Generative Modeling by Estimating Gradients of the Data Distribution

YANG SONG

Progress in generative models of images

Karras, T., Laine, S., Aittala, M., Hellsten, J., Lehtinen, J. and Aila, T., 2020. Analyzing and improving the image quality of stylegan. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (pp. 8110-8119).

Progress in generative models of text

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Talktotransformer.com

(prompt) The best generative model is

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Talktotransformer.com

(prompt) The best generative model is

one that can learn over time and which predicts the structure and functionality of the brain as a whole.

Introduction to generative models

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$$\mathbf{x}_i \overset{\text{i.i.d.}}{\sim} p_{\text{data}}$$

$$i = 1, 2, \cdots, N$$

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Models of Probability distributions

$\boldsymbol{\theta} \in \Theta$

Introduction to generative models

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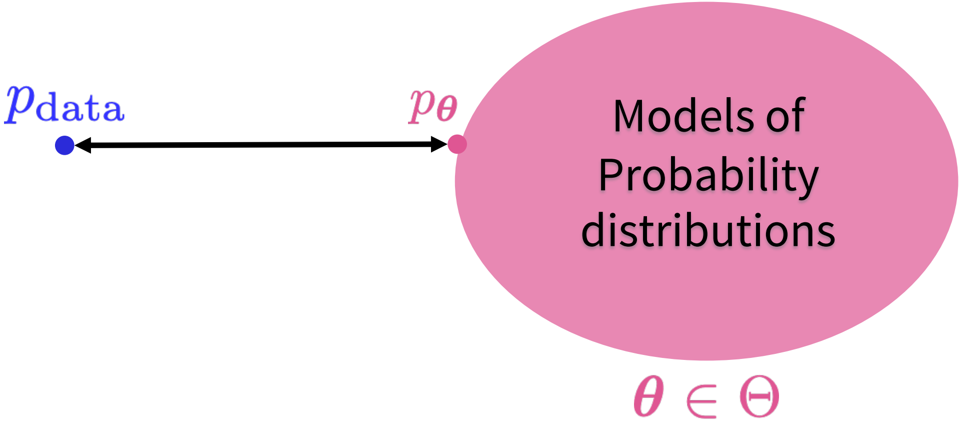

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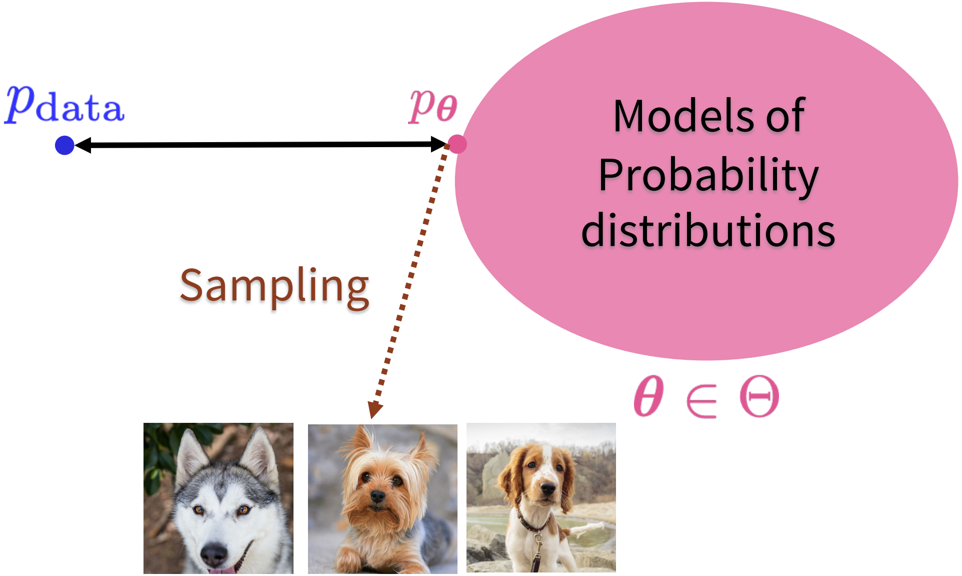
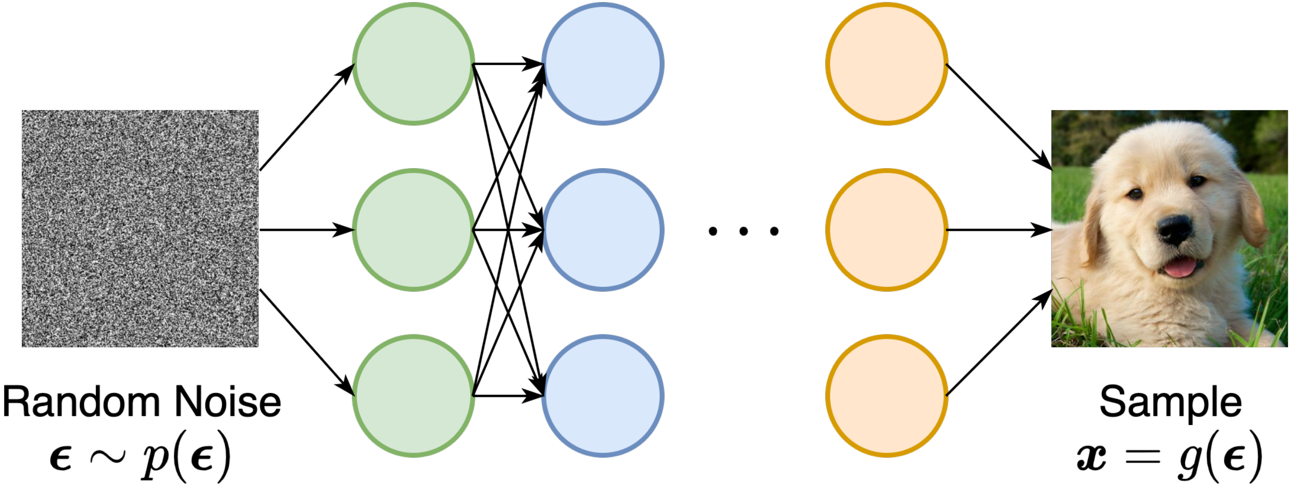


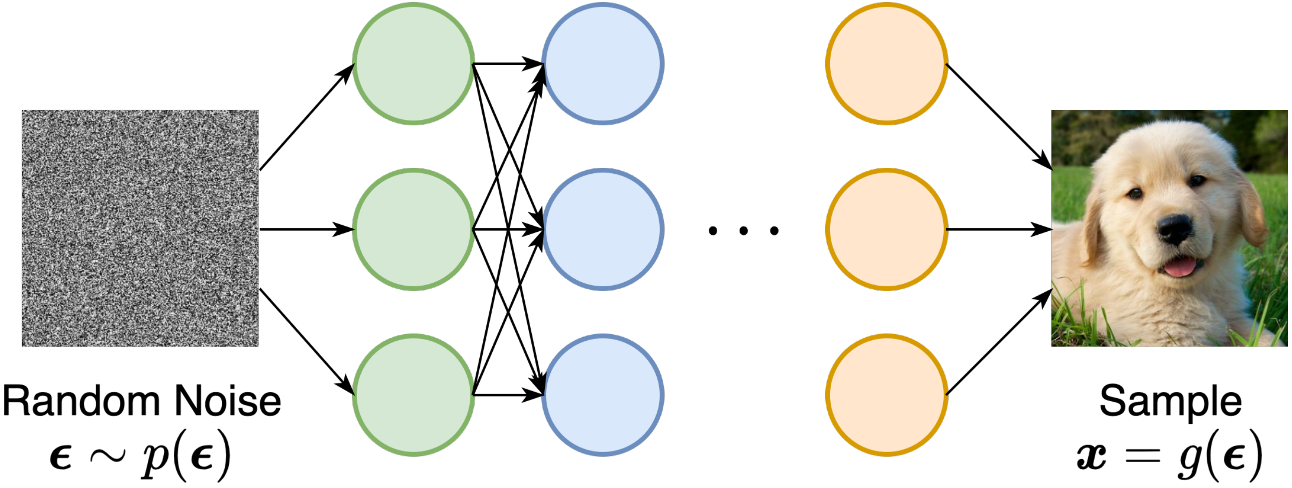
Representations of probability distributions

