Sampling with Mirrored Stein Operators

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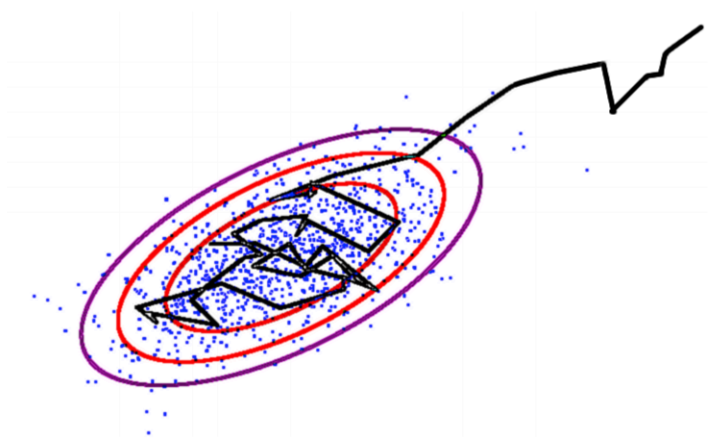
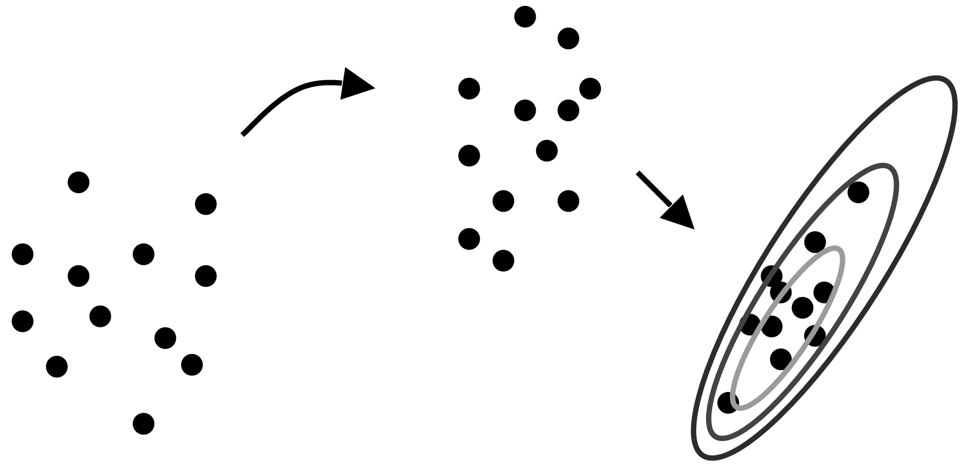
Joint work with Chang Liu, Lester Mackey

Sampling from an Unnormalized Distribution

Fig. from Murray (2009)



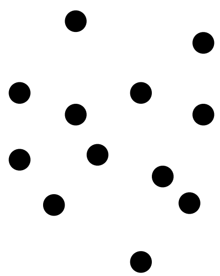


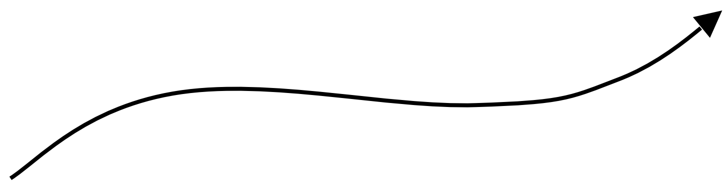
MCMC

Particle evolution methods
e.g., Stein Variational Gradient Descent

Stein Variational Gradient Descent (SVGD)

$$T(\theta) = \theta + \epsilon g(\theta)$$

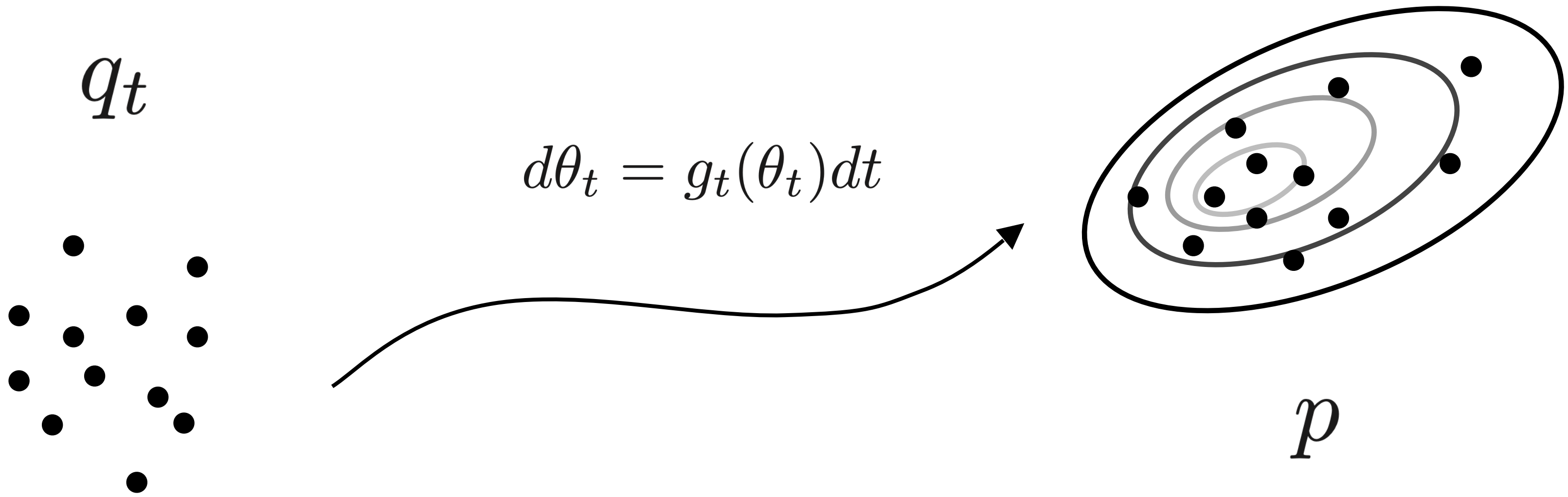




$$\epsilon \to 0$$

$$\theta^1, \theta^2, \ldots, \theta^n$$

Stein Variational Gradient Descent (SVGD)



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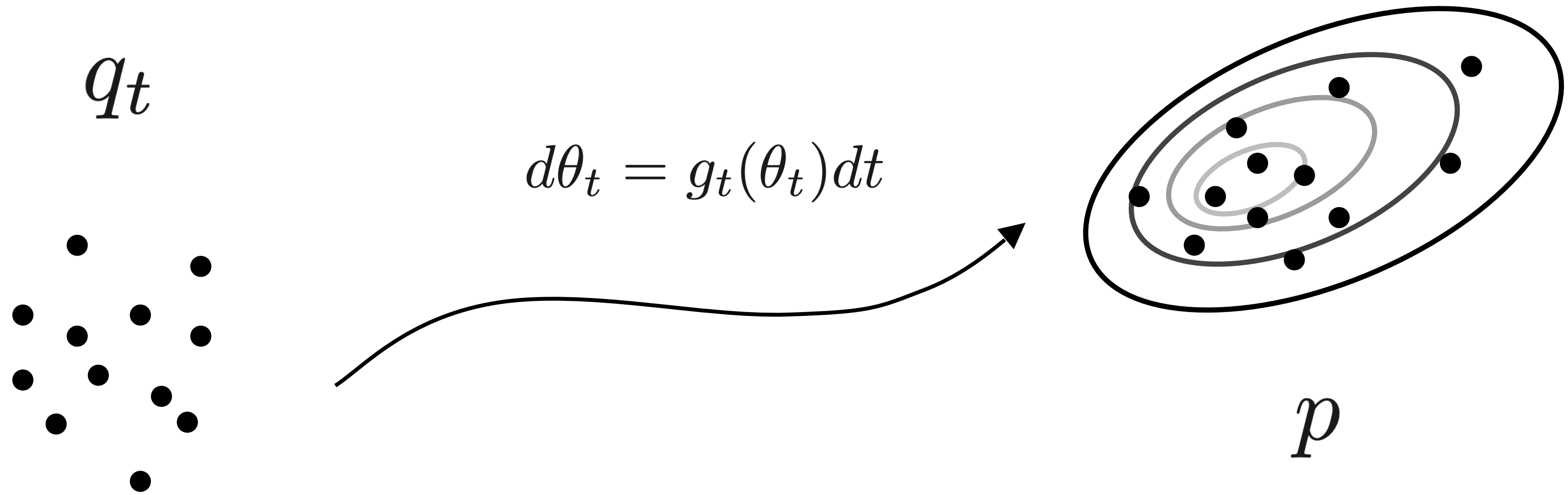

(Liu & Wang, 2016)

$$\frac{d}{dt}\mathrm{KL}(q_t \| p) = -\mathbb{E}_{q_t}[(\mathcal{S}_p g_t)(\theta)]$$

