"Self-concordant Schrödinger operators"

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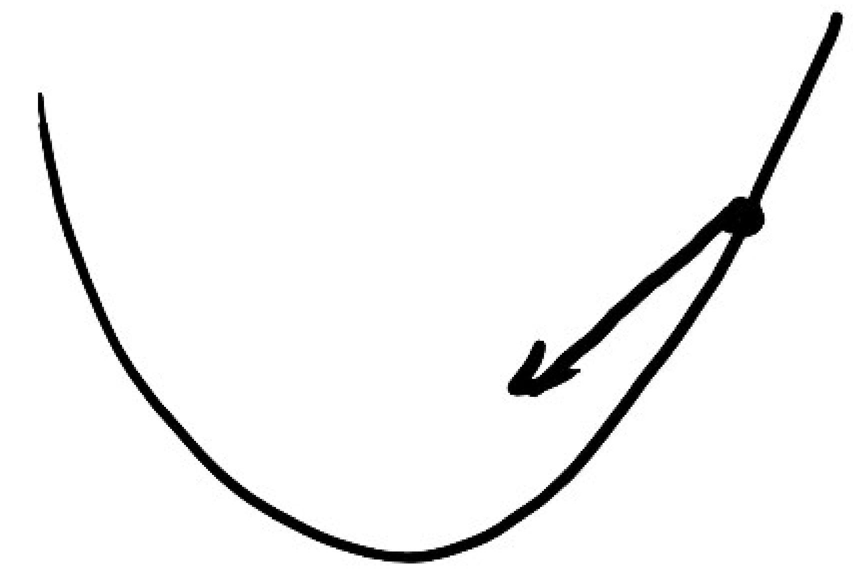
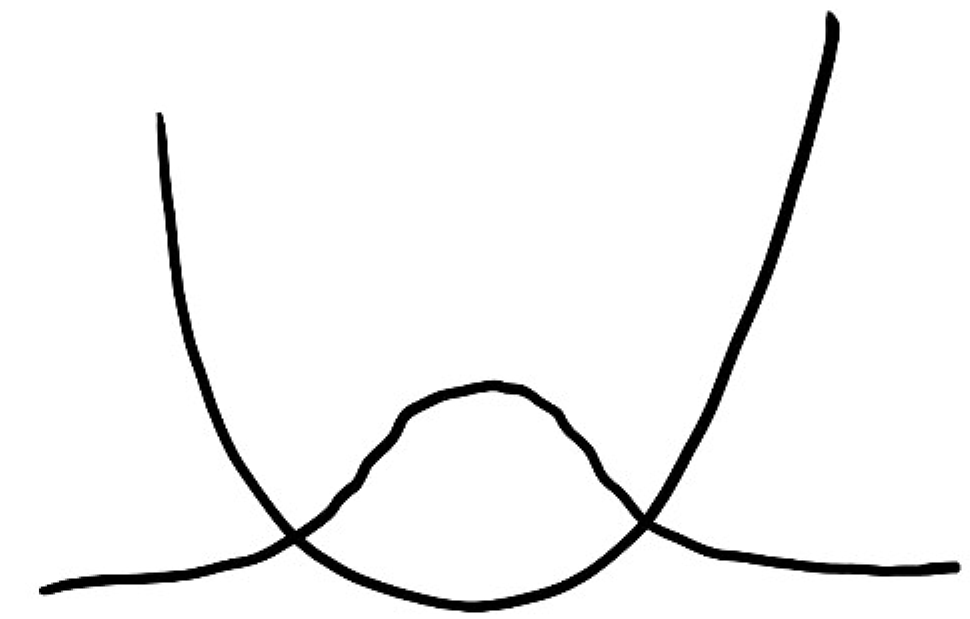
October '25, TU Münich