Implicit models: represent the sampling process



Representations of probability distributions

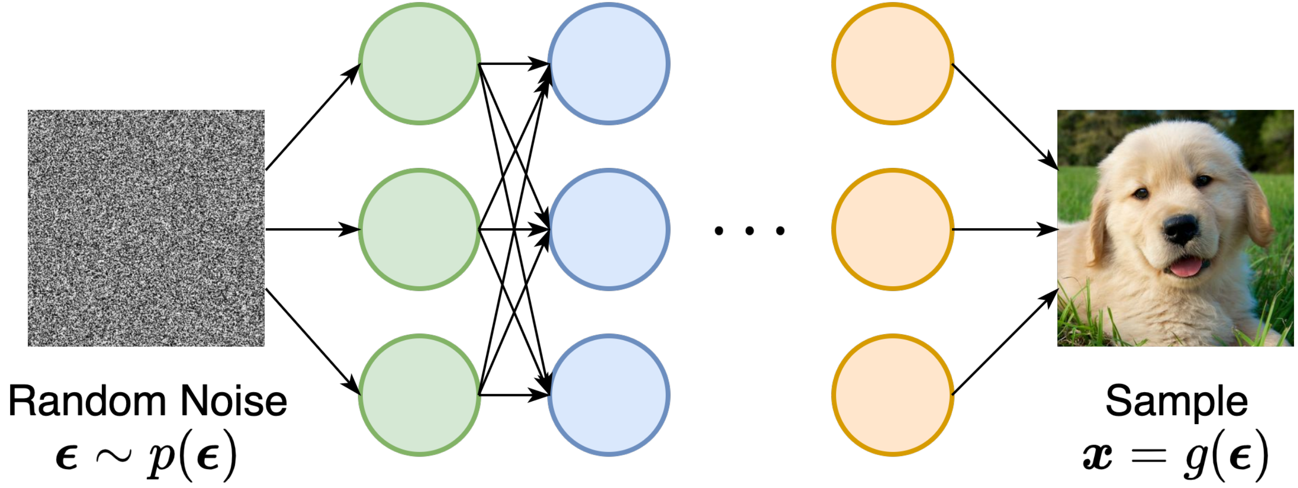
Implicit models: represent the sampling process



Pros: flexible architecture, high sample quality.

Representations of probability distributions

Implicit models: represent the sampling process

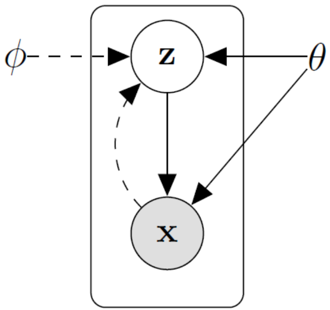


Pros: flexible architecture, high sample quality.

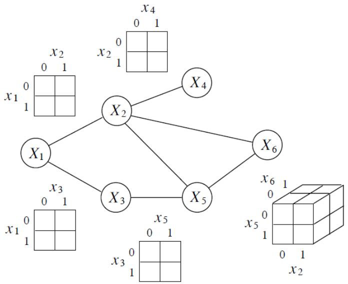
Cons: hard to train, no likelihood, no principled model comparisons

Representations of probability distributions

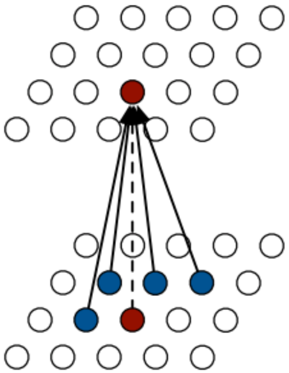
Explicit models: represent a probability density/mass function



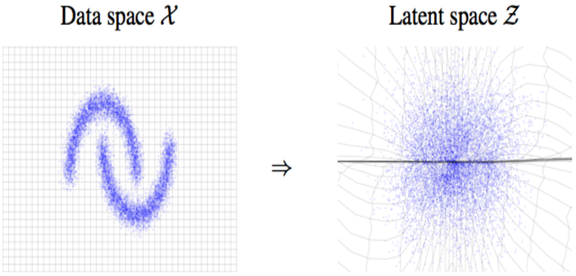
Bayesian networks (e.g., VAEs)



MRF



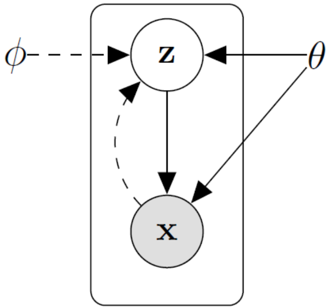
Autoregressive models



Flow models

Representations of probability distributions

Explicit models: represent a probability density/mass function



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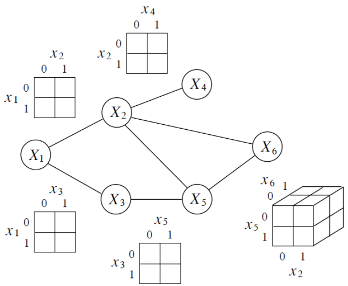

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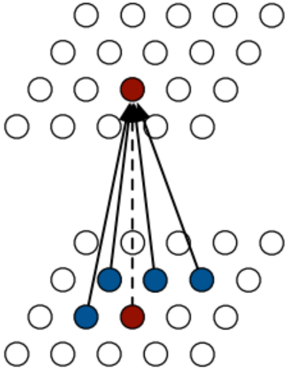

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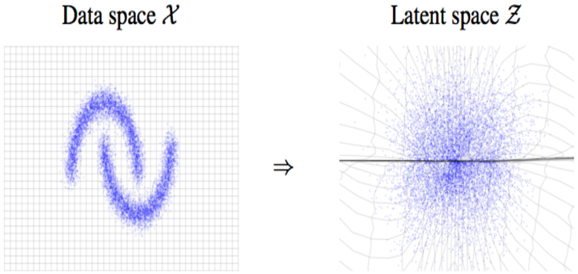
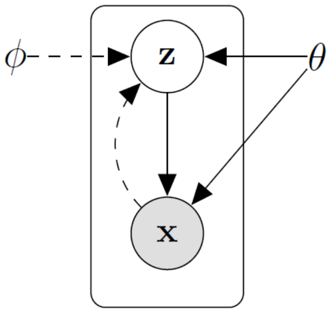


Flow models

Pros: likelihoods

Representations of probability distributions

Explicit models: represent a probability density/mass function



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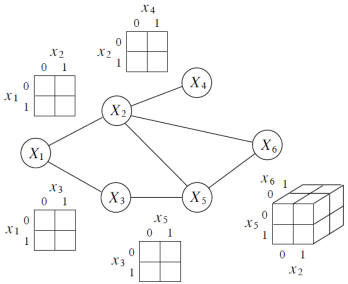

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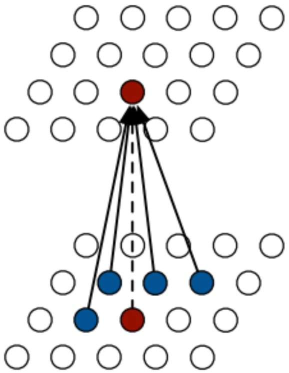

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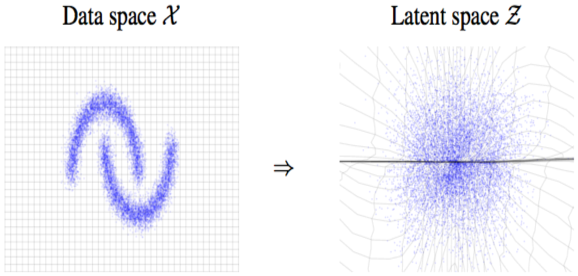

Flow models

Pros: likelihoods

Cons: need to be normalized, expressivity-tractability trade-off

Representation of probability distributions

This talk: The gradient of log probability density

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$$\nabla_{\mathbf{x}} \log p(\mathbf{x})$$

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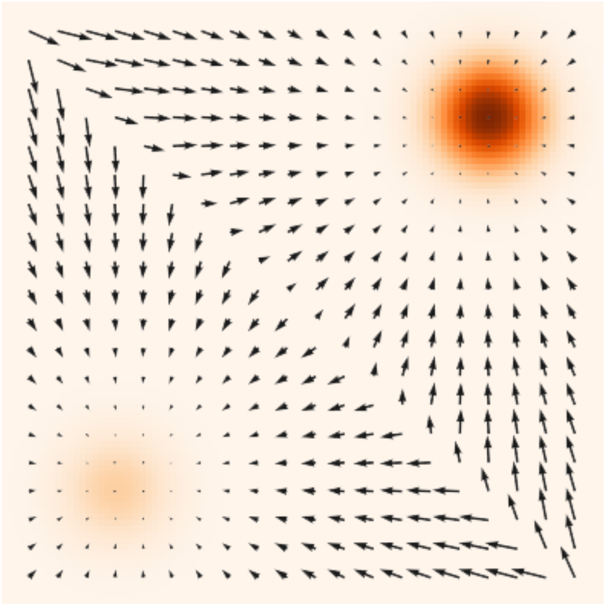

(PDF and score)

Why scores?