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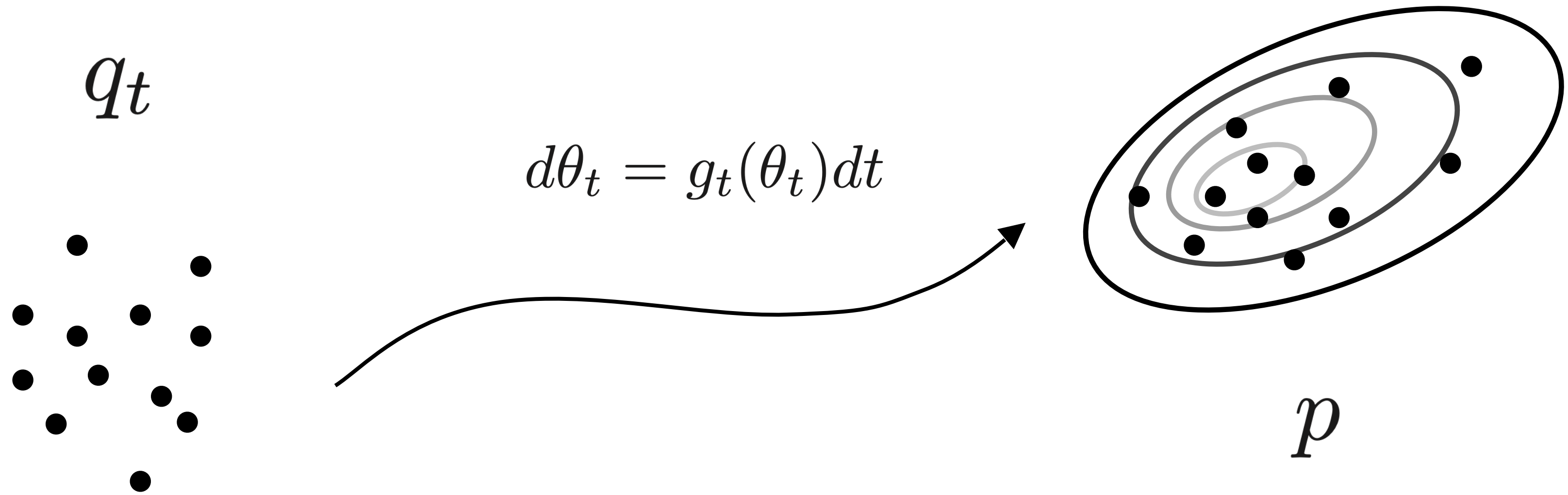

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Langevin Stein Operator: $(\mathcal{S}_p g)(\theta) = g(\theta)^\top \nabla \log p(\theta) + \nabla \cdot g(\theta)$

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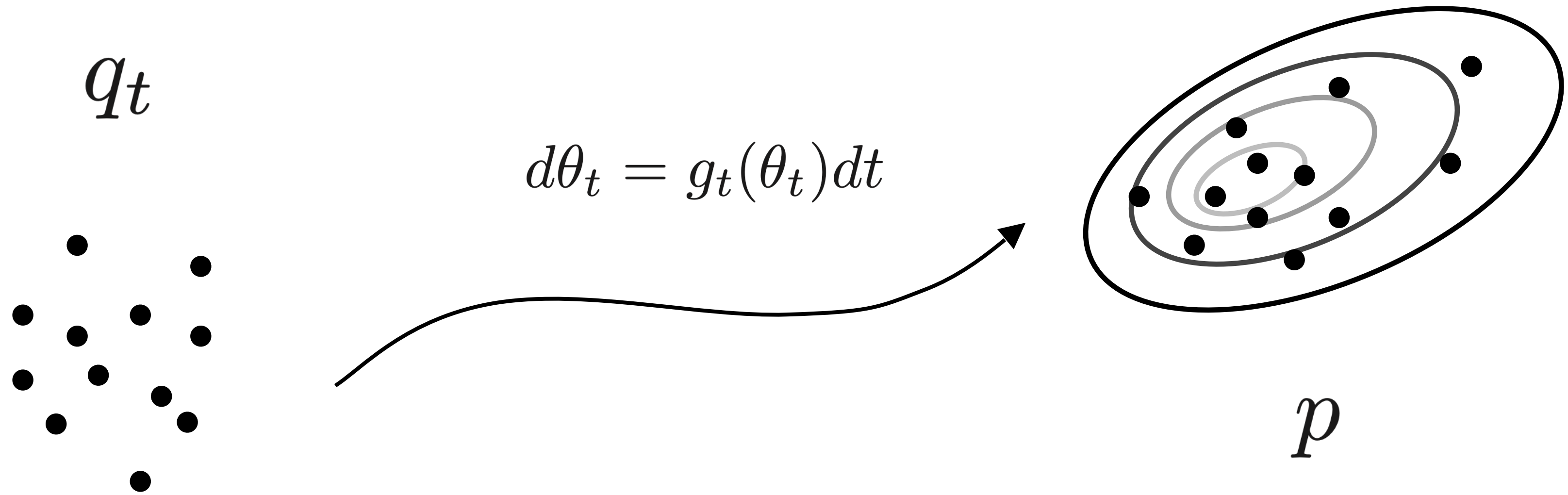

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Find the direction that **most quickly** decreases the KL divergence to p

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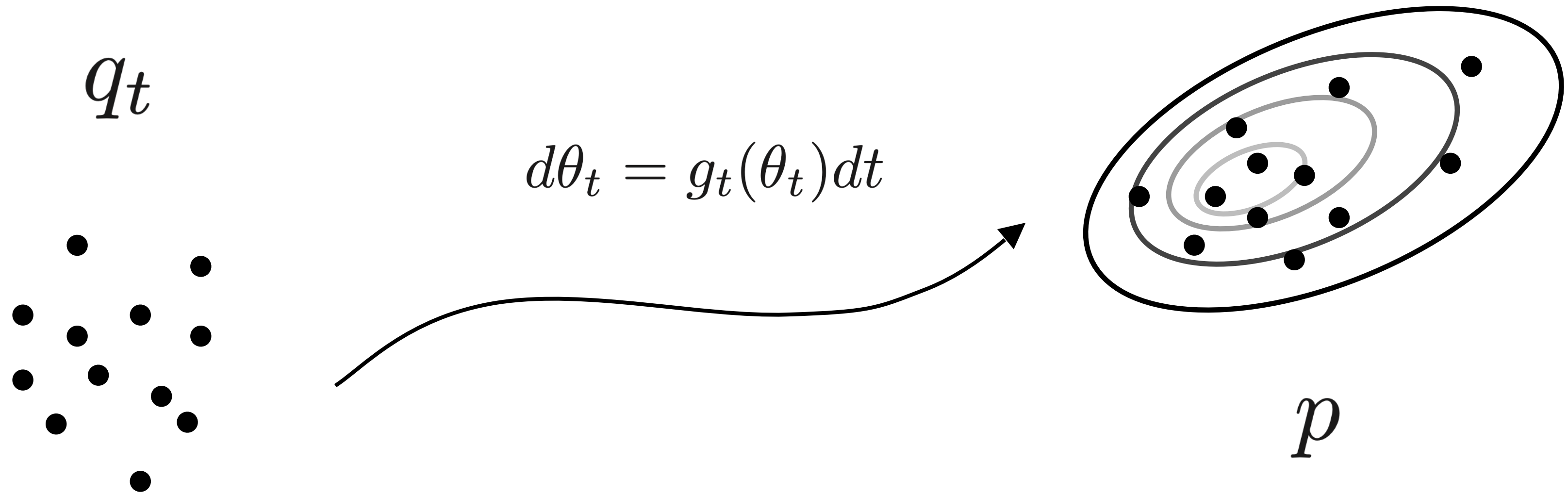

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$$g_t^* = \underset{g_t \in \mathcal{H}, \|g_t\|_\mathcal{H} \leq 1}{\arg\min} \frac{d}{dt} \mathrm{KL}(q_t \| p) \propto \mathbb{E}_{q_t}[\mathcal{S}_p K(\cdot, \theta)]$$

Optimal direction in the RKHS of kernel K.

Two Regimes of SVGD

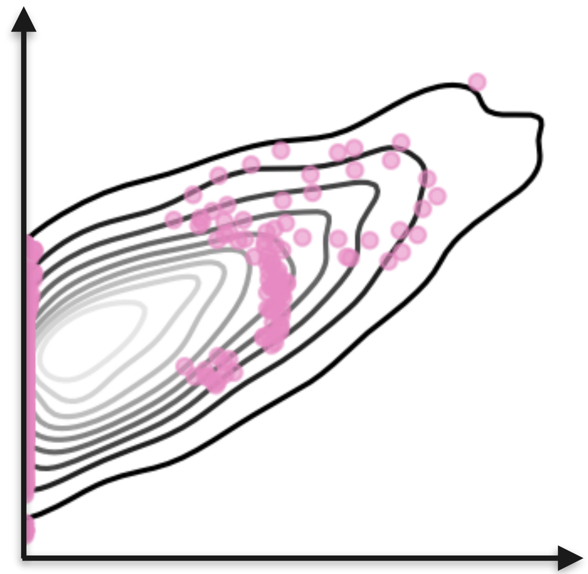
(Liu & Wang, 2016)

$$\theta_{t+1}^i \leftarrow \theta_t^i + \epsilon_t \frac{1}{n} \sum_{j=1}^{n} \Big(K(\theta_t^i, \theta_t^j) \nabla \log p(\theta_t^j) + \nabla_{\theta_t^j} \cdot K(\theta_t^j, \theta_t^i) \Big)$$

- $n = 1$: reduces to gradient descent on $-\log p(\theta)$ if $\nabla \cdot K(\theta, \theta) = 0$.
- $n \to \infty$: weak convergence to p under certain conditions.

(Gorham & Mackey, 2017; Liu 2017; Gorham et al., 2020)

They Break Down for Constrained Targets



SVGD + Projection: Samples end up collecting on the boundary.

Langevin Stein Operators

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$$\int_\Theta \nabla \cdot ((p(\theta)g(\theta))d\theta = 0 \Leftrightarrow \int_{\partial\Theta} p(\theta)g(\theta)^\top n(\theta)d\theta = 0$$

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For unconstrained domain, since p vanishes at infinity, this holds under very mild conditions, such as bounded Lipschitz g.

Therefore, $q_t = p$ is a stationary point of the SVGD dynamics.

