Stein's Method for Modern Machine Learning

From Gradient Estimation to Generative Modeling

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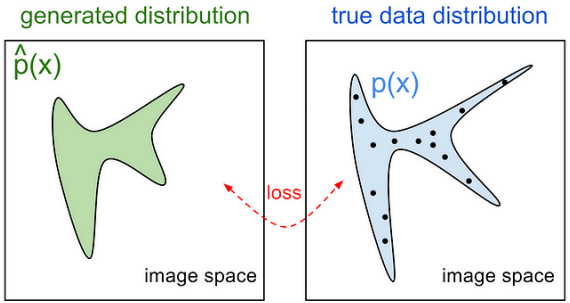
Outline

- Stein's method: Foundations
- Stein's method and machine learning
  - Sampling
  - Gradient estimation
  - Score-based modeling

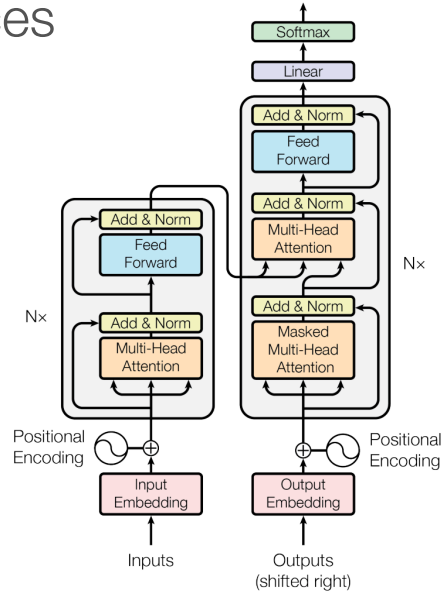
Divergences between Probability Distributions

- How well does my model fit the data?
- Parameter estimation by minimizing divergences
- Sampling as optimization



https://openai.com/blog/generative-models/

GANs, Diffusion models



Transformers

Integral Probability Metrics (IPM)

$$d_{\mathcal{H}}(q, p) = \sup_{h \in \mathcal{H}} | \mathbb{E}_q[h(X)] - \mathbb{E}_p[h(Y)] |$$

- When $\mathcal{H}$ is sufficient large, convergence in $d_{\mathcal{H}}(q_n, p)$ implies q_n weakly converges to p
- Examples: Total variation distance, Wasserstein distance
- **Problem**: Often p is our model and integration under p is intractable
- **Idea**: Only consider functions with $\mathbb{E}_p[h(Y)] = 0$

Stein's Method

- Identify an operator $\mathcal{T}$ that generates mean-zero functions under target distribution p.

$$\mathbb{E}_p[(\mathcal{T}g)(X)] = 0 \text{ for all } g \in \mathcal{G}$$

- Define the Stein discrepancy:

$$\mathcal{S}(q, \mathcal{T}, \mathcal{G}) \triangleq \sup_{g \in \mathcal{G}} \mathbb{E}_q[(\mathcal{T}g)(X)] - \mathbb{E}_p[(\mathcal{T}g)(X)]$$

- Show that the Stein discrepancy is lower bounded by an IPM. For example, if for any $h \in \mathcal{H}$, a solution $g \in \mathcal{G}$ exists for the equation $h(x) - \mathbb{E}_p[h(Y)] = (\mathcal{T}g)(x)$, then $d_{\mathcal{H}}(q, p) \leq \mathcal{S}(q, \mathcal{T}, \mathcal{G})$.

[Stein, 1972]

Identifying a Stein Operator

Stein's Lemma

If p is a standard normal distribution, then

$$\mathbb{E}_p[g'(X) - Xg(X)] = 0 \text{ for all } g \in C_b^1$$

The corresponding Stein operator: $\mathcal{T}(g) = g'(x) - xg(x)$

Identifying a Stein Operator

Barbour's generalization via stochastic processes

- The (infinitesimal) generator A of a stochastic process $(X_t)_{t\geq 0}$ is defined as

$$(Af)(x) = \lim_{t\to 0} \frac{\mathbb{E}[f(X_t)\,|\,X_0 = x] - f(x)}{t}\,.$$

- The generator of a stochastic process with stationary distribution p satisfies $\mathbb{E}_p[(Af)(X)] = 0$.