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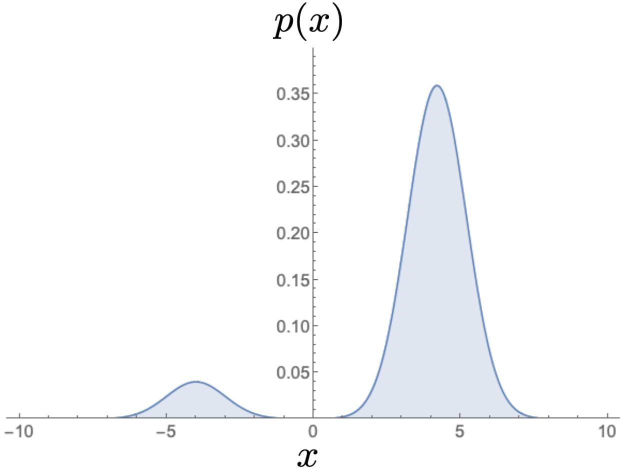

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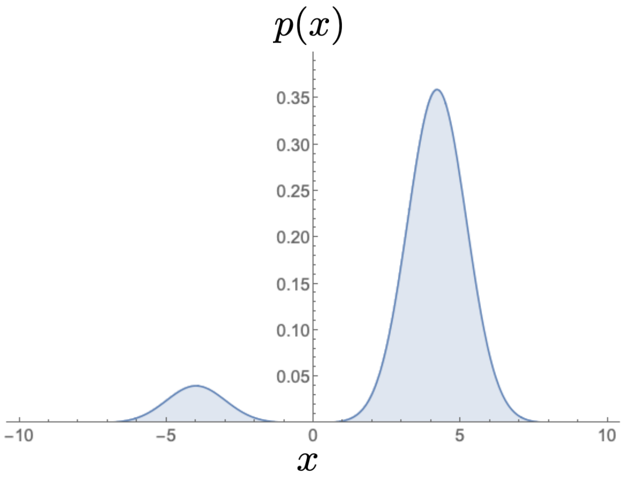
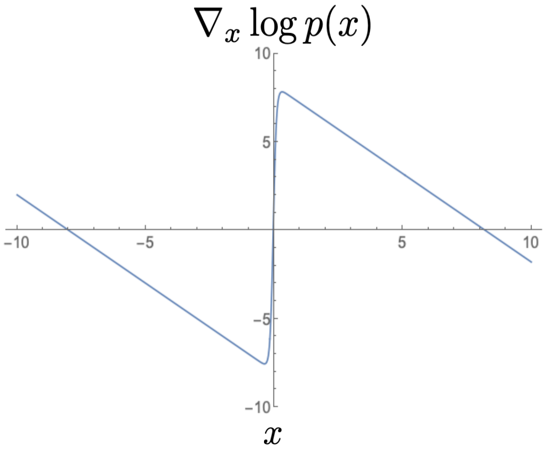

$p(x)$
0.35
0.30
0.25
0.20
0.15
0.10
0.05
−10
−5
0
5
10
x


$\nabla_x \log p(x)$
10
5
−5
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x

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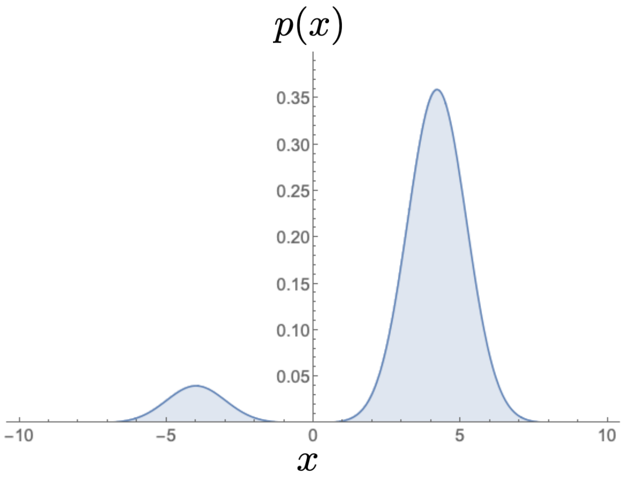

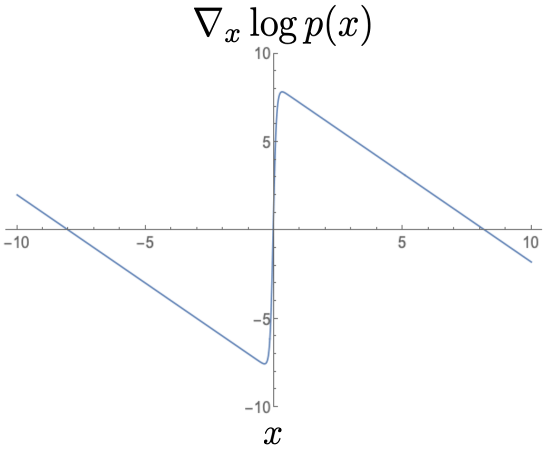

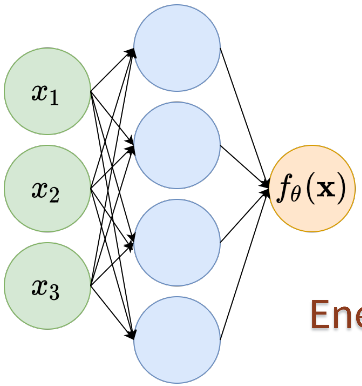

$$\Longrightarrow p_\theta(\mathbf{x}) = \frac{e^{-f_\theta(\mathbf{x})}}{Z_\theta}$$

Energy-Based Model (EBM)

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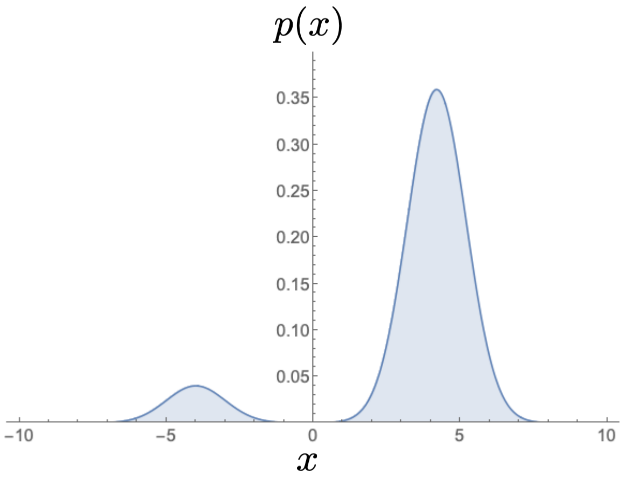

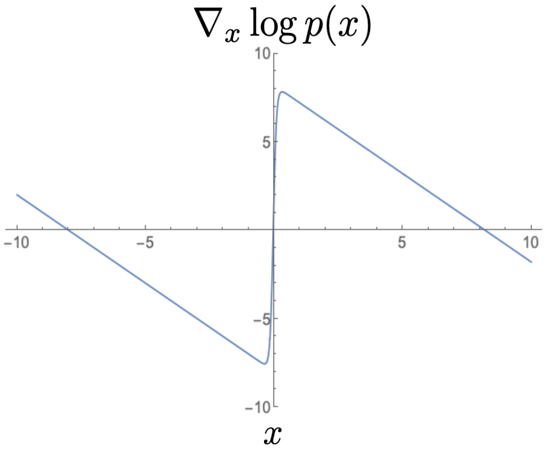

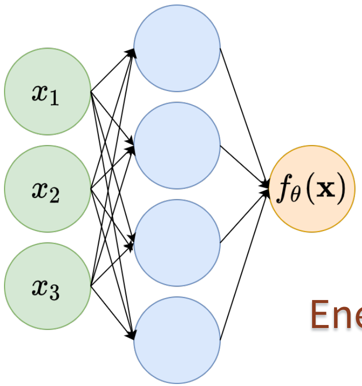

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Energy-Based Model (EBM)

$$\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) = -\nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \underbrace{\nabla_{\mathbf{x}} \log Z_\theta}_{=0}$$
$$= -\nabla_{\mathbf{x}} f_\theta(\mathbf{x})$$