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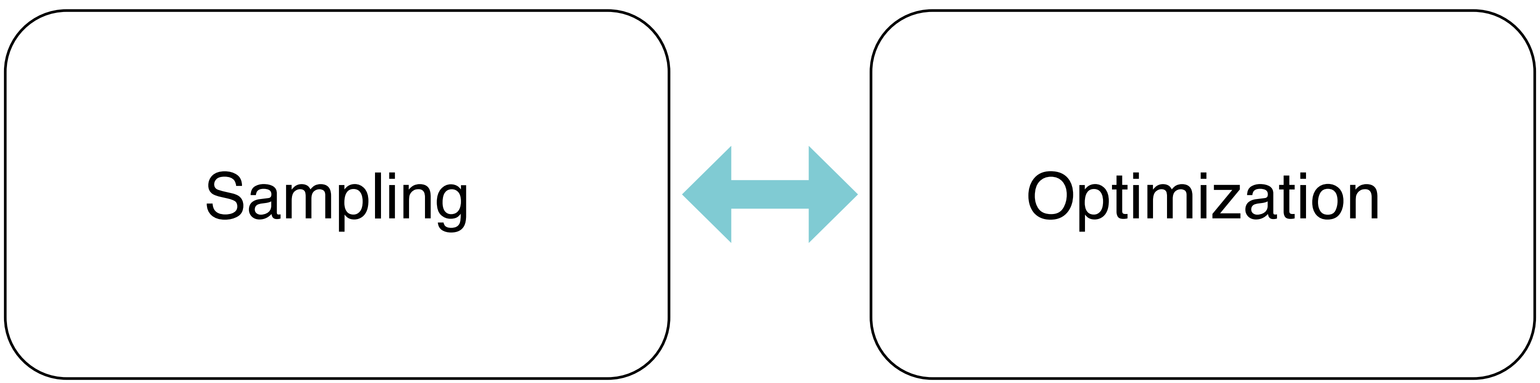
- Standard SVGD updates can push the particles outside of its support
    - Result: Future updates undefined.
- The boundary conditions may fail to hold for g in the RKHS
    - This happens when p is non-vanishing or explosive on the boundary
    - Result: SVGD need not converge to p since p is not a stationary point.

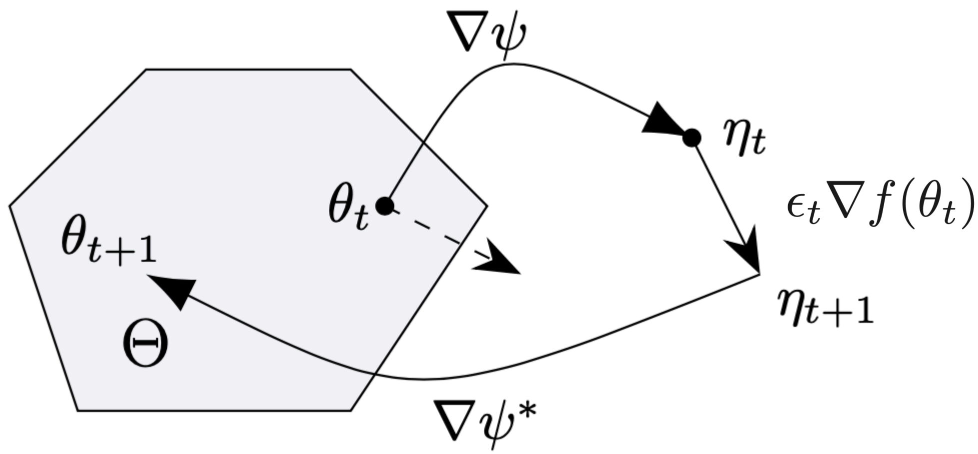
This Talk is About



Particle evolution samplers

Mirror descent

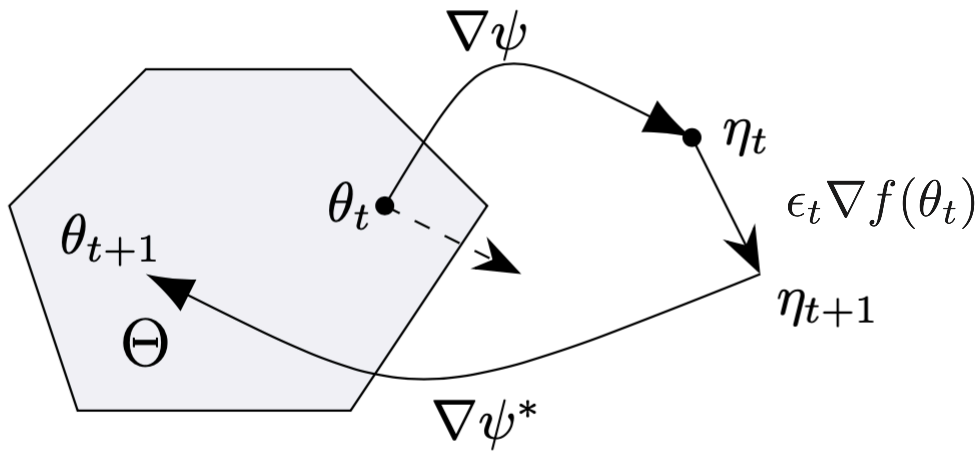
Mirror Descent



Strictly convex $\psi : \Theta \to \mathbb{R} \cup \{\infty\}$

$$(\nabla\psi)^{-1} = \nabla\psi^*$$

Mirror Descent



Strictly convex $\psi : \Theta \to \mathbb{R} \cup \{\infty\}$

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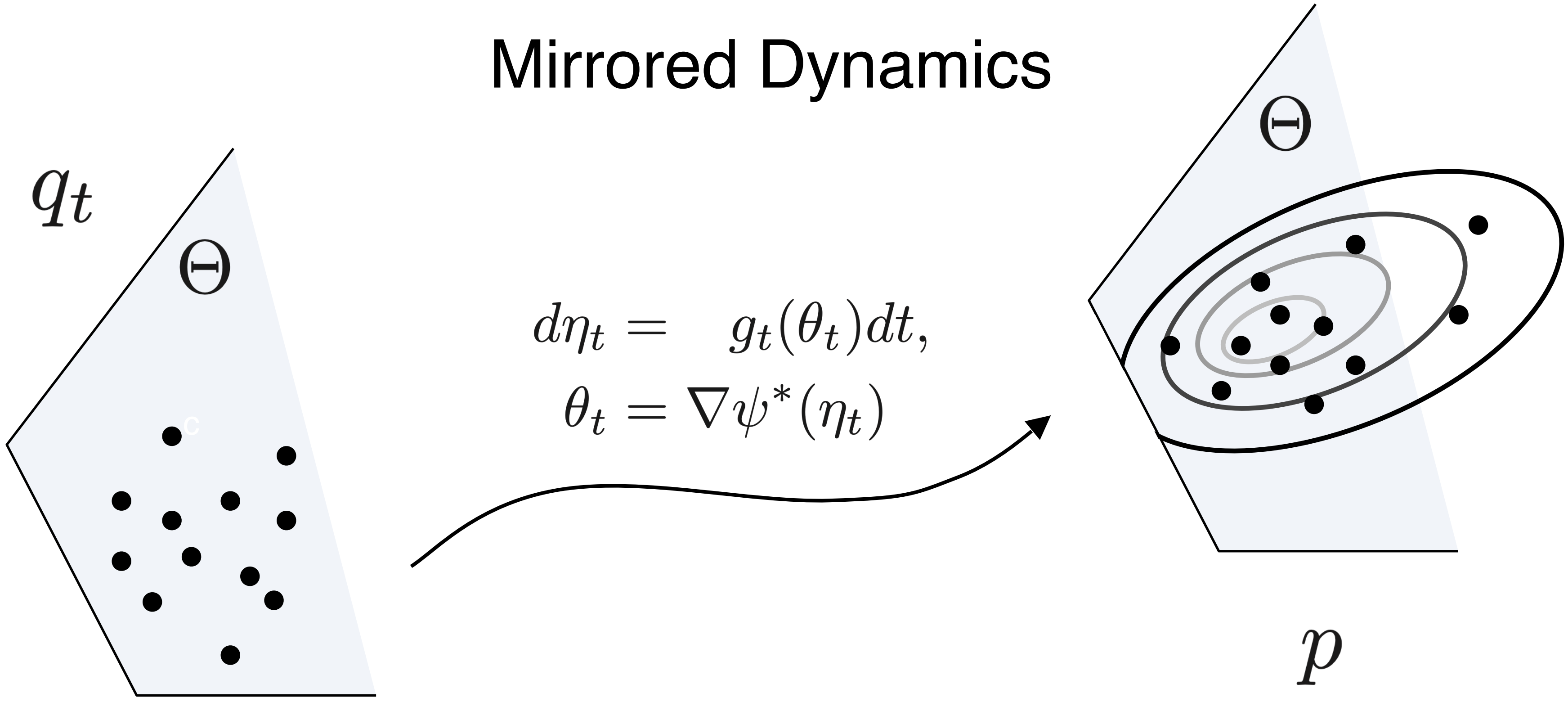
Continuous time limit: mirror flow

$$d\eta_t = -\nabla f(\theta_t)dt, \;\; \theta_t = \nabla\psi^*(\eta_t)$$

Equivalent Riemannian gradient flow: $d\theta_t = -\nabla^2\psi(\theta_t)^{-1}\nabla f(\theta_t)dt$