[Barbour, 1988 & 1990]

Langevin Stein Operator

- Langevin diffusion on $\mathbb{R}^d$: $dX_t = \nabla \log p(X_t) dt + \sqrt{2} dW_t$
- Generator:

$$(Af)(x) = \nabla \log p(x)^\top \nabla f(x) + \nabla \cdot \nabla f(x)$$

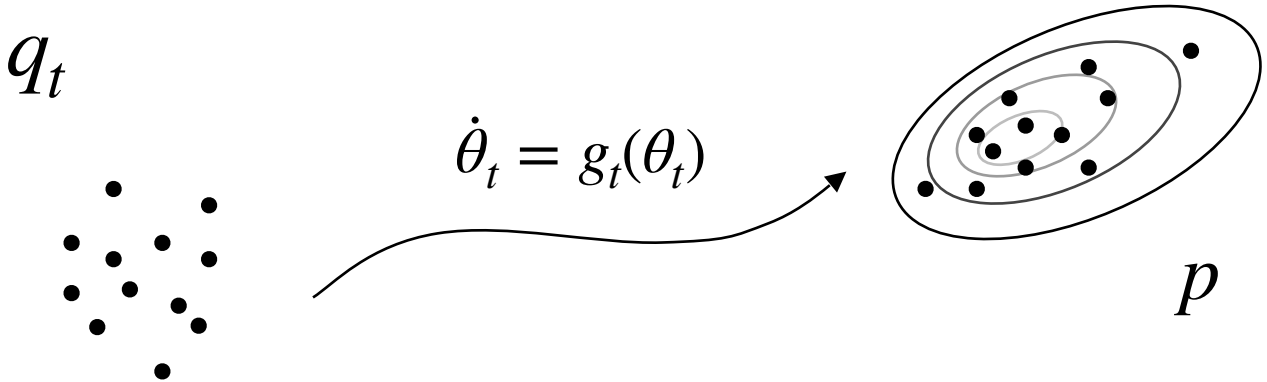
- Convenient form with a vector-valued function $g : \mathbb{R}^d \to \mathbb{R}^d$:

$$(\mathcal{T}_p g)(x) = \nabla \log p(x)^\top g(x) + \nabla \cdot g(x)$$

- Depends on p only through $\nabla \log p$, computable even for unnormalized p

[Gorham & Mackey, 2015]

Stein Operators and Sampling



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

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

[Liu & Wang, 2016]

Wasserstein Gradient Flow and SVGD

$$\inf_{g_t \in \mathcal{G}} \frac{d}{dt} \mathrm{KL}(q_t \| p) = - \sup_{g_t \in \mathcal{G}} \mathbb{E}_{q_t}[(\mathcal{T}_p g_t)(X)]$$

- $\mathcal{G} = \mathcal{L}^2(q_t)$: Wasserstein Gradient Flow

$$g_t^* \propto \nabla \log p - \nabla \log q_t,$$

  Same density evolution as Langevin diffusion

- $\mathcal{G} =$ RKHS of kernel K: Stein Variational Gradient Descent [Liu & Wang, 2016]

$$g_t^* \propto \mathbb{E}_{q_t}[K(\cdot, X) \nabla \log p(X) + \nabla_X \cdot K(\cdot, X)]$$

Convergence Analysis of SVGD

- Korba, A., Salim, A., Arbel, M., Luise, G., & Gretton, A. A non-asymptotic analysis for Stein variational gradient descent. *NeurIPS* (2020).

- Chewi, S., Le Gouic, T., Lu, C., Maunu, T., & Rigollet, P. SVGD as a kernelized Wasserstein gradient flow of the chi-squared divergence. *NeurIPS* (2020).