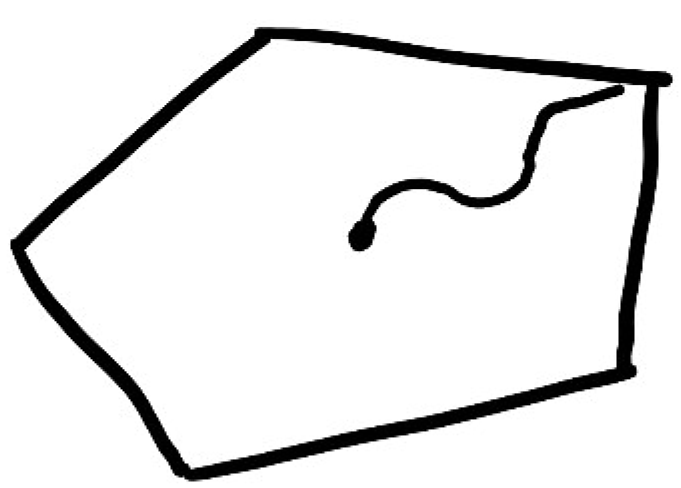
OUTLINE



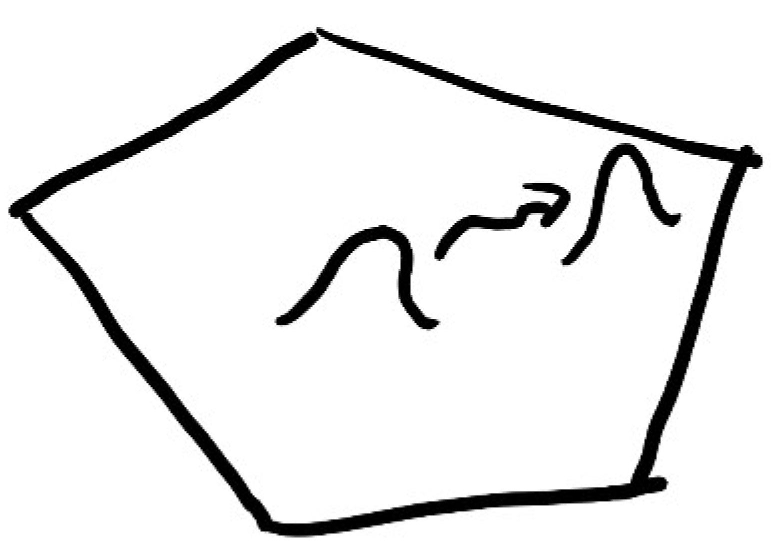
- (2nd order) optimization



- (2nd order) quantum optimization



- interior point methods



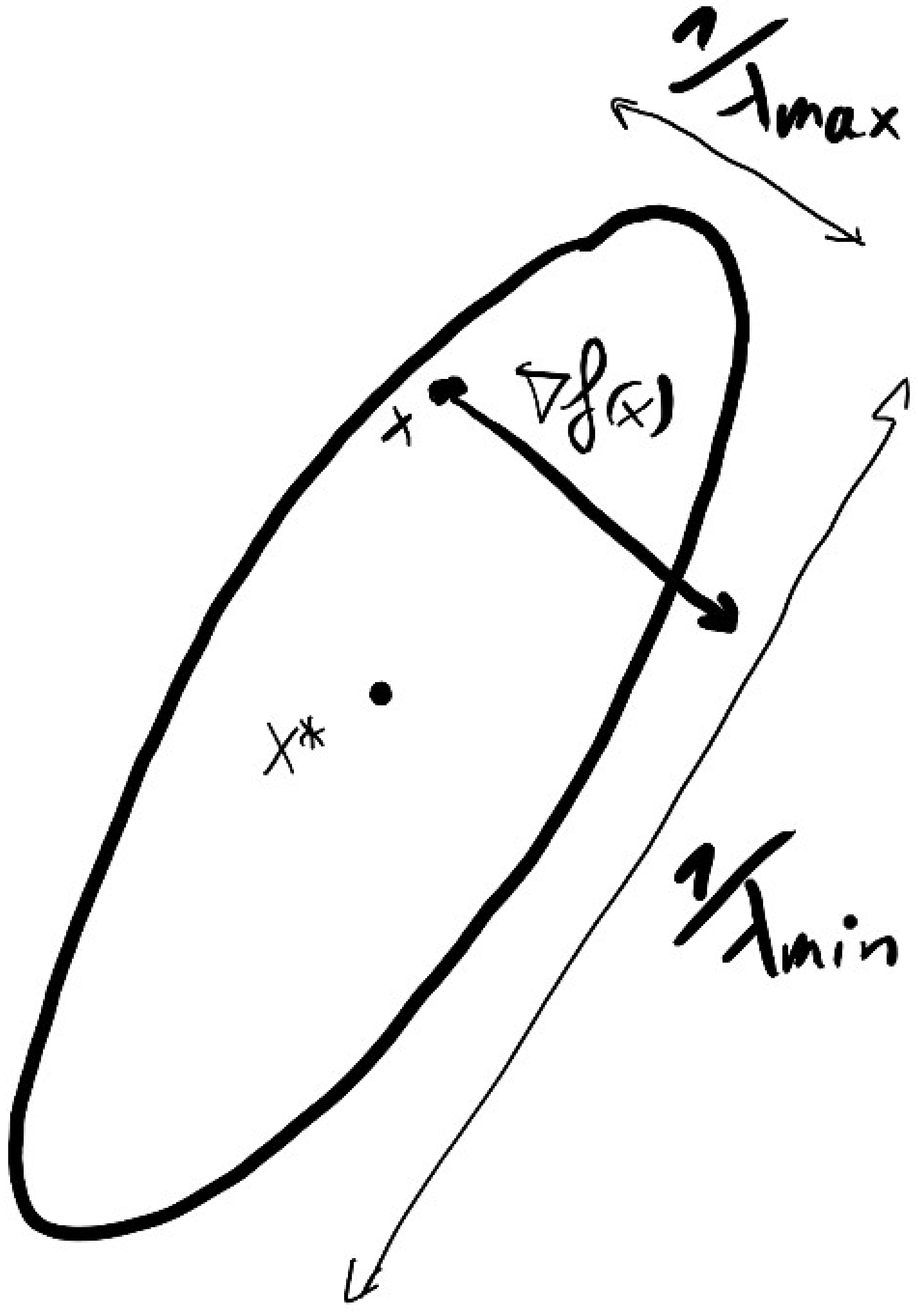
- quantum interior point method

(1st order) optimization

convex, smooth $f : \mathbb{R}^n \to \mathbb{R}$

"1st order" information

$\rightsquigarrow$ gradient descent: $\boxed{x' = x - \eta \nabla f(x)}$



basecase:

quadratic $f(x) = \frac{1}{2} x^T A x$, $A > 0$

! # steps $\sim \frac{\lambda_{max}(A)}{\lambda_{min}(A)} = \kappa(A)$

2^{nd} order optimization:

Hessian $H(x) = \Delta f(x) > 0$

smooth, (strongly) convex $f: \mathbb{R}^n \to \mathbb{R}$

↳ Newton step:

$$\boxed{x' = x - \eta\, H(x)^{-1} \nabla f(x)}$$

"2nd order" information

e.g., quadratic $f(x) = \frac{1}{2} x^T A x$:

$$x' = x - \eta A^{-1}(Ax) = x - \eta x \quad \rightsquigarrow \# \text{steps} \sim 1$$

2nd order optimization:

$$\boxed{x' = x - \eta H(x)^{-1} \nabla f(x)}$$

? general convex f

— f is SELF-CONCORDANT if $H(x)$ is "stable":

$$\|\delta\|_x \le \varepsilon \implies H(x+\delta) \approx_\varepsilon H(x)$$

$$\left(= \sqrt{\langle \delta, H(x)\delta \rangle} \right)$$

— [Nesterov-Nemirovski '94] : f self-concordant and x suff. close

f self-concordant,
x_0 "sufficiently close" to x^* $\Bigg\} \Rightarrow f(x_k) - f(x^*) \le 1/2^{2^k}$ — ! independent of cond. number (and dimension)

"(1st order) Quantum optimization"

smooth, convex

Schrödinger operator $\boxed{\mathcal{H} = -\frac{1}{2}\Delta + f}$ on $\mathrm{dom}(\mathcal{H}) \supseteq C_c^\infty(\mathbb{R}^n)$

— if $f \geq 0$ and $f(x) \to \infty$ as $x \to \infty$:

ground state energy

$\mathcal{H}$ has discrete, nonnegative spectrum $0 \leq \underbrace{\lambda_0 \leq \lambda_1}_{\lambda_1 - \lambda_0 \,=\, \text{spectral gap} \; \delta(\mathcal{H})} \leq \lambda_2 \leq \dots$

