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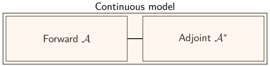
Stochastic Zeroth-Order Method for Computing Operator Quantities

Jonas Bresch | Technical University Berlin | joint work with
Dirk Lorenz, Oleh Melnyk, Felix Schneppe, Martin Schoen, Gabriele Steidl, Maximilian Winkler

Funded by:
Berlin Mathematical School BMS
DAAD

Motivation: Adjoint Mismatch in Inverse Problems



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Continuous model

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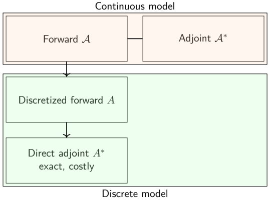

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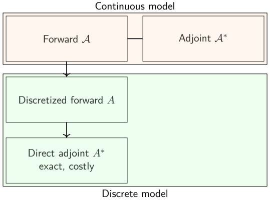

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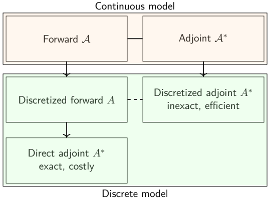

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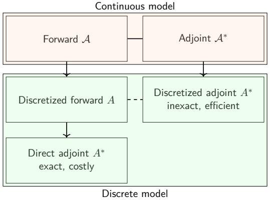

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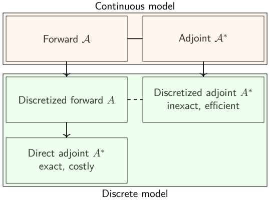

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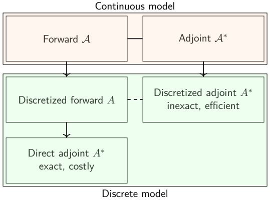

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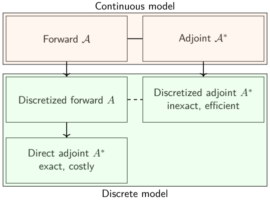

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- It holds: $\mathcal{A}_\alpha^* = \mathcal{A}_{-\alpha}$ and $\mathcal{A}_\alpha^{-1} = \mathcal{A}_{-\alpha}$, such that $\|\mathcal{A}_\alpha\| = 1$ in the continuous setting.

Motivation: Toy Example for Adjoint Mismatch

- Rotations of a function $f : \mathbb{D} \coloneqq \{x \in \mathbb{R}^2 : \|x\| \leq 1\} \to \mathbb{R}$ in $\mathbb{R}^2$,
- given by $\mathcal{A}_\alpha f(x) = f(R_\alpha x)$, where

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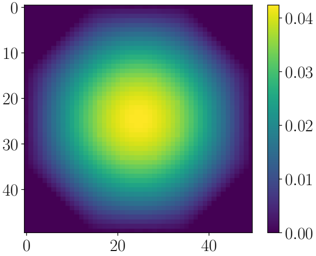
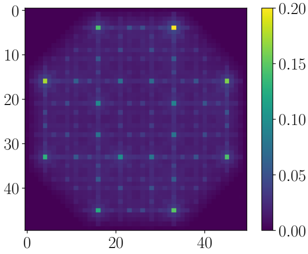
n	α	$\sqrt{\|A_{-\alpha} A_\alpha\|}$	$\|A_\alpha\|$
25	10	0.99999	1.00463
25	30	1.00002	1.05930
25	45	0.99996	1.17387
50	10	1.00080	0.99804
50	30	0.99998	1.05314
50	45	1.00000	1.16840





Adjoint Mismatch Operator – Riemannian Geometry

Focus on the maximization of the shifted Rayleigh quotient of $A \in \mathbb{R}^{m \times d}$ by $V \in \mathbb{R}^{m \times d}$

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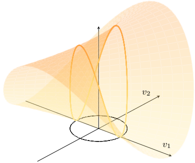