Score

Score estimation

- **Given:** i.i.d. samples $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p_{\text{data}}(\mathbf{x})$
- **Goal:** Estimating the score $\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$

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- **Objective:** How to compare two vector fields of scores?

$$\frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2]$$

(Fisher divergence)

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- Integration by parts → **Score Matching (**Hyvärinen 2005)

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\frac{1}{2}\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2 + \text{trace}(\underbrace{\nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})}_{\text{Jacobian of } \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})})\right]$$

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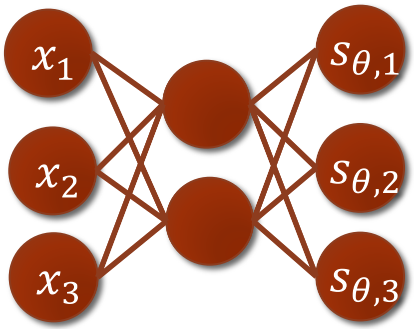
Not scalable

Stanford University

Score Matching is not scalable

- Deep score models



$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

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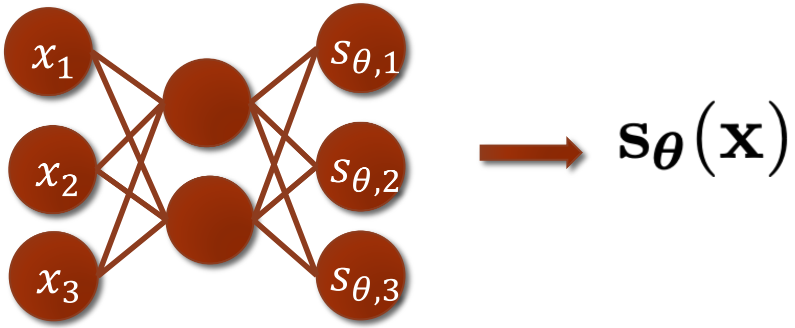

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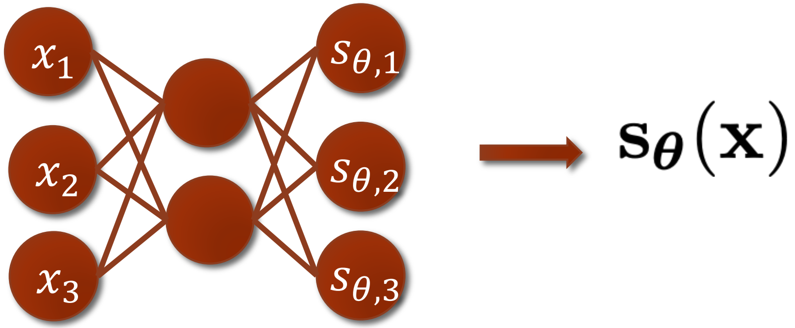

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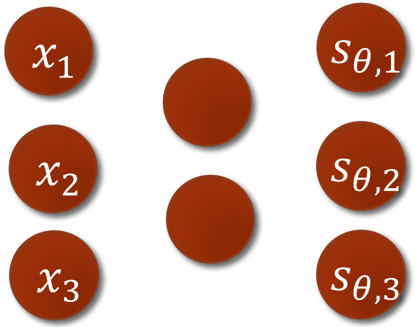

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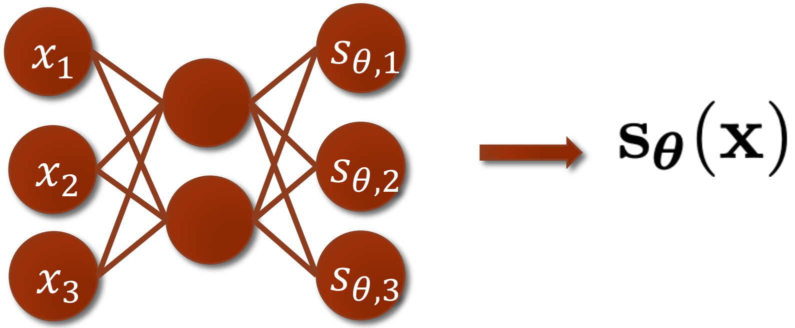

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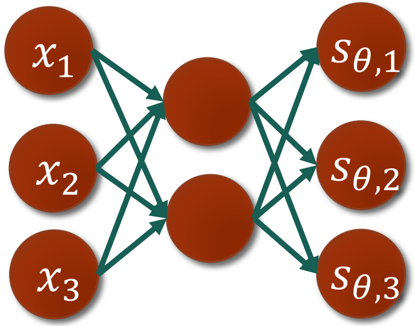

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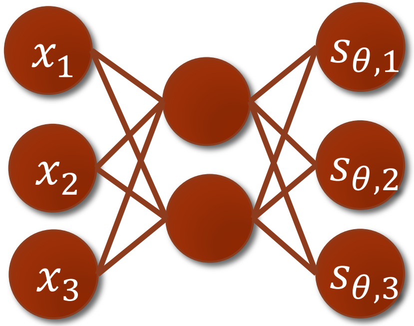

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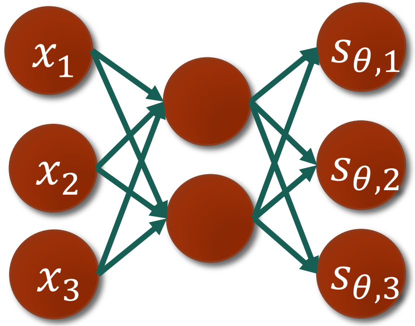

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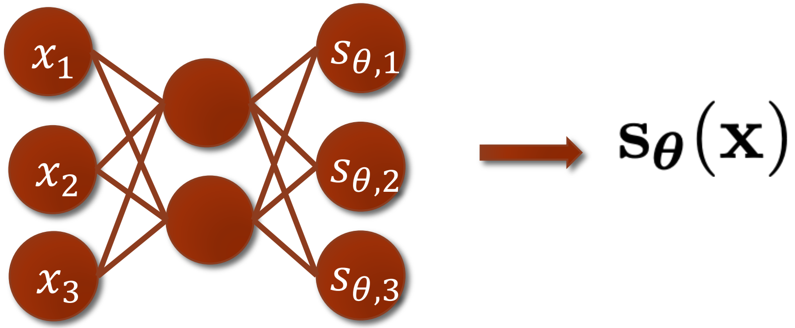

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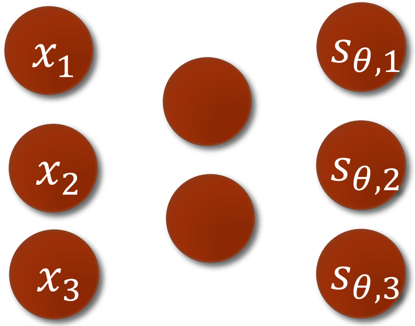

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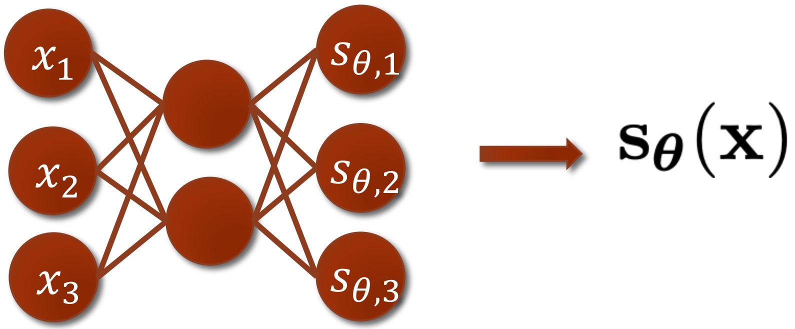