- Shi, J., & Mackey, L. A finite-particle convergence rate for Stein variational gradient descent. *NeurIPS* (2023).

  Convergence rate for discrete-time, finite-particle SVGD

Stein's Method and Gradient Estimation

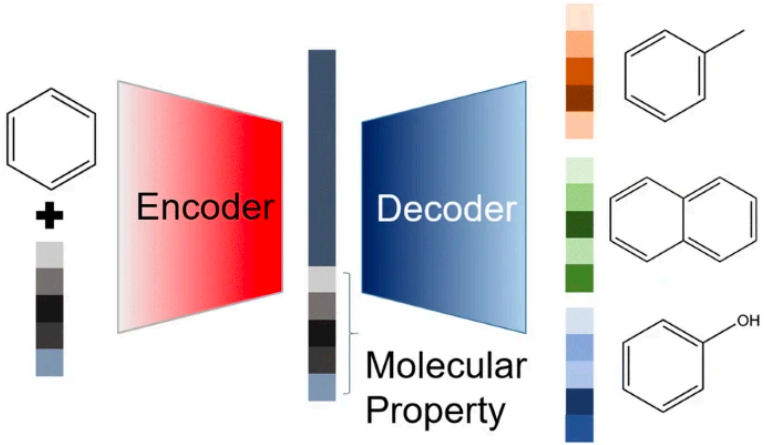
The Gradient Estimation Problem

A common problem in training generative models and reinforcement learning

$$\nabla_\eta \mathbb{E}_{q_\eta}[f(X)]$$

Encoder

Decoding error



[Lim et al., 2018]

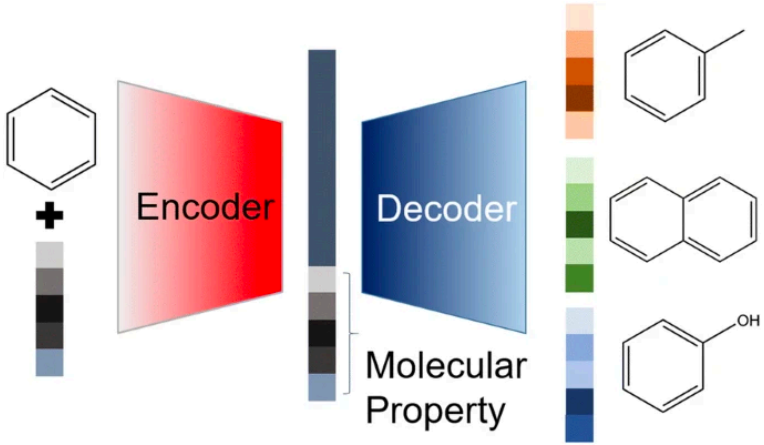
The Gradient Estimation Problem

A common problem in training generative models and reinforcement learning

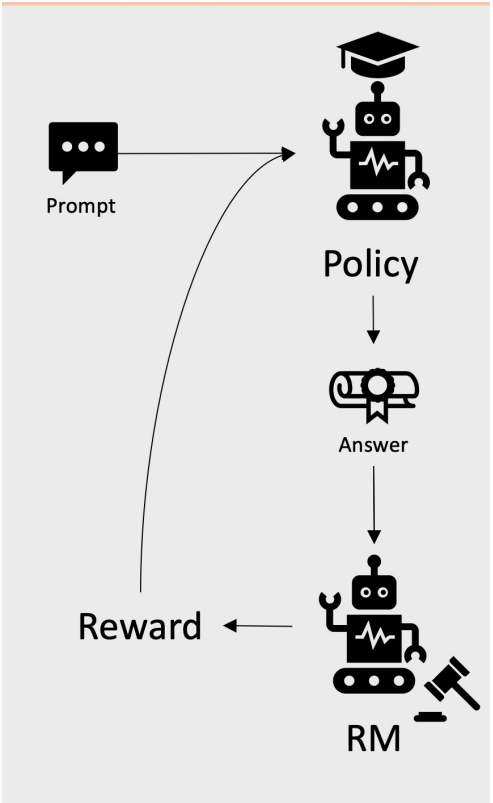
$$\nabla_\eta \mathbb{E}_{q_\eta}[f(X)]$$