Mirrored Dynamics



$$d\eta_t = \quad g_t(\theta_t)dt,$$
$$\theta_t = \nabla\psi^*(\eta_t)$$

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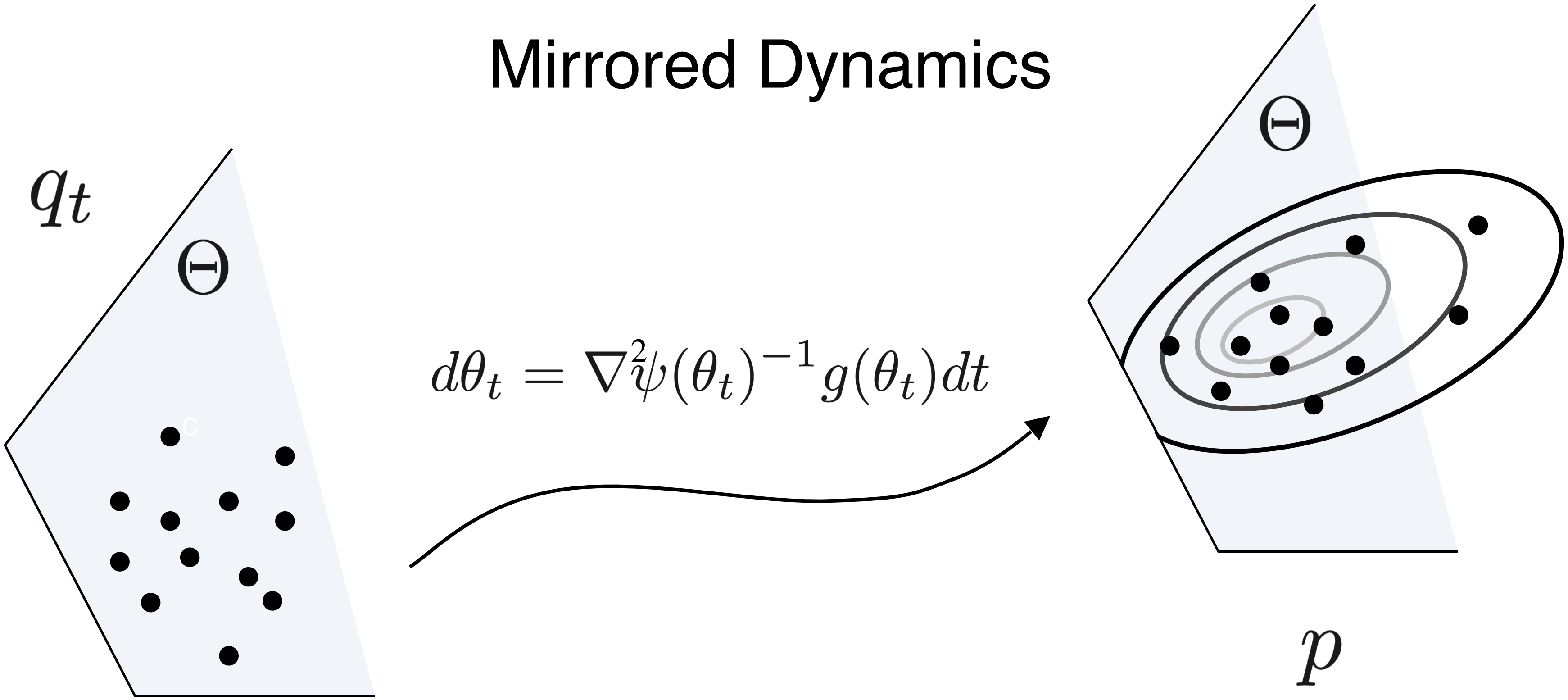

$$d\theta_t = \nabla^2\psi(\theta_t)^{-1} g(\theta_t)dt$$

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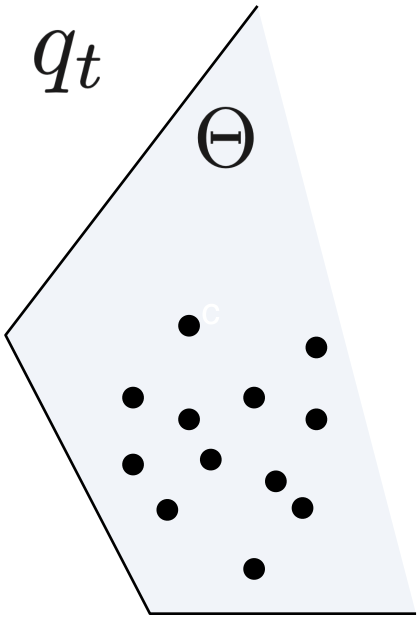

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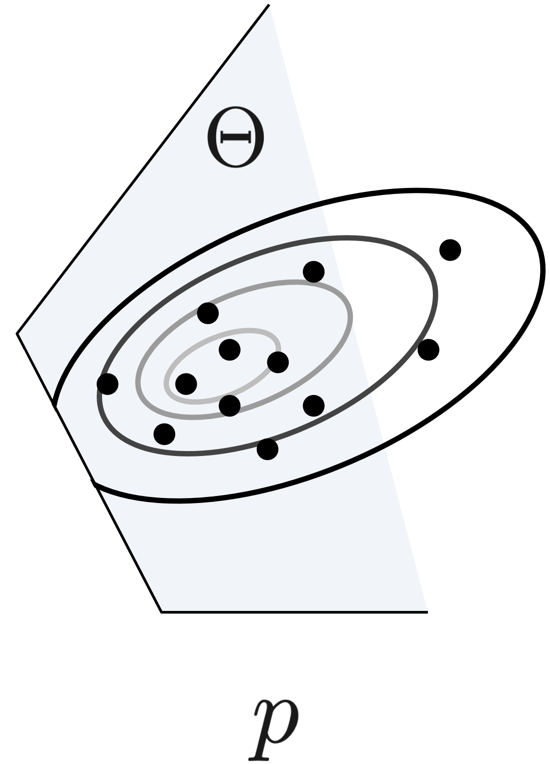

Mirrored Stein Operator

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A Stein Operator for Constrained Targets

Mirrored Stein Operator*

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Proposition 1 (informal) $\mathcal{M}_{p,\psi}$ generates mean-zero functions under p if

$$\int_{\partial\Theta} p(\theta) \|\nabla^2 \psi(\theta)^{-1} n(\theta)\|_2 d\theta = 0$$

and $g \in C^1$ is bounded Lipschitz.

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Intuitively, we expect $\nabla^2 \psi(\theta)^{-1}$ to **cancel the growth** of p at the boundary.

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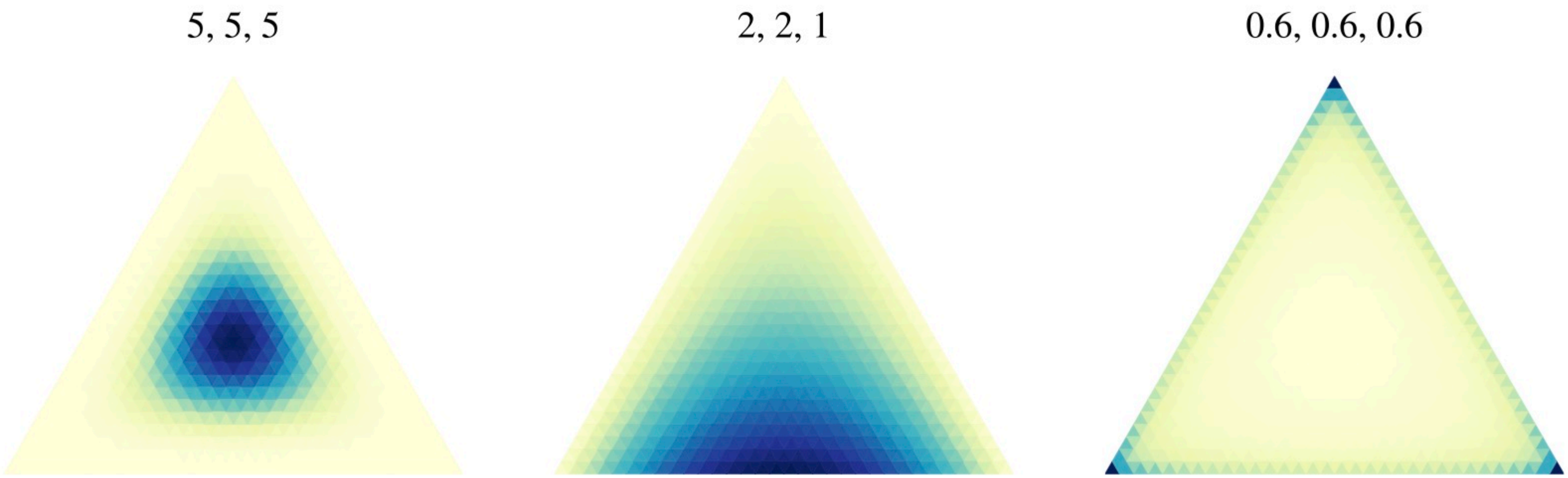
Example: The Dirichlet Distribution



$$p(\theta) \propto \prod_{j=1}^{d+1} \theta_j^{\alpha_j - 1} \qquad \begin{cases} \alpha_j < 1 : \theta_j \to 0, \theta_{-j} = \dfrac{1-\theta_j}{d} \Rightarrow p(\theta) \to \infty, \\ \alpha_j = 1 : \theta_j \to 0, \theta_{-j} = \dfrac{1-\theta_j}{d} \Rightarrow p(\theta) > 0. \end{cases}$$

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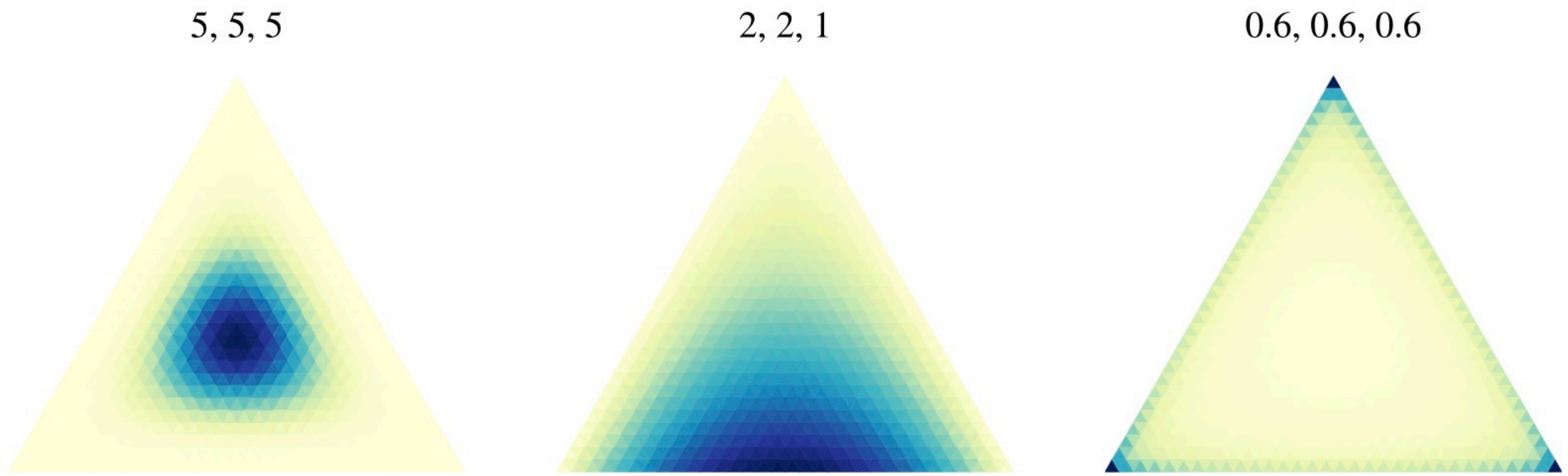

