\big(\langle v, Av\rangle + \langle A^*v, v\rangle\big) = \langle v, A^{\mathsf{H}}v\rangle$

→ $B = I_d$ → top **spectral problem**

→ general B → leading **generalized eigenvector** of $B^{-1}A^{\mathsf{H}}$

↔ max λ s.t. $\begin{cases} A^{\mathsf{H}}v = \lambda Bv \\ \langle v, Bv\rangle = 1 \end{cases}$

Rieman. Grad.: First & Zeroth Order

→ Riemannian gradient, retraction

→ **requires** adjoint A^*, inverse B^{-1}

- **Surrogate** stochastic gradient
- Sample $\tilde{x} \sim \mathcal{N}(0, I_d)$, $x^k = P_{v^k}\tilde{x}$
- **Estimate** $\widehat{\nabla}_1 f(v^k) = \frac{f(R_{v^k}(\mu_k x^k)) - f(v^k)}{\mu_k} x^k$
- **Choice** of the step size!

Specific Construction, Estimator

- **Solve** quadratic subproblem

$$\arg\min_{\tau\in\mathbb{R}} \frac{\langle R_{v^k}(\tau x^k), AR_{v^k}(\tau x^k)\rangle}{\langle R_{v^k}(\tau x^k), BR_{v^k}(\tau x^k)\rangle}, \quad \begin{cases} a_k := \langle v^k, A^{\mathsf{H}}v^k\rangle \\ b_k := 2\langle x^k, A^{\mathsf{H}}v^k\rangle \end{cases}$$

- **Estimator** $\mathbb{E}[b_k x^k] = \frac{1}{d-1}\nabla_{\mathbb{S}_B^{d-1}} f(v^k)$,

$$\mathbb{E}[b_k^2 \mid v^k] = \frac{4}{d-1}\|P_{v^k}A^{\mathsf{H}}v^k\|^2 = \frac{1}{d-1}\|\nabla_{\mathbb{S}_B^{d-1}} f(v^k)\|^2$$

Riemannian Formulation

- Work on the ellipsoid
  $\mathbb{S}_B^{d-1} = \{v \in \mathbb{R}^d \mid \langle v, Bv\rangle = 1\} = h^{-1}(\{0\})$
- smooth, embedded Riemannian manifold $h(v) = \langle v, Bv\rangle - 1$
- tangent space
  $\mathbb{T}_v = \ker(Dh[v]) = \{x \in \mathbb{R}^d \mid \langle x, Bv\rangle = 0\}$
- Then $\mathcal{R}(A, B) = \max_{v\in\mathbb{S}_B^{d-1}} \langle v, A^{\mathsf{H}}v\rangle$

Convergence, Rates

$\operatorname{dist}(G_{\max}, v^k) \to 0$, $r(A, B, v^k) \nearrow \lambda_{\max}$, $k \to \infty$, a.s.

$$\min_{k=0,\dots,n} \mathbb{P}(\|A^{\mathsf{H}}v^k - a_k Bv^k\|^2 \geq \varepsilon) \in \mathcal{O}(1/n)$$

$$\min_{k=0,\dots,n} \mathbb{E}[b_k^2] = \min_{k=0,\dots,n} \mathbb{E}[\|\nabla_{\mathbb{S}_B^{d-1}} f(v^k)\|^2] \in \mathcal{O}(1/n)$$