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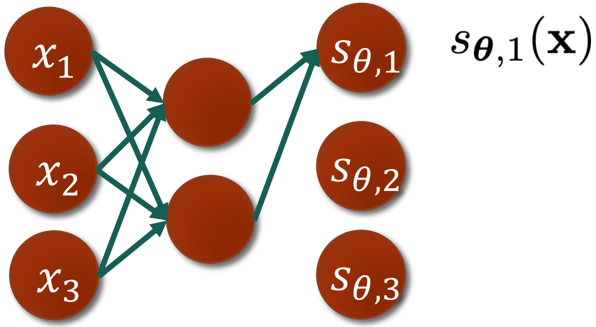

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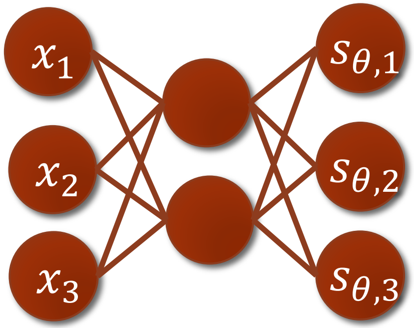
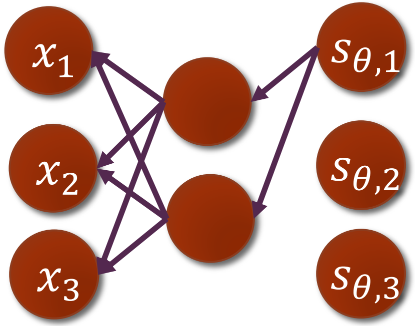


$$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$$

- Compute $\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2$ and $\operatorname{trace}(\nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$

$$\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}$$



$$\nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{pmatrix} \boxed{\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3} \end{pmatrix}$$

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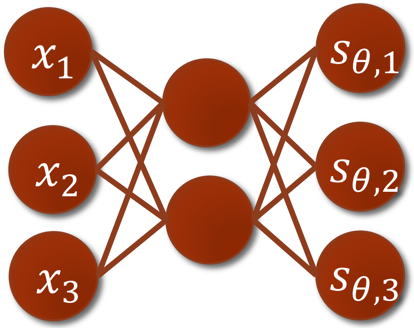
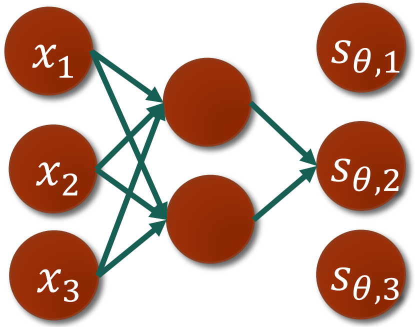


$$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$$

- Compute $\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2$ and $\operatorname{trace}(\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$

$$\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}$$

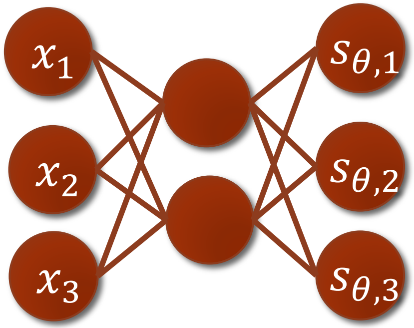


$$s_{\boldsymbol{\theta},2}(\mathbf{x})$$

$$\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{pmatrix} \boxed{\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3} \end{pmatrix}$$

Score Matching is not scalable

- Deep score models



$$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$$

- Compute $\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2$ and $\mathrm{trace}(\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$

$$\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}$$

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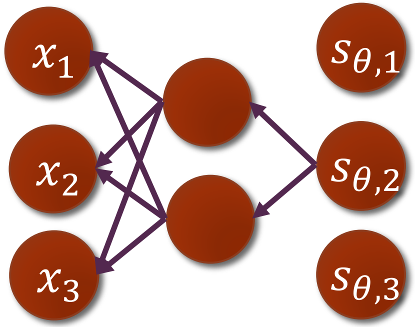

$$\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{pmatrix} \boxed{\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_1} & \boxed{\frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_2}} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3} \end{pmatrix}$$

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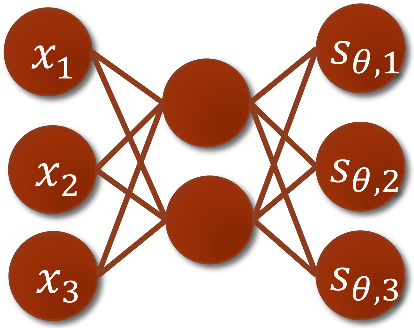

$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

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$$\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}$$

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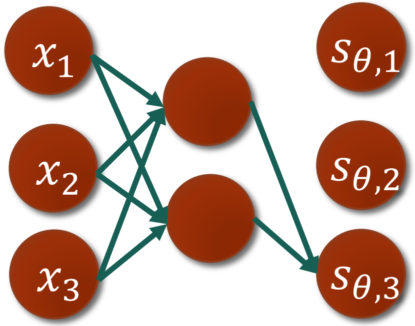
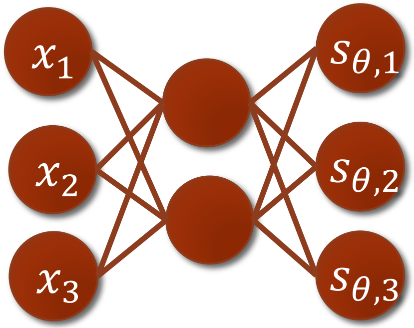


$s_{\boldsymbol{\theta},3}(\mathbf{x})$

$$\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{pmatrix} \boxed{\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_1} & \boxed{\frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_2}} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3} \end{pmatrix}$$

Score Matching is not scalable

- Deep score models



$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

- Compute $\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2$ and $\operatorname{trace}(\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$

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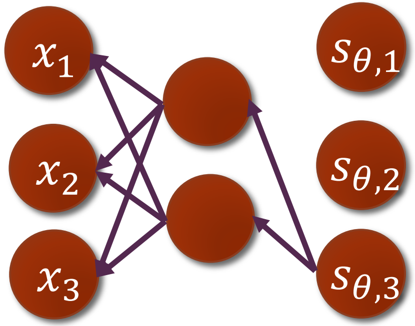
$$\frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3}$$



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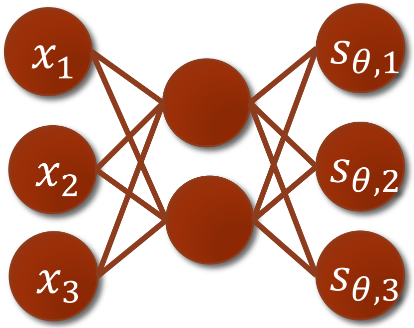

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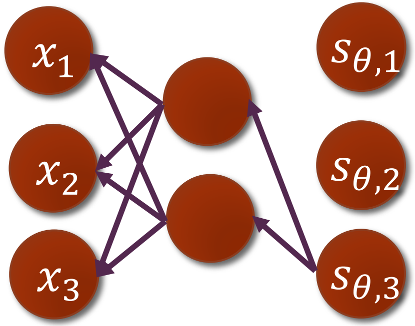

$O(D)$ Backprops!

$$\nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{pmatrix} \boxed{\frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_1}} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_2} & \frac{\partial s_{\boldsymbol{\theta},1}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_1} & \boxed{\frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_2}} & \frac{\partial s_{\boldsymbol{\theta},2}(\mathbf{x})}{\partial x_3} \\ \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_1} & \frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_2} & \boxed{\frac{\partial s_{\boldsymbol{\theta},3}(\mathbf{x})}{\partial x_3}} \end{pmatrix}$$

Score Matching is not scalable

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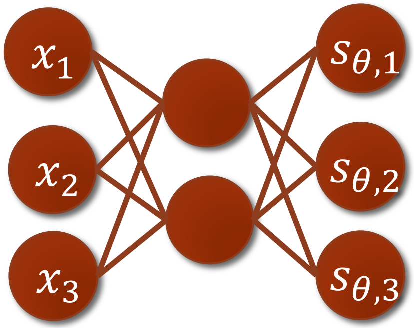

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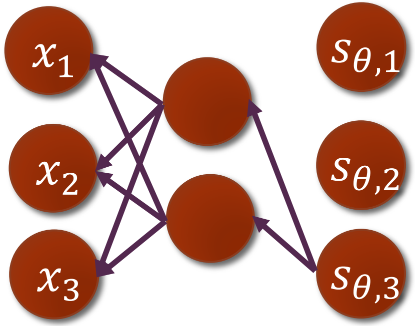

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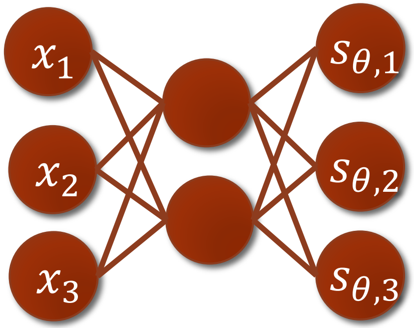
Score Matching is not scalable

- Deep score models



$\longrightarrow \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

Score Matching is not Scalable!