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Negative entropy $\psi(\theta) = \sum_{j=1}^{d+1} \theta_j \log \theta_j$ satisfies the boundary condition

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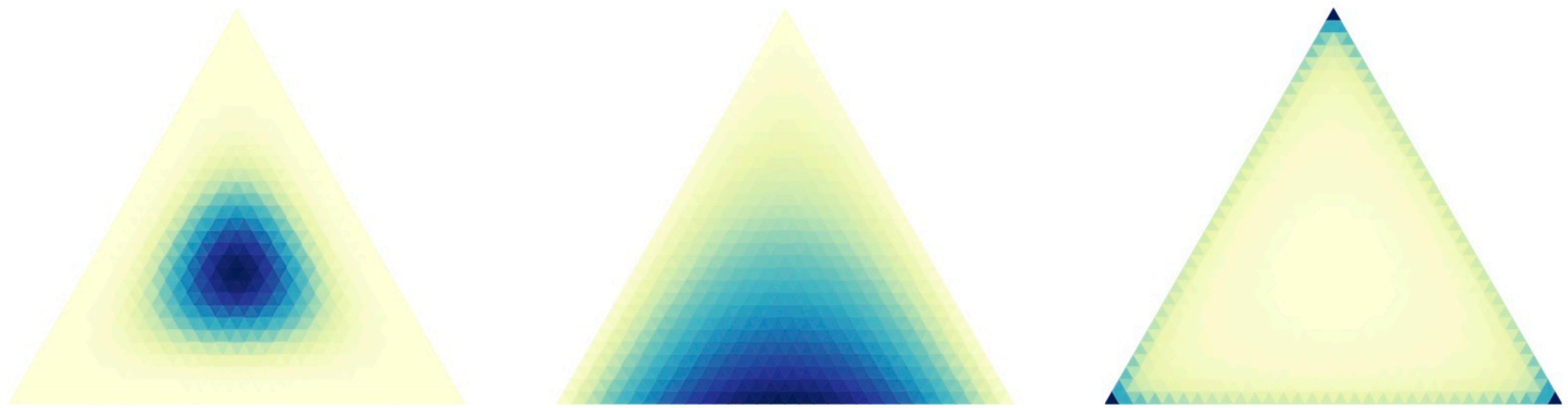

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$$\nabla^2 \psi(\theta)^{-1} = \mathrm{diag}(\theta) - \theta\theta^\top$$

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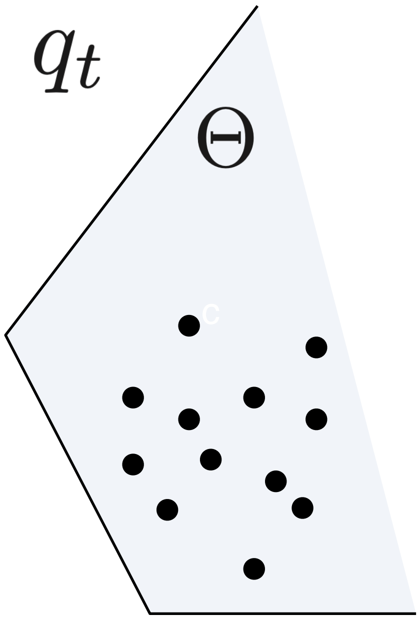

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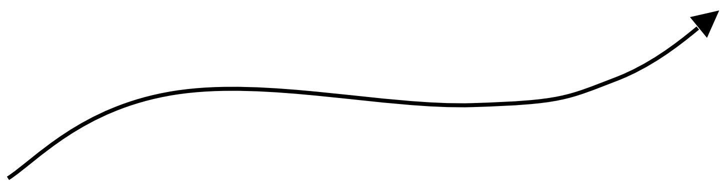

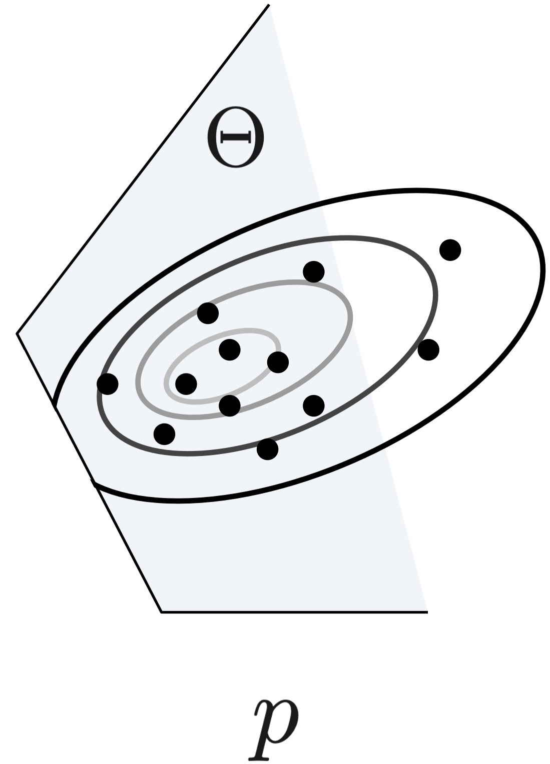

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Two Algorithms

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Choosing optimal g_t in

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Choosing optimal g_t in

- the RKHS of a fixed kernel

- **Mirrored SVGD**: SVGD in the η space.
- $n = 1$: GD on $-\log p_H(\eta)$.

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- the RKHS of an adaptive kernel that incorporates the geometry

- **Stein Variational Mirror Descent** (SVMD)
- $n = 1$: Mirror Descent on $-\log p(\theta)$.

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Mirrored SVGD (MSVGD)

Theorem 4 If $K(\theta, \theta') = k(\theta, \theta')I$, then the optimal mirrored updates can alternatively be expressed as

$$g^*_{q_t, kI}(\theta_t) = \mathbb{E}_{q_{t,H}}[k_\psi(\eta, \eta_t)\nabla \log p_H(\eta) + \nabla_\eta k_\psi(\eta, \eta_t)].$$

where $k_\psi(\eta, \eta') = k(\nabla\psi^*(\eta), \nabla\psi^*(\eta'))$

transformed density of p in dual space

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transformed density of p in dual space

- MSVGD is SVGD in η space with the **transformed kernel** k_ψ.
- When only a single particle is used $(n = 1)$, Mirrored SVGD reduces to gradient ascent on the log transformed density $\log p_H(\eta)$.

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Single Particle MSVGD is Not Mirror Descent

Still want an algorithm that reduces to mirror descent when $n = 1$?

- θ space is the space we are primarily interested in.
- Mode in θ space need not match mode in η space
- Using $\log p(\theta)$ to guide the evolution could work better if $p(\theta)$ is better behaved than $p_H(\eta)$.

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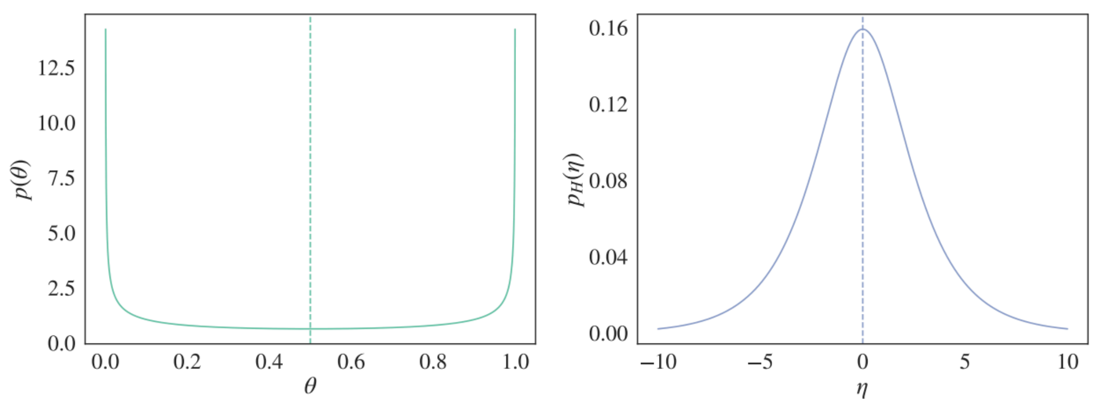


$\theta \sim \mathrm{Beta}(0.5, 0.5)$

Stein Variational Mirror Descent (SVMD)

Key idea: Construct an **adaptive kernel** that

① incorporates the metric induced by ψ ② evolves with q_t

Definition (Kernels for SVMD)

Given a reference kernel k, we write it in Mercer's representation:

$$k(\theta, \theta') = \sum_{i \geq 1} \lambda_i u_i(\theta) u_i(\theta'),$$

where u_i is an eigenfunction satisfying:

$$\mathbb{E}_{q_t(\theta')}[k(\theta, \theta') u_i(\theta')] = \lambda_i u_i(\theta).$$

Kernels for SVMD:

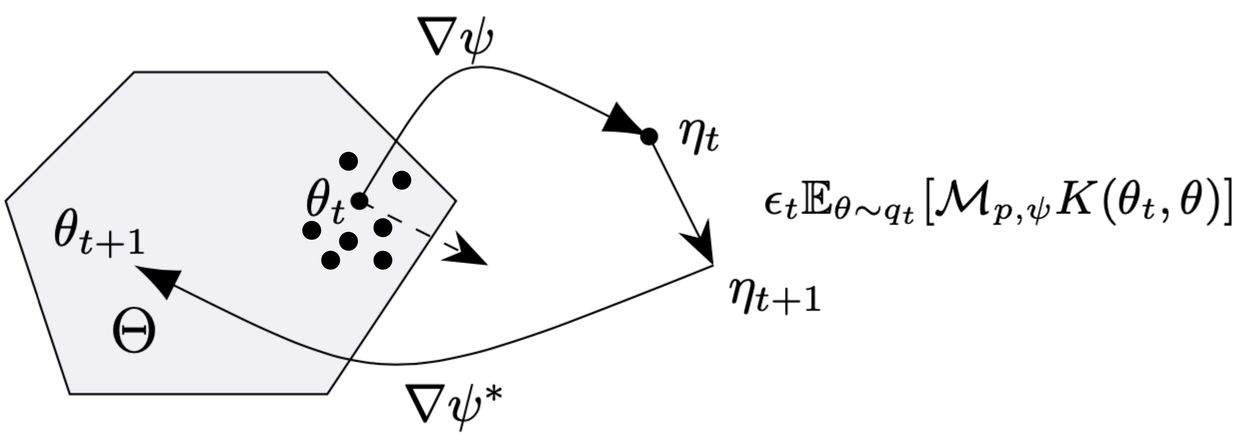
$$k^{1/2}(\theta, \theta') \triangleq \sum_{i \geq 1} \lambda_i^{1/2} u_i(\theta) u_i(\theta')$$

$$K_{\psi,t}(\theta, \theta') \triangleq \mathbb{E}_{\theta_t \sim q_t}[k^{1/2}(\theta, \theta_t) \nabla^2 \psi(\theta_t) k^{1/2}(\theta_t, \theta')]$$

A Multi-Particle Generalization of Mirror Descent

If $n = 1$, then one-step of SVMD becomes

$$\eta_{t+1} = \eta_t + \epsilon_t \left(k(\theta_t, \theta_t) \nabla \log p(\theta_t) + \nabla k(\theta_t, \theta_t) \right),$$
$$\theta_{t+1} = \nabla \psi^*(\eta_{t+1}).$$



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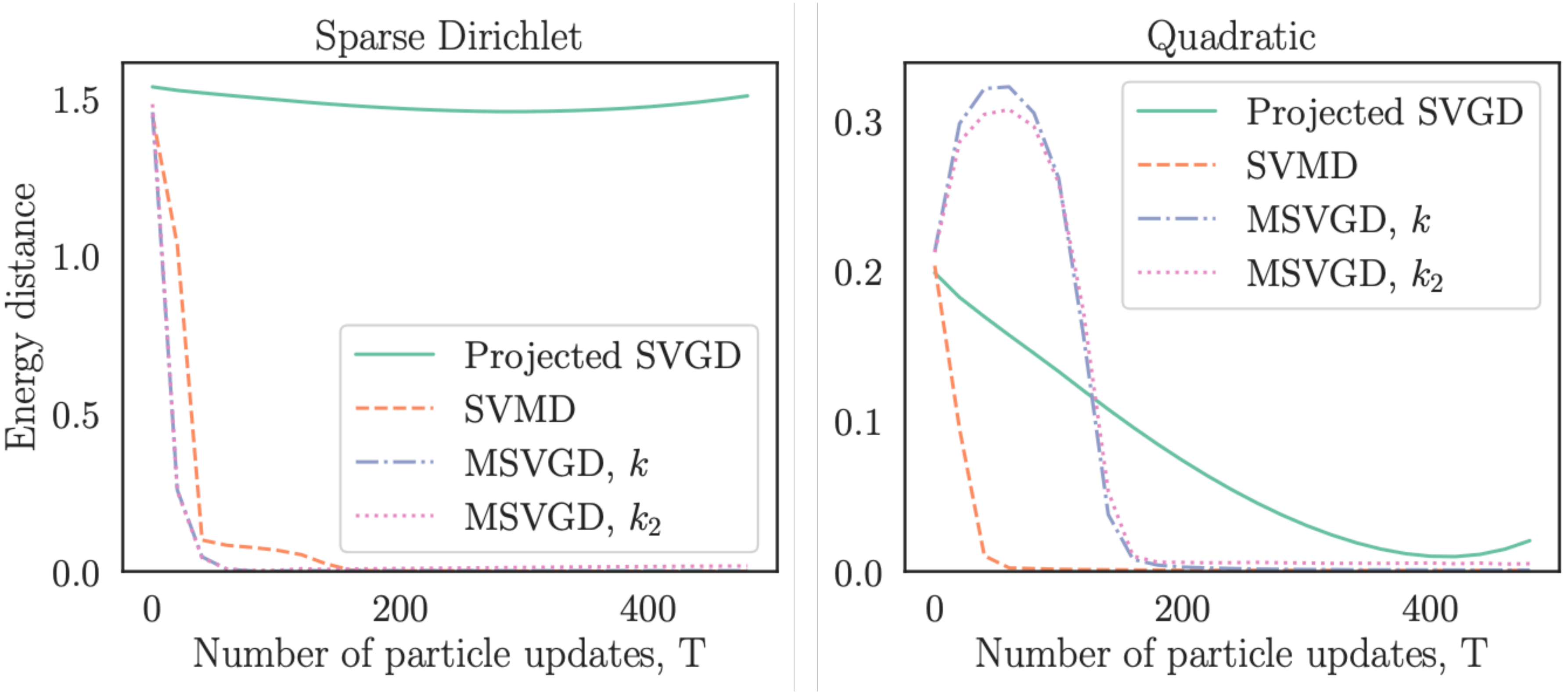
Approximation Quality on the Simplex



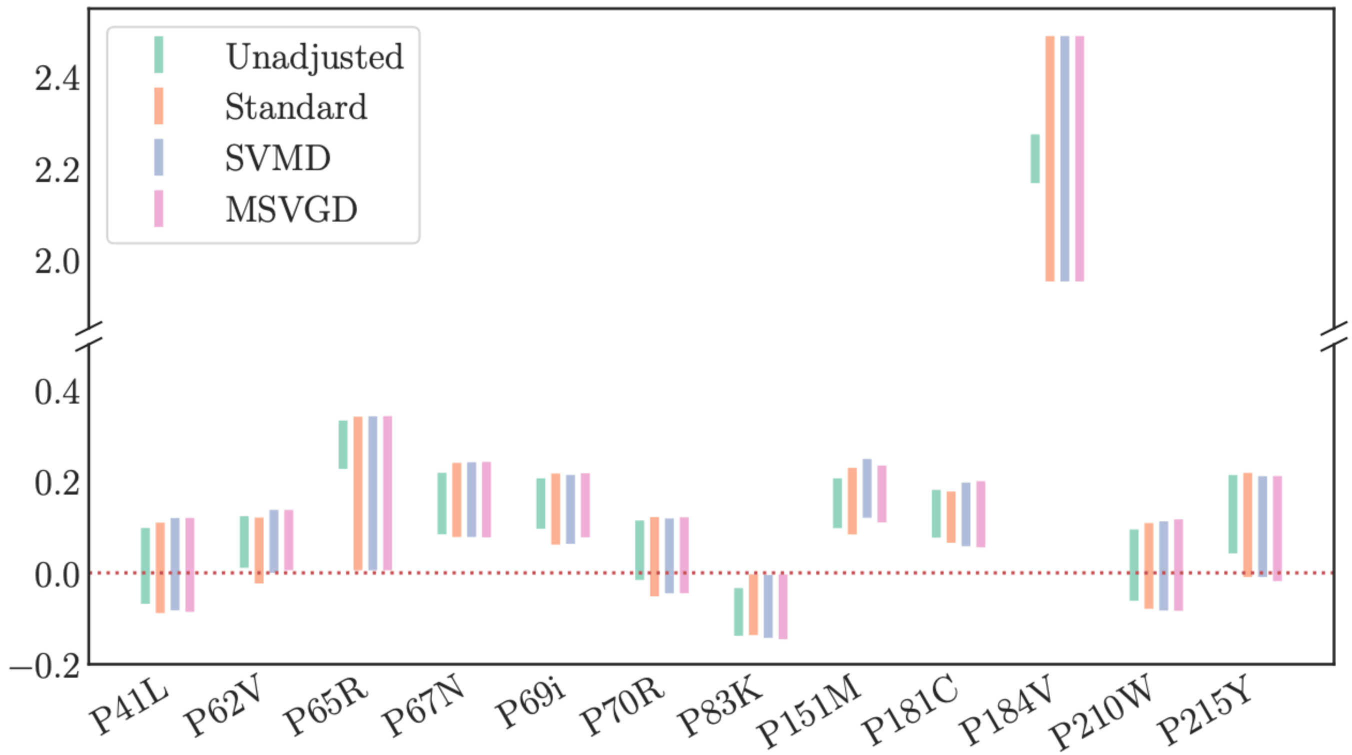
Quality of 50-particle approximations to 20-dimensional distributions on the simplex.

Application: Post-Selection Inference

Task: Generate valid confidence intervals (CIs) for parameters after data-driven model (feature) selection.