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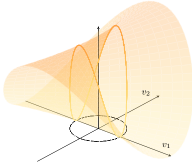

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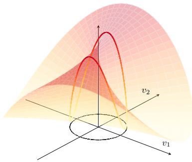

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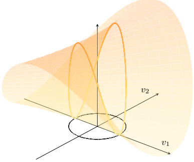

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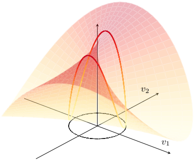

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The tangent space with orthogonal projection is given as

$$\mathbb{T}_v := \ker\big(Dh\big) = \Big\{x \in \mathbb{R}^d : \langle x,v\rangle = 0\Big\} = \operatorname{span}\{v\}^\perp \quad \text{and} \quad P_v : \mathbb{R}^d \to \mathbb{T}_v, \quad x \mapsto \big(I_d - vv^*\big)x.$$

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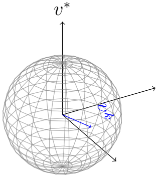
1. Idea: reduce to the problem to $\|A\|$ with $r(A,0,\cdot)^2 = \|A\cdot\|^2$, on $\mathbb{S}^{d-1}$[9]



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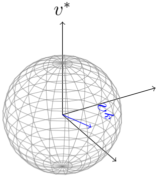

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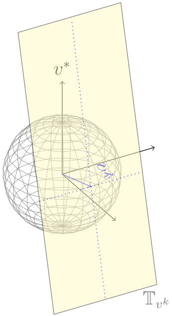

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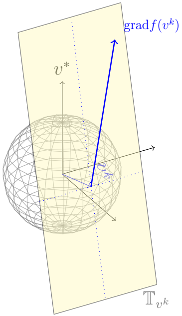

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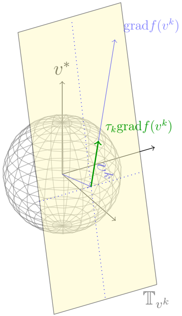

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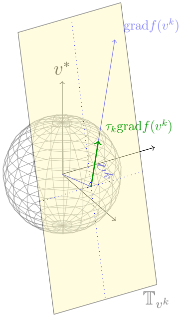

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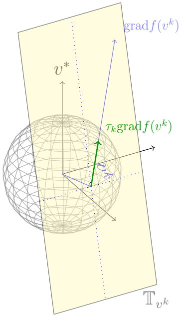

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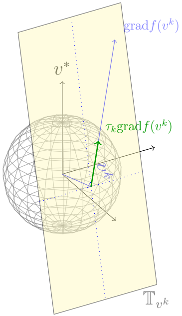

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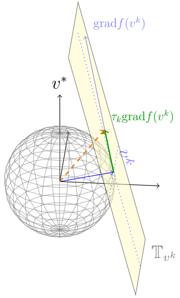

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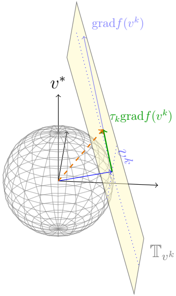

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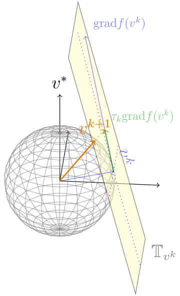
$$v^{k+1} = R_{v^k}\left(\tau_k y^k\right) \quad \text{with} \quad y^k \in \left\{\operatorname{grad} r(A,0,v^k)^2, \widehat{\operatorname{grad}}_m r(A,0,v^k)^2\right\}, \text{ where } R_v(\tau x) := \frac{v+\tau x}{\|v+\tau x\|}.$$



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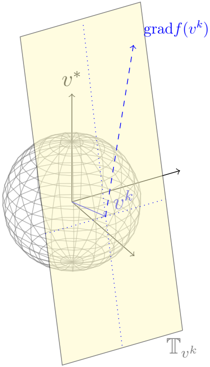