Policy

Reward Model



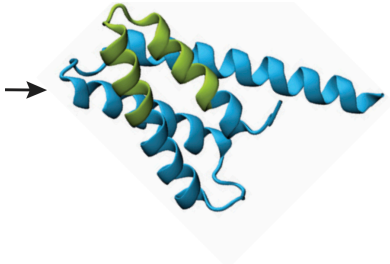
[Lim et al., 2018]



https://aws.amazon.com/de/what-is/reinforcement-learning-from-human-feedback/

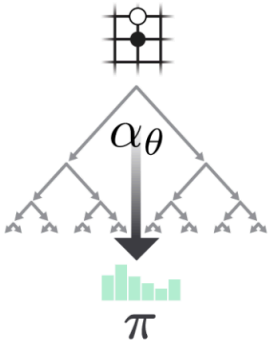
Discrete Gradient Estimation

- Discrete data, states, and actions



MDDTLFSILNSELLSLINDMPITNDQK
KLMSNNFVKMANDLKGEFGDENVY
YVNQTTKYVYIYEEARQLLGFPTLSD
KIYQKILIRINEKLSRNFNIEIQKNKI

[Alamdari et al., 2023]



[Silver et al., 2017]

Model Input

Q: Roger has 5 tennis balls. He buys 2 more cans of tennis balls. Each can has 3 tennis balls. How many tennis balls does he have now?

A: Roger started with 5 balls. 2 cans of 3 tennis balls each is 6 tennis balls. 5 + 6 = 11. The answer is 11.

Q: The cafeteria had 23 apples. If they used 20 to make lunch and bought 6 more, how many apples do they have?

Model Output

A: The cafeteria had 23 apples originally. They used 20 to make lunch. So they had 23 - 20 = 3. They bought 6 more apples, so they have 3 + 6 = 9. The answer is 9. ✓

[Wei et al., 2022]

- Computing exact gradients is often intractable

Intractable sum over 2^d configurations

$$\nabla_\eta \mathbb{E}_{q_\eta}[f(X)] = \nabla_\eta \sum_{x \in \{0,1\}^d} q_\eta(x) f(x)$$

d-dimensional binary vector

Complex, nonlinear function

Gradient Estimation and Variance Reduction

$$\hat{g}_1 = \frac{1}{K}\sum_{k=1}^{K} f(x_k)\nabla_\eta \log q_\eta(x_k) \quad \text{(REINFORCE)}$$

High variance!

Control Variates

$$\hat{g}_2 = \frac{1}{K}\sum_{k=1}^{K} [f(x_k)\nabla_\eta \log q_\eta(x_k) + cv(x_k)] - \mathbb{E}_{q_\eta}[cv(X)]$$

- Strong correlation is required for effective variance reduction
- **Fundamental tradeoff**: cv needs to be very *flexible* but still have *analytic expectation* under q_η.

A: Stein Operator

$$\hat{g}_2 = \frac{1}{K}\sum_{k=1}^{K} [f(x_k)\nabla_\eta \log q_\eta(x_k) + (Ah)(x_k)] - \mathbb{E}_{q_\eta}[(Ah)(X)]$$

$= 0$

Discrete Stein Operators

How: Apply Barbour's idea to discrete-state Markov chains.

$$\mathbb{E}_q[((K-I)h)(X)] = 0 \xrightarrow{\text{cont. time}} \mathbb{E}_q[(Ah)(X)] = 0$$