— <u>key example</u>: $\mathcal{H}_0 = -\frac{1}{2}\Delta + \frac{1}{2} x^T A x$

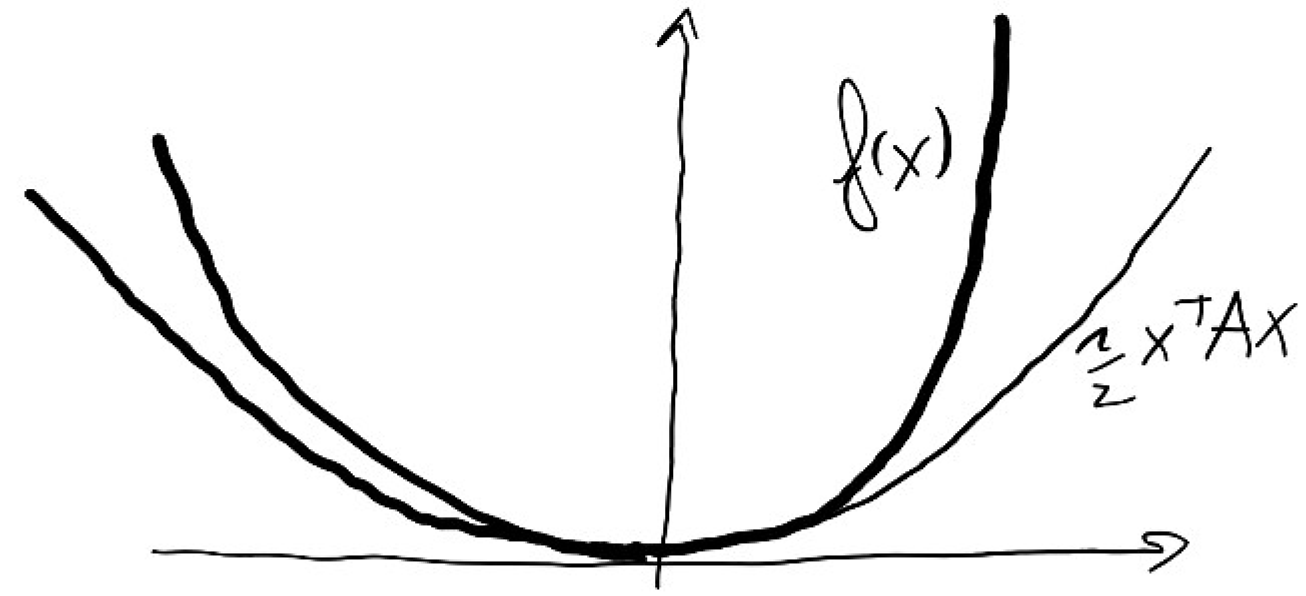
= quantum harmonic oscillator

g.s. energy $\lambda_0(\mathcal{H}_0) = \frac{1}{2}\mathrm{Tr}[\sqrt{A}]$

$\lambda_1(\mathcal{H}_0) = \frac{1}{2}\mathrm{Tr}[\sqrt{A}] + \lambda_{min}[\sqrt{A}]$

$$\left.\begin{aligned} \lambda_0(\mathcal{H}_0) &= \tfrac{1}{2}\mathrm{Tr}[\sqrt{A}] \\ \lambda_1(\mathcal{H}_0) &= \tfrac{1}{2}\mathrm{Tr}[\sqrt{A}] + \lambda_{min}[\sqrt{A}] \end{aligned}\right\} \quad \frac{\delta(\mathcal{H}_0)}{\lambda_0(\mathcal{H}_0)} \geq \frac{1}{n\sqrt{\kappa(A)}}$$

"(1^{st} order) Quantum optimization"



? general convex f

(assume $x^* = 0$, $\nabla f(0) = 0$, $\nabla^2 f(0) = A$)

This work:

NON-ASYMPTOTIC **SEMICLASSICAL ANALYSIS**

$\gamma >> 1$

$$\mathcal{H}^\gamma = -\frac{1}{2}\Delta + \gamma^2 f$$

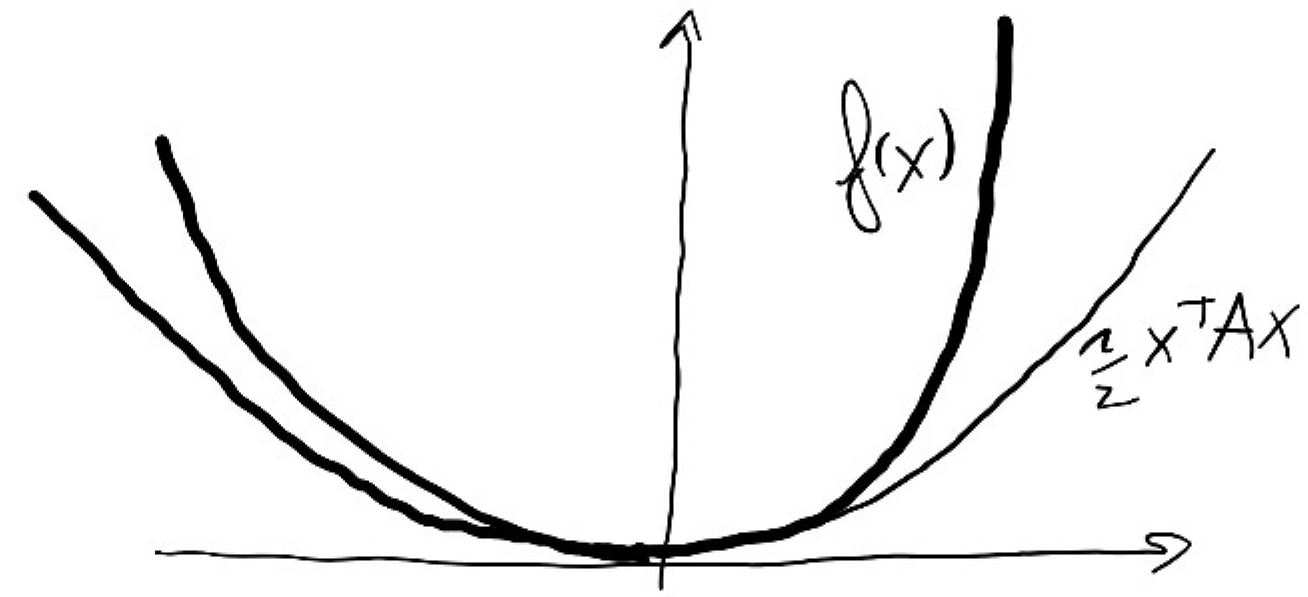
$$\approx -\frac{1}{2}\Delta + \gamma^2 \frac{1}{2} x^T A x = \mathcal{H}_0^\gamma$$

for low energies:

$$\lambda_0(\mathcal{H}^\gamma) \approx \lambda_0(\mathcal{H}_0^\gamma), \quad \lambda_1(\mathcal{H}^\gamma) \approx \lambda_1(\mathcal{H}_0^\gamma)$$

"(1st order) Quantum optimization"

? general convex f



(assume $x^* = 0$, $\nabla f(0) = 0$, $\nabla^2 f(0) = A$)

This work:

NON-ASYMPTOTIC SEMICLASSICAL ANALYSIS

"uniform" over family of fcts.

$$\boxed{\text{Thm.: If } f \text{ self-concordant and } \gamma \geq \mathrm{poly}(n, \|A\|, \|A^{-1}\|), \text{ then } \lambda_0(\mathcal{H}) \approx \gamma \tfrac{1}{2}\mathrm{Tr}[\sqrt{A}] \text{ and } \delta(\mathcal{H}) \approx \gamma \sqrt{\|A^{-1}\|}.}$$

"2nd order quantum optimization"

recall: gradient descent: ∇ $\rightsquigarrow$ Newton step: $H^{-1}\nabla$

! $H^{-1}\nabla$ is "Riemannian gradient"

wrt **Hessian manifold** $\underbrace{M_g = (\mathbb{R}^n, g = H)}$

e.g., $d\,\mathrm{vol}_g(x) = \sqrt{\det H(x)}\, dx$

$\rightsquigarrow$ we define **"2nd order Schrödinger operator"**

$$\boxed{\mathcal{H} = -\tfrac{1}{2} L + f}$$

= Schrödinger operator on Hessian manifold

L = Laplace-Beltrami operator on M_g

"2nd order quantum optimization"