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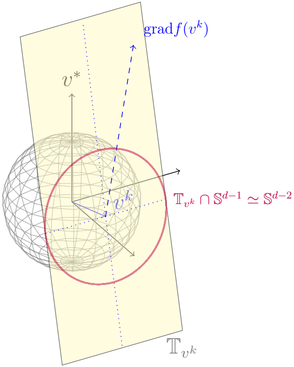

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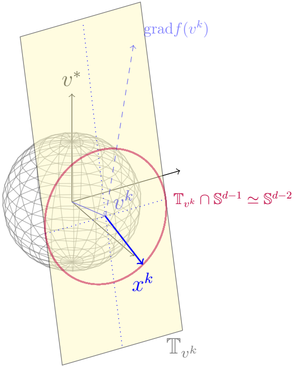

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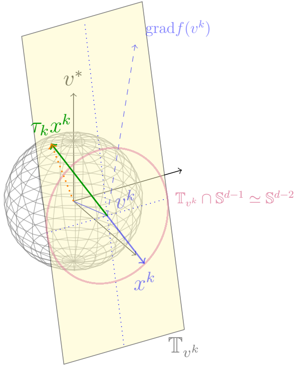

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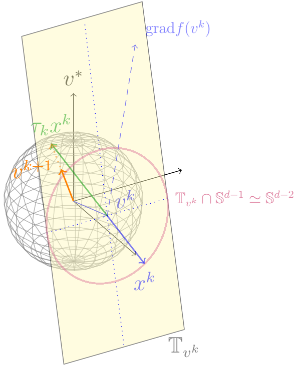

Optimal Stepsize τ_k – Solving a Quadratic Subproblem, sub-generalized Rayleigh Problem

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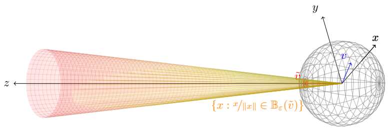

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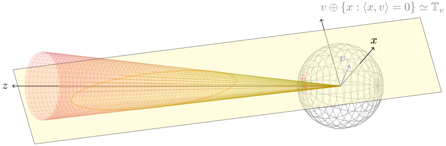

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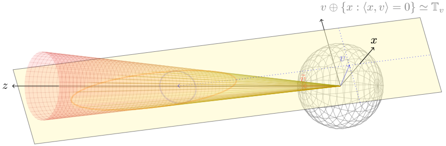

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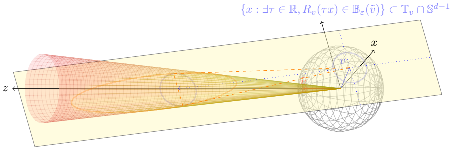

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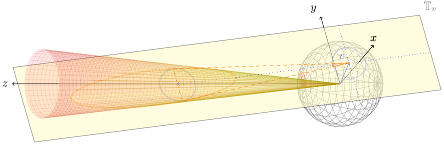

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Let $v^k \in \mathbb{S}^{d-1}$ *and* $x^k = P_{v^k}\tilde{x}/\|P_{v^k}\tilde{x}\| \in \mathbb{T}_{v^k} \cap \mathbb{S}^{d-1}$, $\tilde{x} \sim \mathcal{N}(0, I_d)$. *Then* $\quad v^k \in E_\sigma \quad \Leftrightarrow \quad b_k = 0$ *a.s.*

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

i) *If* $\dim(E_{\sigma_1}) \geq \max\{m,d\} - 1$, *then* $r(A,0,v^k)$ *converges after finitely many iterations, i.e.* $k \in \{0,1\}$.

ii) *If* $\dim(E_{\sigma_1}) < \max\{m,d\} - 1$, v^k *is not a singular vector,* $r(A,0,v^k)$ *converges, strictly increasing, and* $b_k \to 0$.

iii) *It holds* $\operatorname{dist}(E_{\sigma_1}, v^k) \to 0$, $\quad r(A,0,v^k) \nearrow \sigma_1 = \|A\|$, $\quad k \to \infty$, *a.s.* *and* $\quad \min_{k \leq n} \|\operatorname{grad} r(A,0,v^k)^2\|^2 \in \mathcal{O}(1/n)$.