K: transfer operator

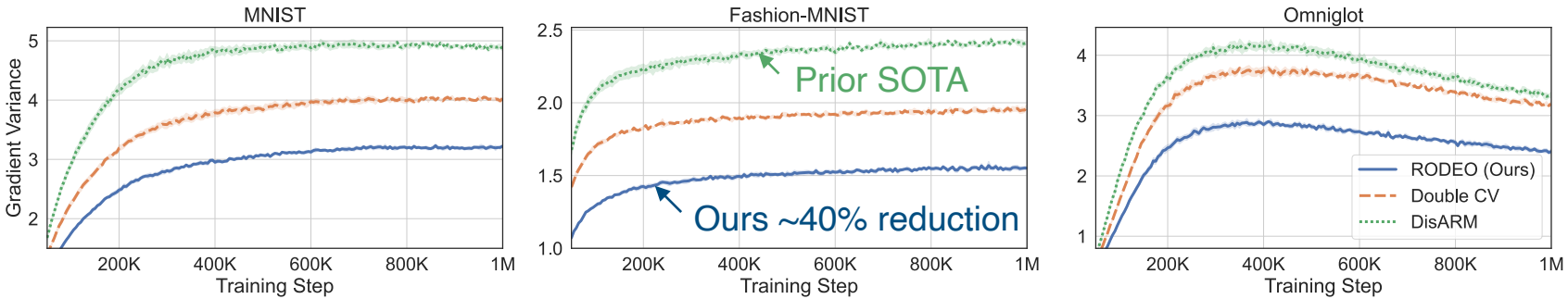
A: generator

Stein Operator	$(Ah)(x)$
Gibbs (4)	$\frac{1}{d}\sum_{i=1}^{d}\sum_{y_{-i}=x_{-i}} q(y_i\|x_{-i})h(y) - h(x)$
MPF (6)	$\sum_{y\in\mathcal{N}_x, y\neq x} \sqrt{q(y)/q(x)}(h(y)-h(x))$
Barker (6)	$\sum_{y\in\mathcal{N}_x, y\neq x} \frac{q(y)}{q(x)+q(y)}(h(y)-h(x))$
Difference (8)	$\frac{1}{d}\sum_{i=1}^{d} h(\mathtt{dec}_i(x)) - \frac{q(\mathtt{inc}_i(x))}{q(x)}h(x)$

Shi, Zhou, Hwang, Titsias & Mackey. Gradient estimation with discrete Stein operators, NeurIPS 2022 Outstanding Paper.

Experiments: Training Binary Latent VAEs

		Bernoulli Likelihoods			Gaussian Likelihoods		
		MNIST	Fashion-MNIST	Omniglot	MNIST	Fashion-MNIST	Omniglot
$K=2$	DisARM	-102.75 ± 0.08	-237.68 ± 0.13	-116.50 ± 0.04	668.03 ± 0.61	182.65 ± 0.47	446.61 ± 1.16
	Double CV	-102.14 ± 0.06	-237.55 ± 0.16	-116.39 ± 0.10	676.87 ± 1.18	186.35 ± 0.64	447.65 ± 0.87
	RODEO (Ours)	$\mathbf{-101.89 \pm 0.17}$	$\mathbf{-237.44 \pm 0.09}$	$\mathbf{-115.93 \pm 0.06}$	$\mathbf{681.95 \pm 0.37}$	$\mathbf{191.81 \pm 0.67}$	$\mathbf{454.74 \pm 1.11}$
$K=3$	ARMS	-100.84 ± 0.14	-237.05 ± 0.12	-115.21 ± 0.07	683.55 ± 1.01	193.07 ± 0.34	457.98 ± 1.03
	Double CV	-100.94 ± 0.09	-237.40 ± 0.11	-115.06 ± 0.12	686.48 ± 0.68	193.93 ± 0.20	457.44 ± 0.79
	RODEO (Ours)	$\mathbf{-100.46 \pm 0.13}$	$\mathbf{-236.88 \pm 0.12}$	$\mathbf{-115.01 \pm 0.05}$	$\mathbf{692.37 \pm 0.39}$	$\mathbf{196.56 \pm 0.42}$	461.87 ± 0.90
RELAX (3 evals)		-101.99 ± 0.04	-237.74 ± 0.12	-115.70 ± 0.08	688.58 ± 0.52	196.38 ± 0.66	$\mathbf{462.23 \pm 0.63}$



Shi, Zhou, Hwang, Titsias & Mackey. Gradient estimation with discrete Stein operators, NeurIPS 2022 Outstanding Paper.