↳ Schrödinger operator $\boxed{\mathcal{H} = -\frac{1}{2}L + f}$ on Hessian manifold M_g

* **key example**: quadratic $f(x) = \frac{1}{2}x^TAx$ ⇝ "flat" manifold $M_g = (\mathbb{R}^n, g=A)$

$$\mathcal{H}_0 = -\frac{1}{2}L + f = -\frac{1}{2}\nabla^T A^{-1}\nabla + \frac{1}{2}x^TAx$$

$$= -\frac{1}{2}\Delta_y + \frac{1}{2}y^Ty \quad \text{for } y = \sqrt{A}x$$

$$\rightsquigarrow \lambda_0(\mathcal{H}_0) = \frac{1}{2}n, \quad \delta(\mathcal{H}_0) = 1$$

! ind. of cond. number

* **our work**:

Thm.: If f self-concordant and $\gamma \geq \mathrm{poly}(n)$,

then $\lambda_0(\mathcal{H}^\gamma) \approx \gamma\frac{1}{2}n$ and $\delta(\mathcal{H}^\gamma) \approx \gamma$.

$\mathcal{H}^\gamma = -\frac{1}{2}L + \gamma^2 f$ ↩

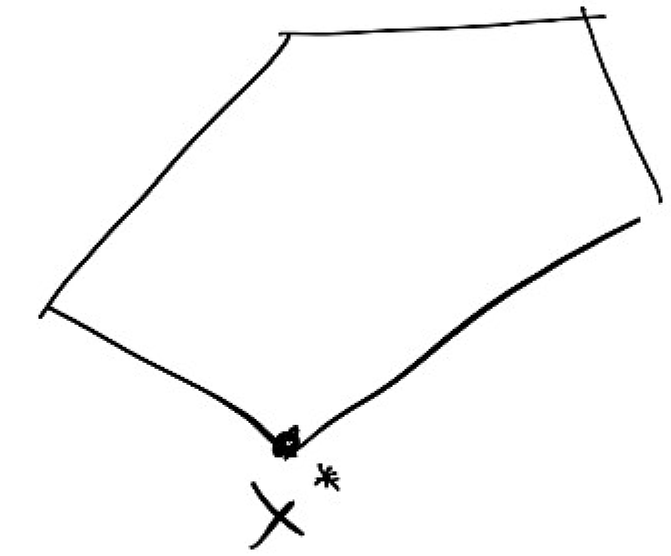
Interior point methods

constrained convex optimization:

↳ gradient descent fails!

$$\boxed{\min_{x \in D} f(x)}$$

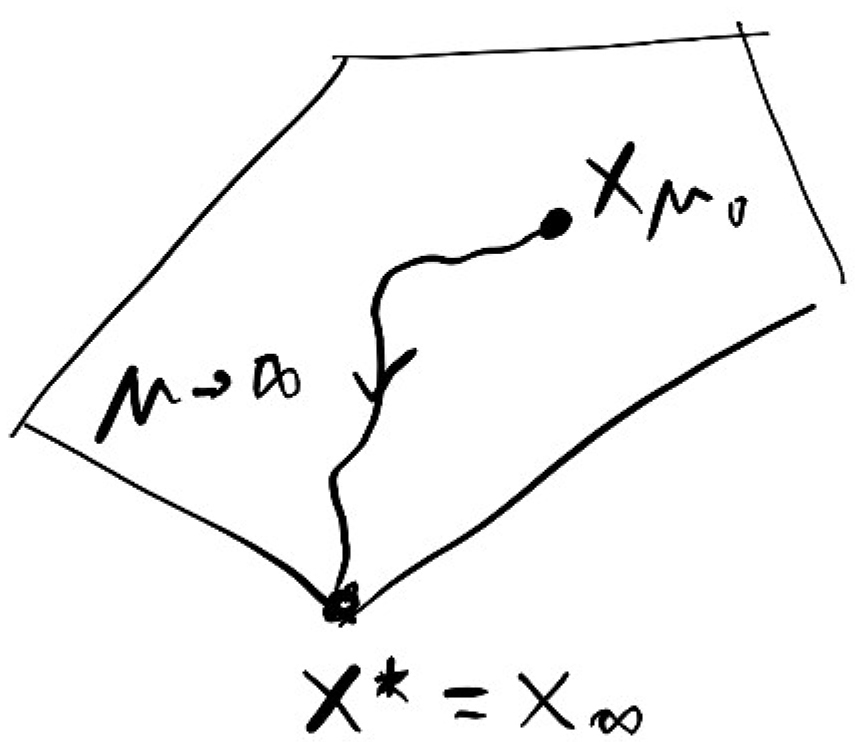
convex subset $D \subseteq \mathbb{R}^n$