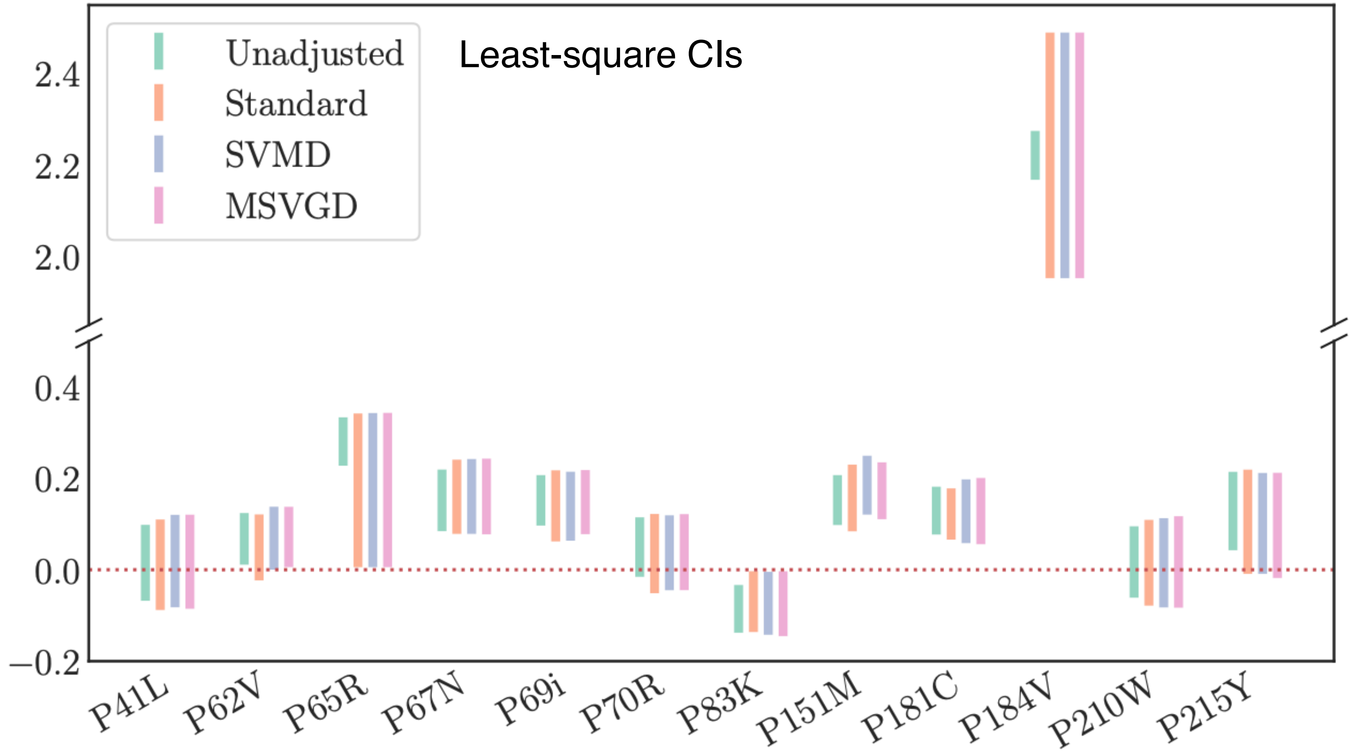
- Need to condition on the selection event.
- Target distributions are log-concave and have constrained support.

Application: Post-Selection Inference



Unadjusted and post-selection CIs for the mutations selected by the randomized Lasso as candidates for HIV-1 drug resistance.

Application: Post-Selection Inference



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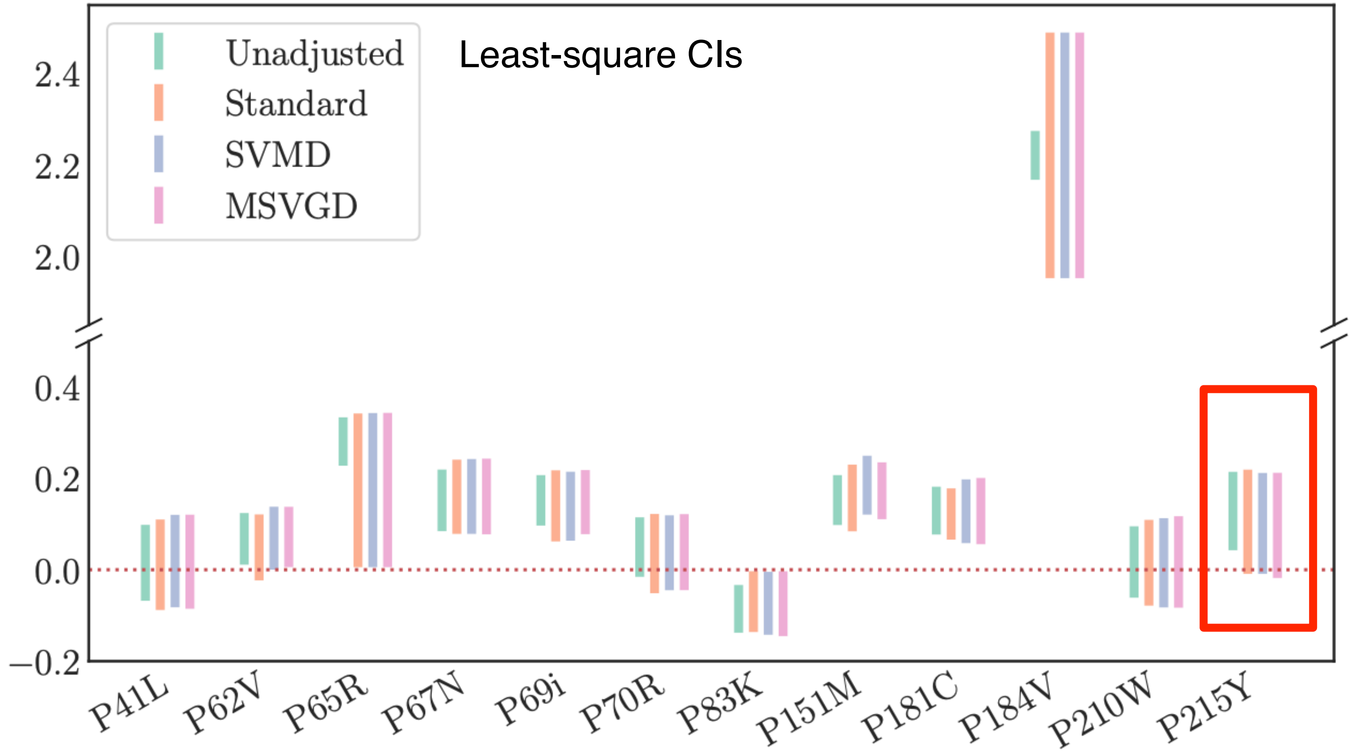

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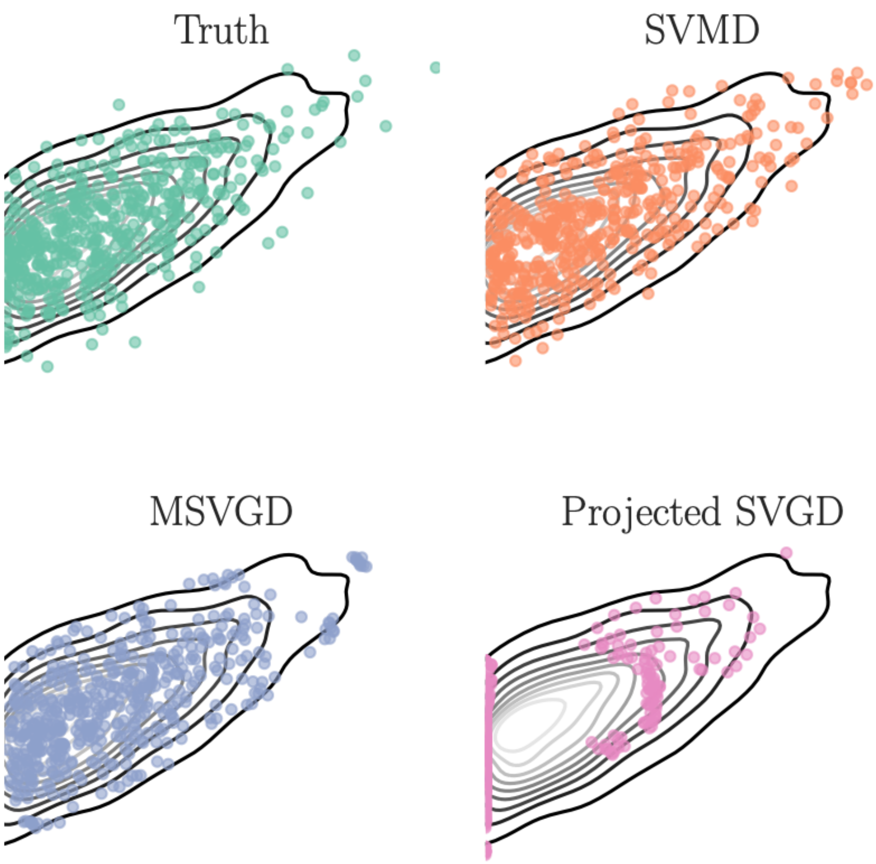
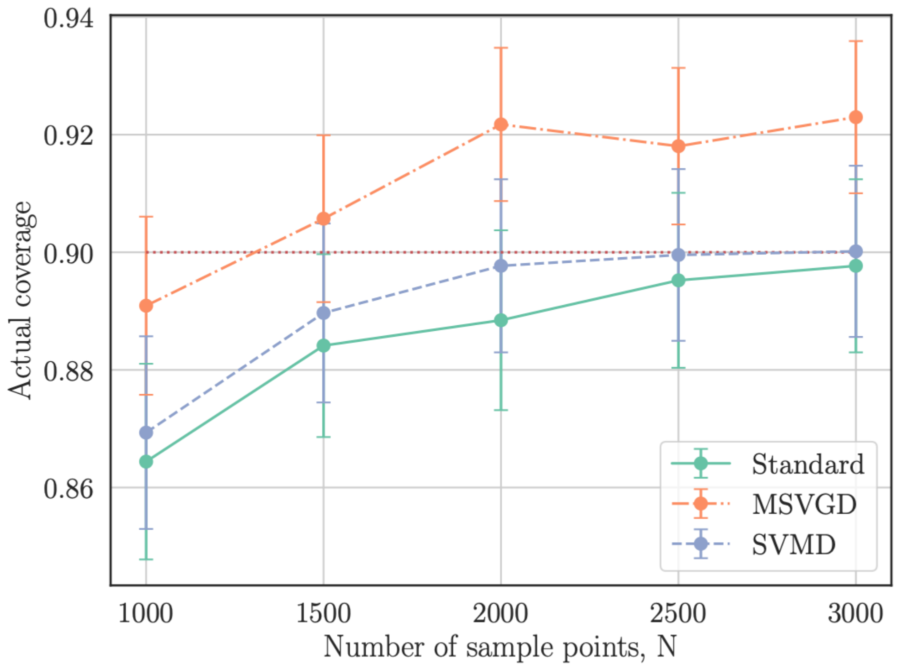
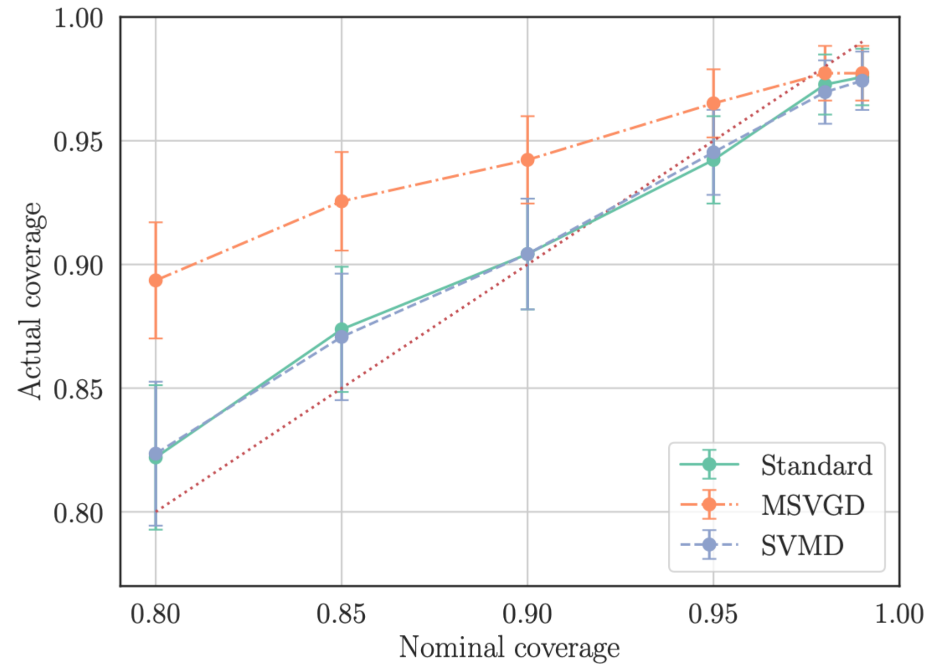