Stein’s Method and Score-Based Modeling

Stein Discrepancy as a Learning Rule

Model fitting: $\min_{\theta} \left| \mathbb{E}_{q}[h(x)^{\top} \nabla_x \log p_{\theta}(x) + \nabla \cdot h(x)] \right|$

?

Data distribution

Model distribution

Score Matching

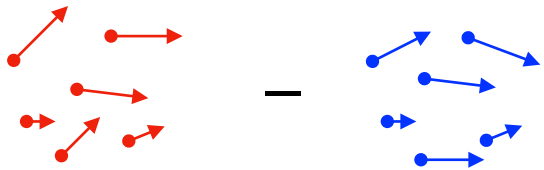
[Hyvärinen, 2005]

Model fitting: $\min_{\theta} \sup_{h \in L^2(q)} \left| \mathbb{E}_q [h(x)^\top \nabla_x \log p_\theta(x) + \nabla \cdot h(x)] \right|$

Data distribution

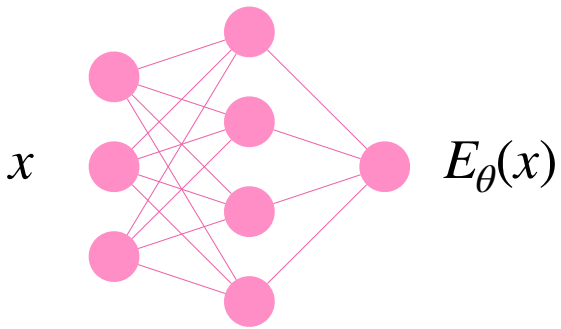
Model distribution

$$\rightarrow \min_{\theta} \mathbb{E}_{q_{\text{data}}} [\| \nabla \log p_\theta(x) - \nabla \log q_{\text{data}}(x) \|^2]$$



Training Energy-Based Models

$$p_\theta(x) = \frac{e^{-E_\theta(x)}}{Z_\theta}$$



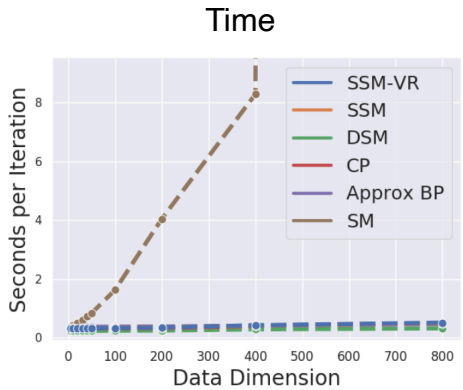
Sliced Score Matching

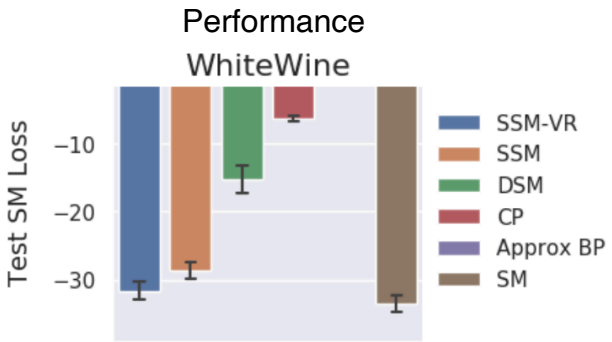
[Song*, Garg*, S & Ermon, UAI'19]

Key insight: The score does not depend on normalizing constant Z_θ

$$\nabla_x \log p_\theta(x) = -\nabla E_\theta(x) + \cancel{\nabla_x \log Z_\theta}$$

- Score Matching is more suitable for training such models than maximum likelihood!