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Connection to Zeroth-Order Methods & Acceleration and Restrictions & Extensions

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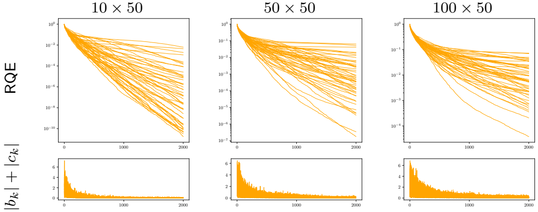

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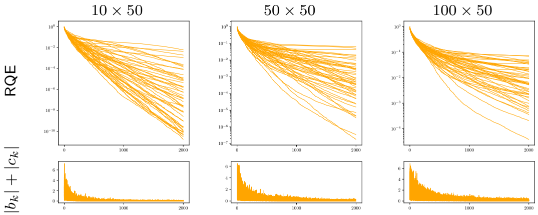

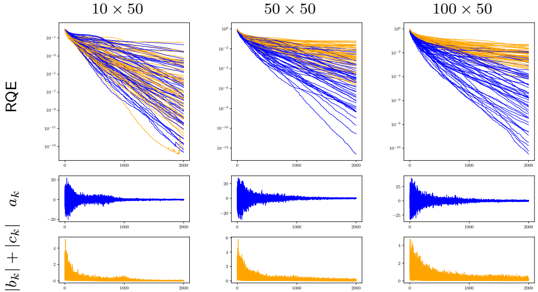

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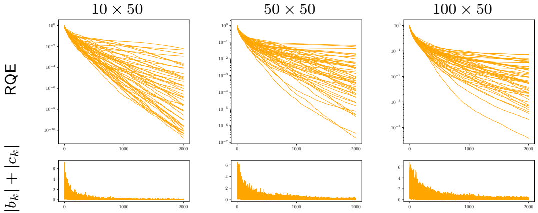

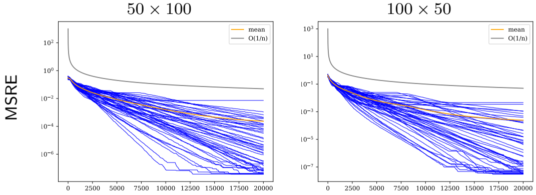

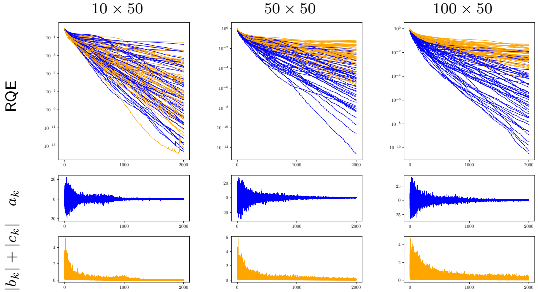

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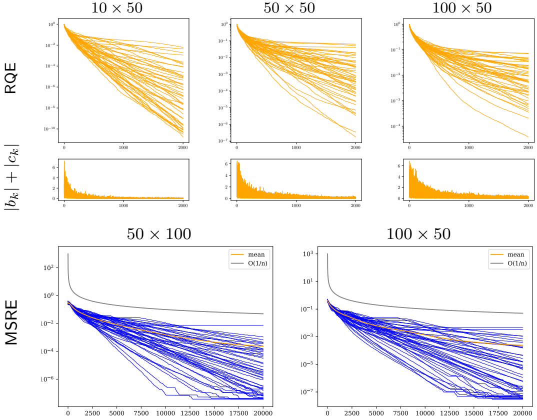

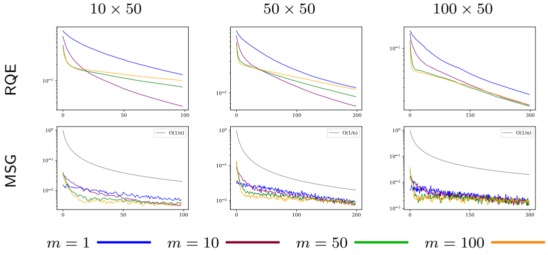

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Thanks for your attention!