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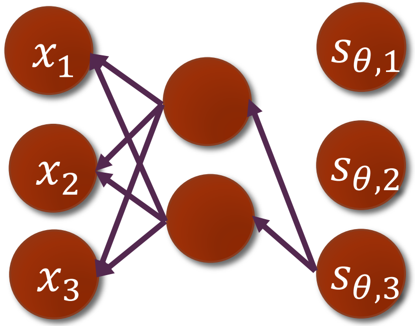

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Sliced score matching

- **Intuition:** one dimensional problems should be easier

Song*, Garg*, Shi, Ermon. "Sliced Score Matching: A Scalable Approach to Density and Score Estimation." UAI 2019.

Sliced score matching

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Sliced score matching

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- **Randomized objective: Sliced Fisher Divergence**

$$\frac{1}{2}\mathbb{E}_{p_{\mathbf{v}}}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\left(\mathbf{v}^{\intercal}\nabla_{\mathbf{x}}\log p_{\text{data}}(\mathbf{x}) - \mathbf{v}^{\intercal}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\right)^2\right]$$

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- Integration by parts → **Sliced Score Matching**:

$$\mathbb{E}_{p_{\mathbf{v}}}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\left[\mathbf{v}^\intercal\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\mathbf{v} + \frac{1}{2}\left(\mathbf{v}^\intercal\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\right)^2\right]$$

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Computing Jacobian-vector products is scalable

$$\mathbf{v}^\intercal \nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) \mathbf{v} = \mathbf{v}^\intercal \nabla_{\mathbf{x}} (\mathbf{v}^\intercal \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$$

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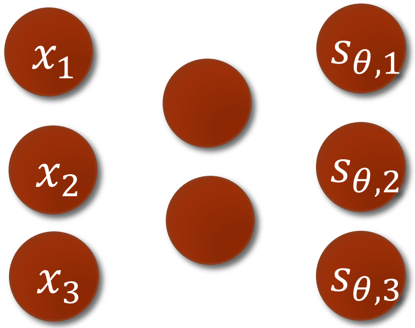

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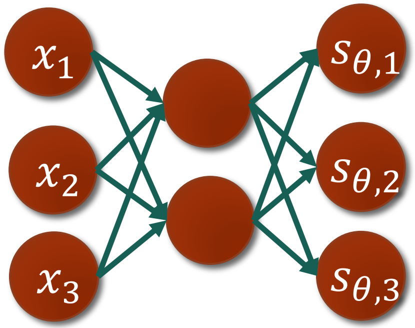

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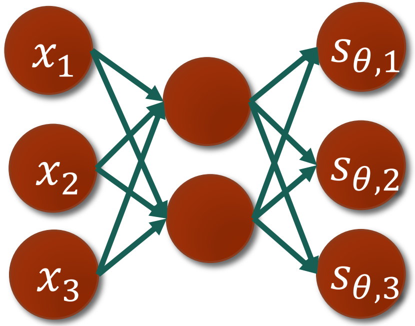

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

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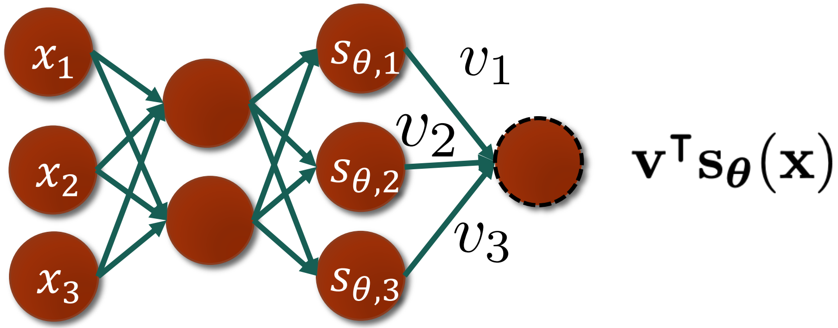

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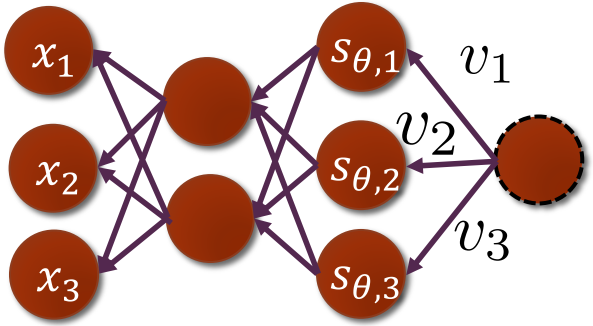
$\nabla_{\mathbf{x}}(\mathbf{v}^\intercal \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}))$



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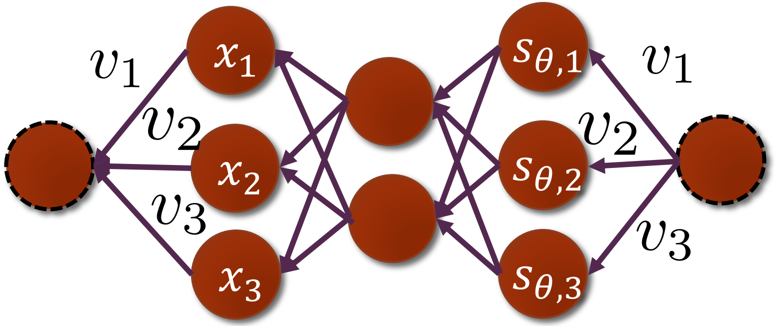

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One Backprop!

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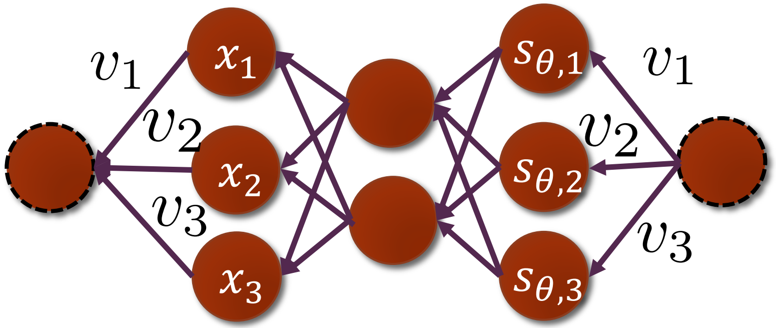

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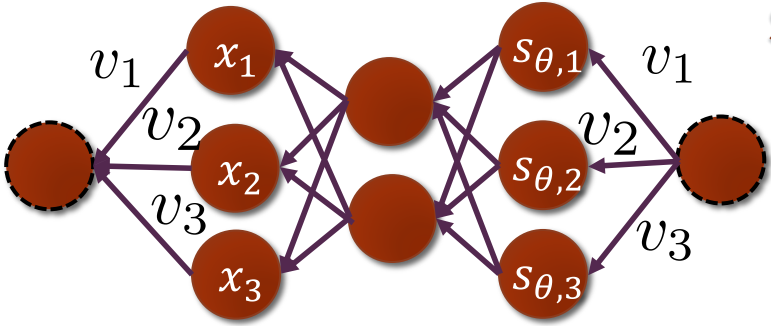

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Sliced Score Matching is scalable