→ interior point methods (IPMs):

1. define barrier function h s.t. $h(x) \to \infty$ as $x \to \partial D$
2. solve "unconstrained" problem $\min_x f_\mu(x) = \min_x \left(\mu f(x) + h(x)\right)$

for increasing μ:



$$\boxed{\begin{array}{l} \text{from } x_{\mu_0} = \operatorname{argmin} f_{\mu_0}(x), \\ \text{repeat} \begin{cases} \text{(a) } \mu' = (1+\nu)\mu \\ \text{(b) from } x_\mu, \text{ solve for } x_{\mu'} \end{cases} \end{array}}$$

= "path-following"

using Newton steps

Quantum interior point method

"self-concordant Schrödinger operator"

$$\boxed{\mathcal{H}_\mu := -\tfrac{1}{2}L + \gamma^2(\mu f + h)} \rightarrow \text{g.s. } |\psi_\mu\rangle, \text{ gap } \delta_\mu$$

Assuming (I) initial state $|\tilde{\psi}_{\mu_0}\rangle \approx |\psi_{\mu_0}\rangle$

(G) estimates of g.s. energies $\lambda_0(\mathcal{H}_\mu)$

(H) (controlled) Hamiltonian simulation $e^{i\mathcal{H}_\mu}$

Thm.: From $|\tilde{\psi}_{\mu_0}\rangle$, prepare $|\psi_\mu\rangle$ concentrated around minimizer x^* while evolving $\mathcal{H}_\mu$ for time $\mathrm{poly}(n, \log(1/\varepsilon))$.

! compared to $\mathrm{poly}(n, \max \chi(A_\mu), \log(1/\varepsilon))$ with 1st order Schrödinger operator

Key ideas

$$R_{\psi_{\mu_j}} = 2|\psi_{\mu_j}\rangle\langle\psi_{\mu_j}| - \mathbb{1}$$

- **quantum annealing**: $|\psi_{\mu_0}\rangle \rightsquigarrow |\psi_{\mu_1}\rangle \rightsquigarrow \dots \rightsquigarrow |\psi_{\mu_T}\rangle$

  $|\langle\psi_{\mu_j}|\psi_{\mu_{j+1}}\rangle| \in \Omega(1)$

- **semiclassical analysis**: triples $(\mathcal{H}_\mu, |\psi_\mu\rangle, \delta_\mu)$

  $\geq 1/\mathrm{poly}(n)$

  $\approx$ Gaussian

- **reflection around unbounded operator**:

  ! QPE on $e^{i\mathcal{H}_\mu}$ fails because of "aliasing"

$\to$ new trick based on "Hubbard-Stratonovich transform":

$$(\mathbb{1}\otimes\langle g|)\, e^{it\mathcal{H}_\mu\otimes\hat{x}}|\varphi\rangle|g\rangle = e^{-\frac{t^2}{2}\mathcal{H}_\mu^2}|\varphi\rangle \approx |\psi_\mu\rangle\langle\psi_\mu|\varphi\rangle$$

Gaussian state

imaginary-time evolution

Summary:

semiclassical analysis of "second-order" Schrödinger operator,

&

"continuous-variable" quantum IPM

independent of cond. number

Open questions:

- sp. gap bounds using global properties
- discretization: Hamiltonian simulation in curved spaces?