Song*, Garg*, Shi & Ermon. Sliced score matching: A scalable approach to density and score estimation. UAI 2019

Score-Based Modeling

Idea: Model the score $s := \nabla \log p$ instead of the density

Advantages:

1. less computation than energy-based modeling
2. enable more flexible models

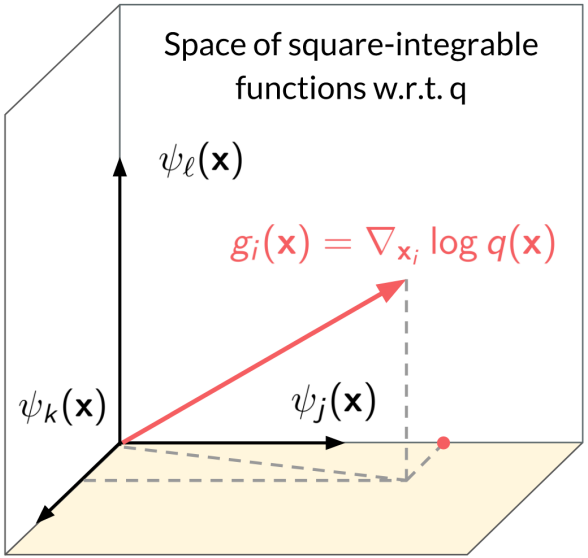
Nonparametric Score Model

$$\min_{s \in \mathcal{H}} \mathbb{E}_{q_{\text{data}}} \|s(x) - \nabla \log q_{\text{data}}(x)\|^2 + \frac{\lambda}{2} \|s\|_{\mathcal{H}}^2$$

The spectral estimator (Shi et al., 18)
is a special case.

Zhou, Shi & Zhu. Nonparametric score estimators. ICML 2020

A Spectral Method for Score Estimation



$$\nabla_{\mathbf{x}} \log q(\mathbf{x}) = -\sum_{j \geq 1} \mathbb{E}_q \left[\nabla \psi_j(\mathbf{x}) \right] \psi_j(\mathbf{x})$$

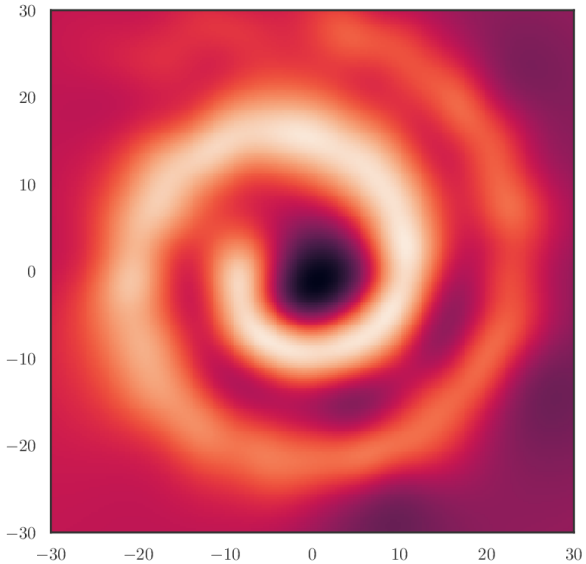
density gradients (score) — eigenfunction

$$\langle \nabla \log q, \psi_j \rangle_{L^2(q)} = -\mathbb{E}_q[\nabla \psi_j(x)]$$

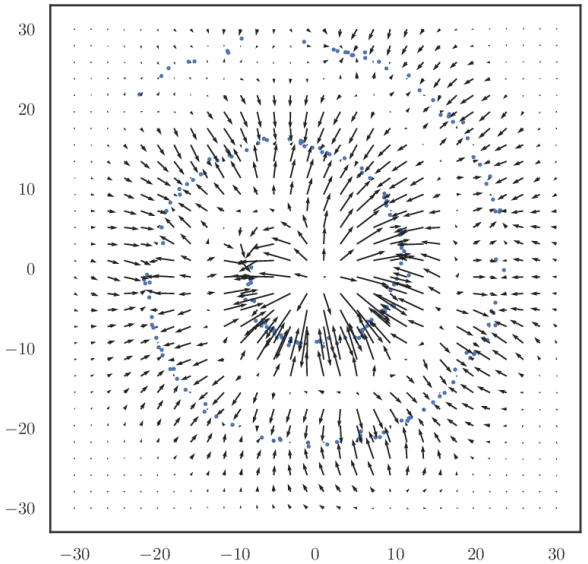
$$\mathbb{E}_{\mathbf{x}' \sim q}[k(\mathbf{x}, \mathbf{x}')\psi_j(\mathbf{x}')] = \lambda_j \psi_j(\mathbf{x})$$