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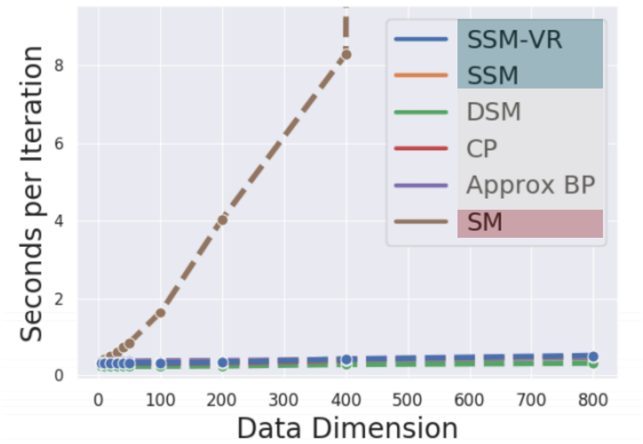
Results: Sliced Score Matching for EBMs

Sliced score matching methods	Other Baselines	Score Matching



Efficiency

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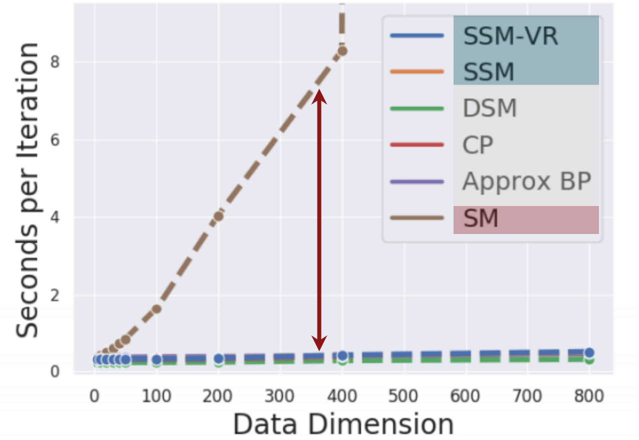

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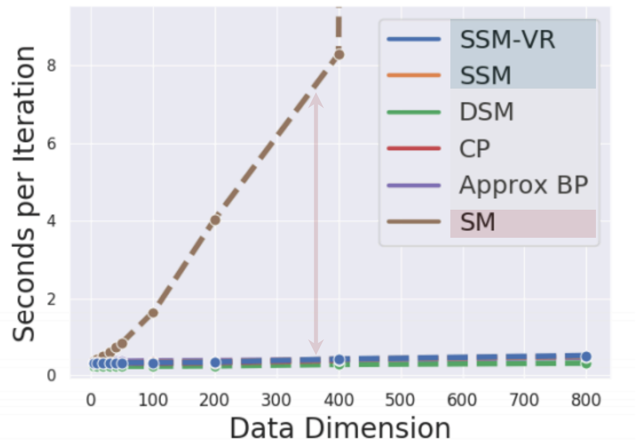

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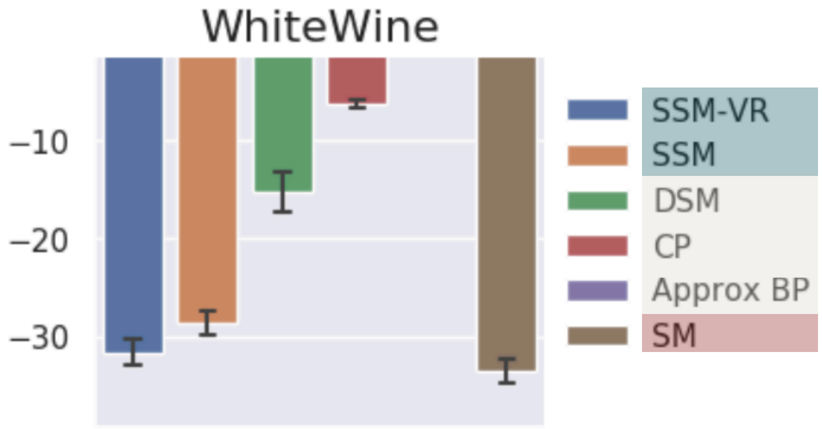

Performance on density estimation

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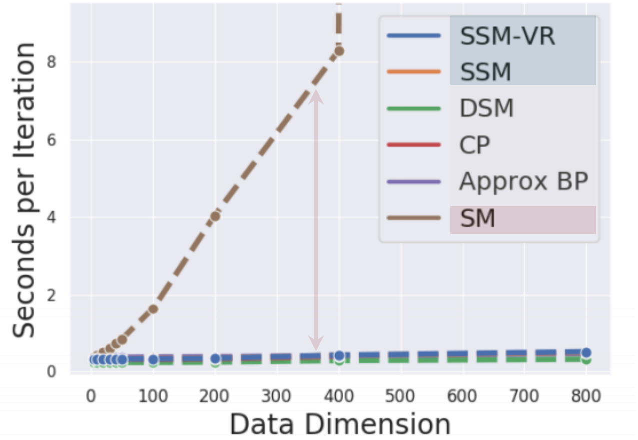

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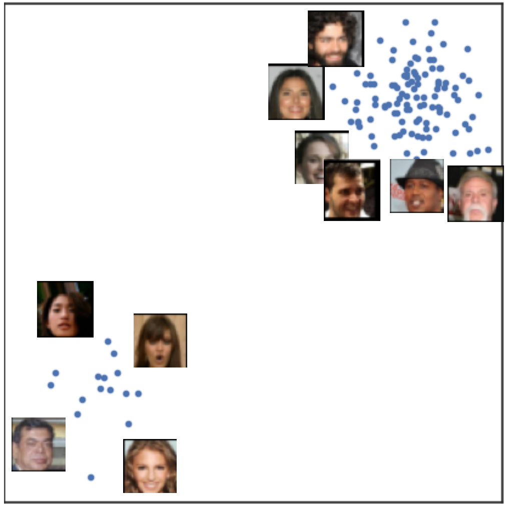
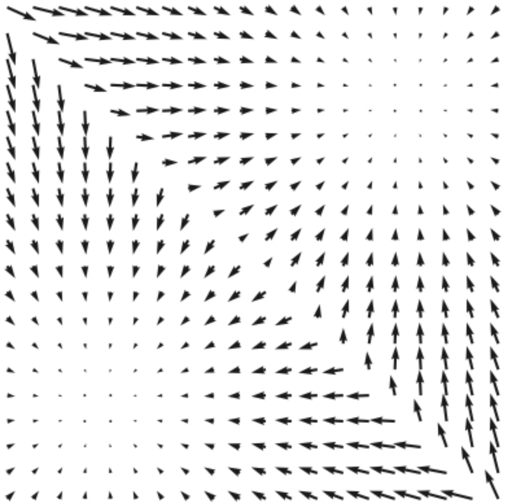
Score-based generative modeling



Data samples

$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p_{\text{data}}(\mathbf{x})$

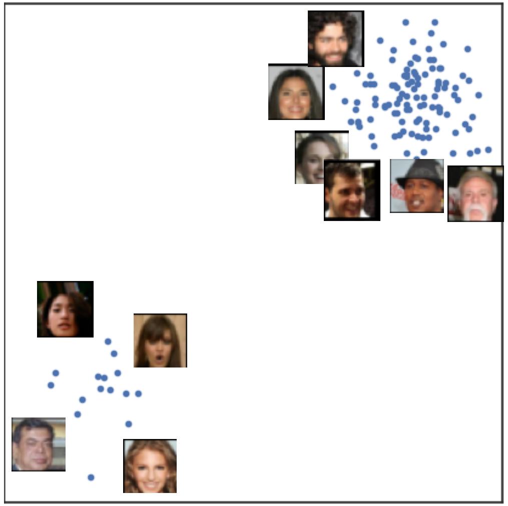
Score Matching



Scores

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$

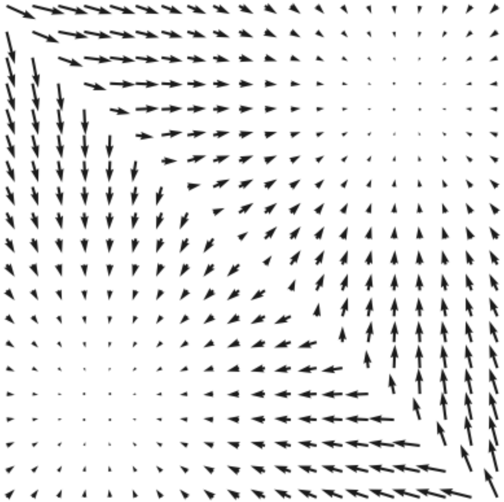
Score-based generative modeling



Data samples

$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p_{\text{data}}(\mathbf{x})$

Score Matching



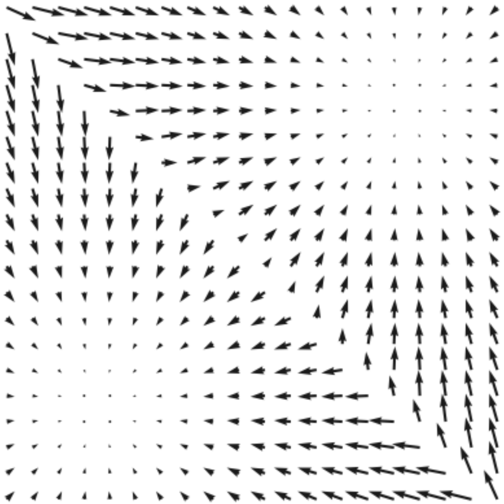
Scores

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$

?