Computing adjoint mismatch of linear maps,
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Included Publications

[1] 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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References III

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  $\min_{x\in\mathbb{X}} \|\mathcal{A}x - y\|_{\mathbb{X}}$ where $\mathcal{A} : \mathbb{X} \to \mathbb{Y}$
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- discretization $A \in \mathbb{R}^{m\times d}$

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

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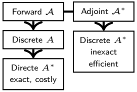

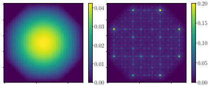

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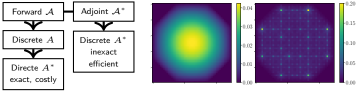

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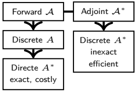

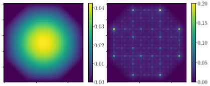

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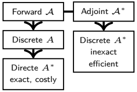

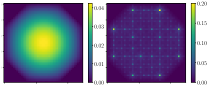

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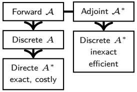

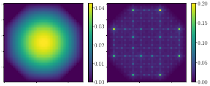

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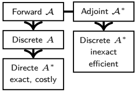

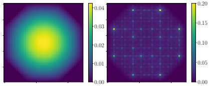

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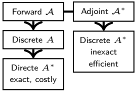

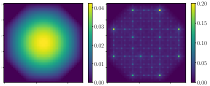

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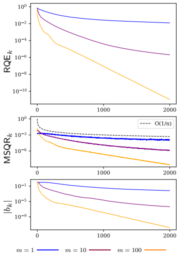

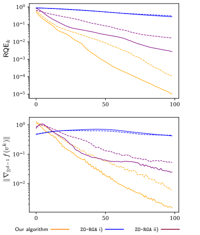

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- **Inverse problems:** $\mathcal{A}x = y$
- might **not solvable**, instead
  $\min_{x\in\mathbb{X}} \|\mathcal{A}x - y\|_{\mathbb{X}}$ where $\mathcal{A}:\mathbb{X}\to\mathbb{Y}$
- **Normal equation:** $\mathcal{A}^*\mathcal{A}x = \mathcal{A}^*y$

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

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

→ exact adjoint A^* may be **expensive** or **unavailable**

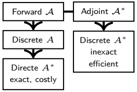
- Replacing A^* by a discretized adjoint V^* → **adjoint mismatch**
- **Affects** convergence $\|V\|, \|A - V\|$

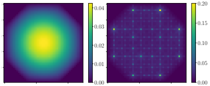
$$\min_{x\in\mathbb{X}} f(\mathcal{A}x) + g(x) = \min_{x\in\mathbb{X}}\max_{y\in\mathbb{Y}} g(x) + \langle \mathcal{A}x, y\rangle - f^*(y)$$

- spectral properties of $V^*A + \kappa I$

$$\min_{x\in\mathbb{X}} \|y - \mathcal{A}x\|_{\mathbb{X}}^2 + g(x) + \tfrac{\kappa}{2}\|x\|_{\mathbb{X}}^2$$

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

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

Riemannian Formulation

- Work on the ellipsoid

$$\mathbb{S}^{d-1} = \{v \in \mathbb{R}^d \mid \langle v, Bv\rangle = 1\} = h^{-1}(\{0\})$$

- 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 $\mathcal{R}(A,B) = \max_{v\in\mathbb{S}^{d-1}} \langle v, A^{\mathsf{H}}v\rangle$

Convergence, Rates

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

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

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