Shi, Sun & Zhu. A spectral approach to gradient estimation for implicit distributions. ICML 2018

A Spectral Method for Score Estimation



$q(\mathbf{x})$ (unknown)



$\{\mathbf{x}^j\}_{j=1}^{M} \overset{\text{i.i.d.}}{\sim} q \rightarrow \nabla_{\mathbf{x}} \log q(\mathbf{x})$

Score function

Shi, Sun & Zhu. A spectral approach to gradient estimation for implicit distributions. ICML 2018
Zhou, Shi & Zhu. Nonparametric score estimators. ICML 2020

Score-Based Modeling

Idea: Model the score $s := \nabla \log p$ instead of the density

Advantages:

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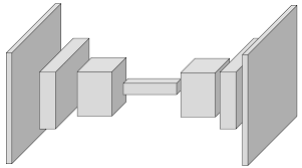
x  $s_\theta(x) \approx \nabla \log q_{\text{data}}(x)$

Nonparametric Score Model

$$\min_{s \in \mathcal{H}} \mathbb{E}_{q_{\text{data}}} \|s(x) - \nabla \log q_{\text{data}}(x)\|^2 + \frac{\lambda}{2} \|s\|_{\mathcal{H}}^2$$

The spectral estimator (Shi et al., 18) is a special case.

Score Network

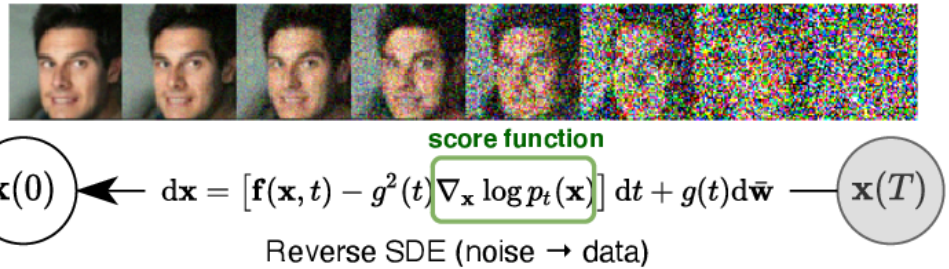
Use neural networks to model score, trained by sliced score matching

$$\min_{\theta} \mathbb{E}_{q_{\text{data}}} \|s_\theta(x) - \nabla \log q_{\text{data}}(x)\|^2$$

Song*, Garg*, Shi & Ermon. Sliced score matching: A scalable approach to density and score estimation. UAI 2019
Zhou, Shi & Zhu. Nonparametric score estimators. ICML 2020

From Score Networks to Diffusion Models

Updates produced by score networks transform noise to data



[Song et al., ICLR'20]

Images created by OpenAI's DALLE-2.
DALLE-2 is based on diffusion models.

Open Problems

- Improving finite-particle rates of SVGD
- Approximately solving the Stein equation for improved gradient estimation
- Lower bounding the discrete Stein discrepancy
- Learning the features in nonparametric score models
- Finding the “right” discrete correspondence of the score matching objective

Joint work with Yuhao Zhou, Jessica Hwang, Shengyang Sun, Yang Song, Sahaj Garg, Michalis K. Titsias, Lester Mackey, Jun Zhu

Main References

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- Alamdari, S., Thakkar, N., van den Berg, R., Lu, A. X., Fusi, N., Amini, A. P., & Yang, K. K. (2023). Protein generation with evolutionary diffusion: sequence is all you need. bioRxiv, 2023-09.
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