A 2D selective density example.

Application: Post-Selection Inference



Nominal Coverage: 0.9



5000 sample points

Coverage of post-selection CIs.

Convergence Results

① Convergence of mirrored updates as $n \to \infty$.

② Infinite-particle mirrored Stein updates decrease KL with sufficiently small step size and drive Mirrored Kernel Stein Discrepancy (MKSD) to 0.

③ MKSD determines weak convergence under suitable conditions.

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Convergence Results

① Convergence of mirrored updates as $n \to \infty$.

Theorem Suppose $q^n_{0,H} = \frac{1}{n}\sum_{i=1}^n \delta_{\eta_0^i}$ satisfying $W_1(q^n_{0,H}, q^\infty_{0,H}) \to 0$. Define the η-induced kernel $K_{\nabla\psi^*,t}(\eta, \eta') := K_t(\nabla\psi^*(\eta), \nabla\psi^*(\eta'))$. If, for some $c_1, c_2 > 0$:

$$\|\nabla(K_{\eta,t}(\cdot\,,\eta)\nabla\log p_H(\eta) + \nabla\cdot K_{\eta,t}(\cdot\,,\eta))\|_{\mathrm{op}} \leq c_1(1 + \|\eta\|_2),$$
$$\|\nabla(K_{\eta,t}(\eta',\cdot\,)\nabla\log p_H(\cdot\,) + \nabla\cdot K_{\eta,t}(\eta',\cdot\,))\|_{\mathrm{op}} \leq c_2(1 + \|\eta'\|_2),$$

Then $W_1(q^n_{t,H}, q^\infty_{t,H}) \to 0$ for each round of t

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Convergence Results

② Infinite-particle mirrored Stein updates decrease KL with sufficiently small step size and drive Mirrored Kernel Stein Discrepancy (MKSD) to 0.

Theorem Assume $\kappa_1 := \sup_\theta \|K_t(\theta,\theta)\|_{\mathrm{op}} < \infty$, and $\kappa_2 := \sum_{i=1}^d \sup_\theta \|\nabla^2_{i,d+i} K_t(\theta,\theta)\|_{\mathrm{op}} < \infty$, $\nabla \log p_H$ is L-Lipschitz, and ψ is α-strongly convex. If ϵ_t is sufficiently small, then

$$\mathrm{KL}(q_{t+1}^\infty \| p) - \mathrm{KL}(q_t^\infty \| p) \leq -\left(\epsilon_t - \left(\frac{L\kappa_1}{2} + \frac{2\kappa_2}{\alpha^2}\right)\epsilon_t^2\right) \mathrm{MKSD}_{K_t}(q_t^\infty \| p)^2 .$$

$$\mathrm{MSD}(q, p, \mathcal{G}) \triangleq \sup_{g \in \mathcal{G}} \mathbb{E}_q[(\mathcal{M}_{p,\psi} g)(\theta)] \quad \text{and} \quad \mathrm{MKSD}_K(q, p) \triangleq \mathrm{MSD}(q, p, \mathcal{B}_{\mathcal{H}_K}).$$

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From Constrained to Unconstrained Targets

Continuous Time	Discretization
Mirror flow: $d\eta_t = -\nabla f(\theta_t)dt,$ $\theta_t = \nabla\psi^*(\eta_t)$	Mirror descent
Riemannian gradient flow with metric tensor $\nabla^2\psi$: $d\theta_t = -\nabla^2\psi(\theta_t)^{-1}\nabla f(\theta_t)dt$	Natural gradient descent with metric tensor $\nabla^2\psi$

Stein Variational Natural Gradient (SVNG)

- Replacing $\nabla^2 \psi(\cdot)$ in SVMD with a general metric tensor
- In Bayesian inference $p(\theta) \propto \pi(\theta)\pi(y|\theta)$, it is common to choose

FIM: $G(\theta) = \mathbb{E}_{\pi(y|\theta)}[\nabla \log \pi(y|\theta) \nabla \log \pi(y|\theta)^\top]$

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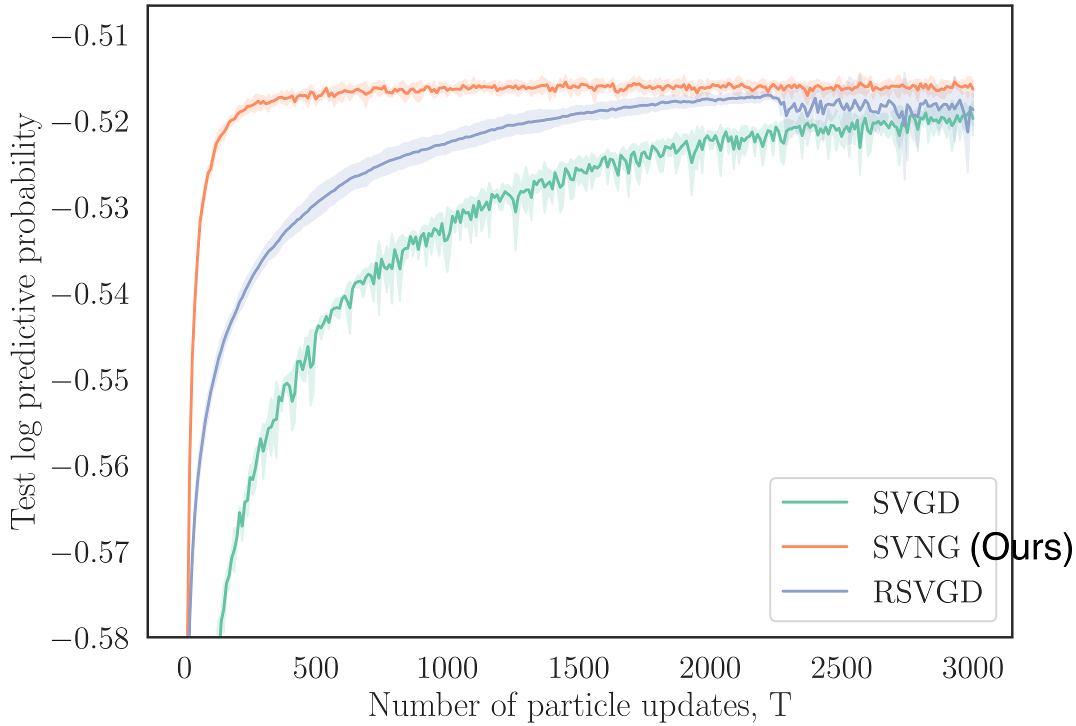
Exploiting Geometry in Bayesian Inference



Posterior inference for large-scale Bayesian Logistic Regression

$581,012$ datapoints, $d = 54$

Takeaways

- A new family of particle evolution samplers suitable for **constrained domains** and **non-Euclidean geometries**.
- SVMD is a multi-particle generalization of **mirror descent** for constrained sampling problems
- SVNG can exploit the geometry of unconstrained sampling problems with user-specified metric tensors.

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Future Work

- Complexity can be cubic w.r.t. the number of particles.
- Where you need mirror descent before, would it benefit from using a variant that is aware of uncertainty?

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Thanks to you and my coauthors

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