New samples

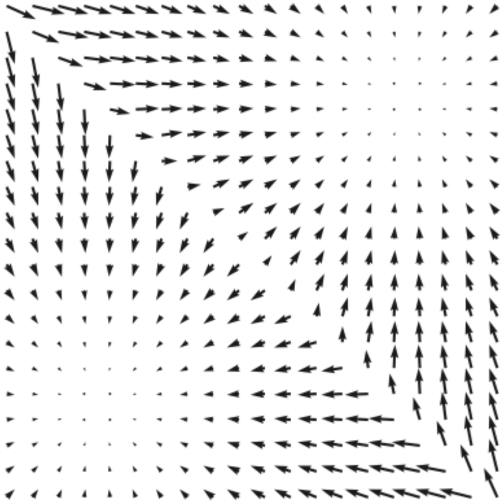
From scores to samples: Langevin MCMC



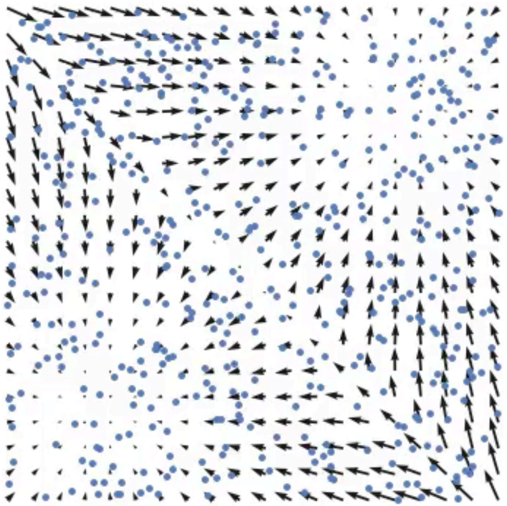
Scores

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

From scores to samples: Langevin MCMC



Scores

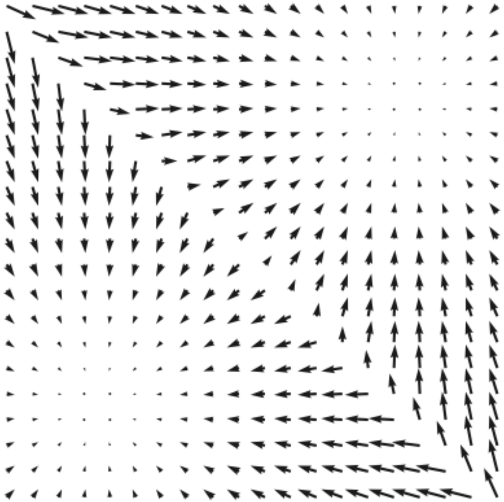


Follow the scores

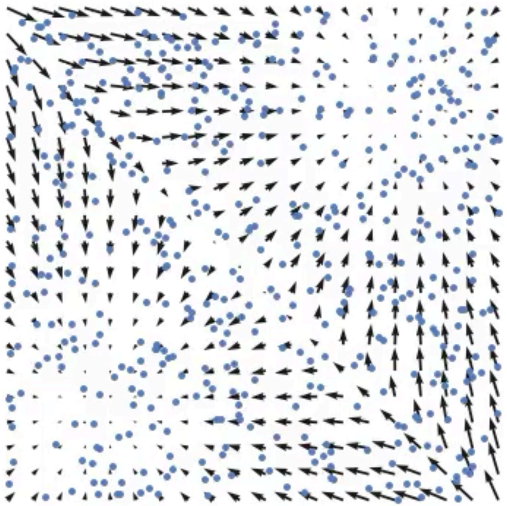
$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$

$$\tilde{\mathbf{x}}_{t+1} \leftarrow \tilde{\mathbf{x}}_t + \frac{\epsilon}{2}\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_t)$$

From scores to samples: Langevin MCMC



Scores



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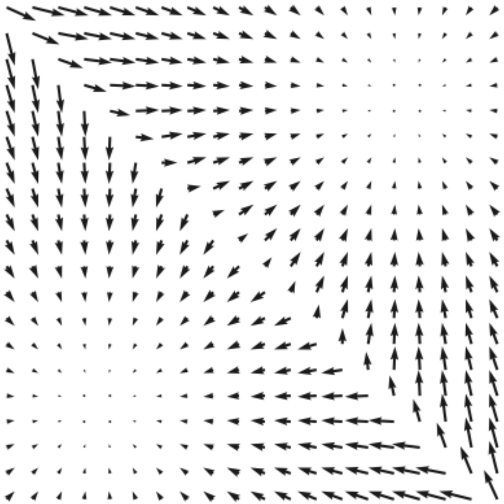
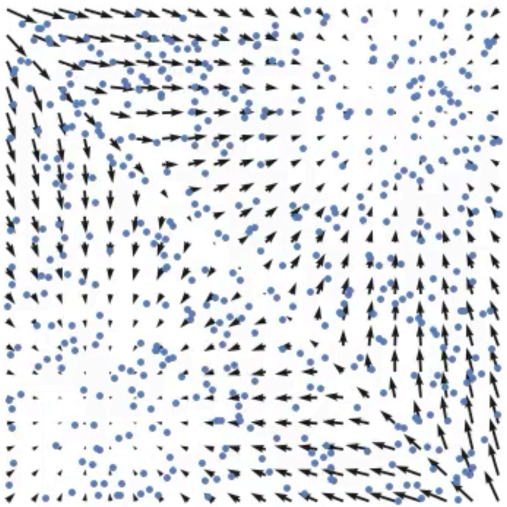


Scores

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$



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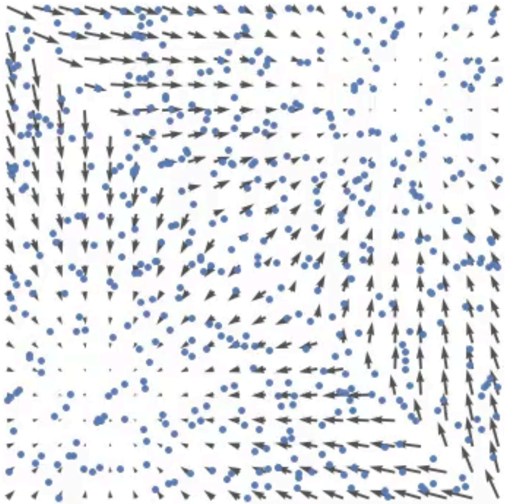
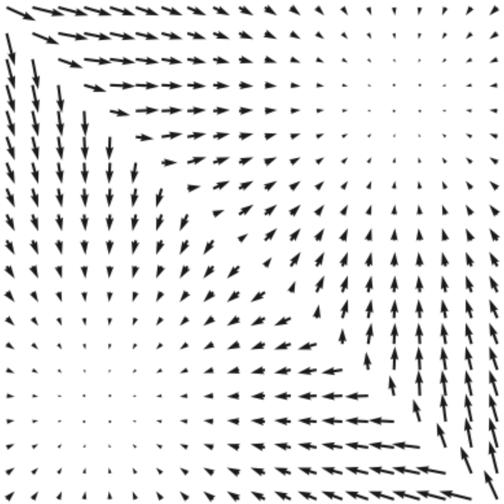


Follow noisy scores:
Langevin MCMC

$$\mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

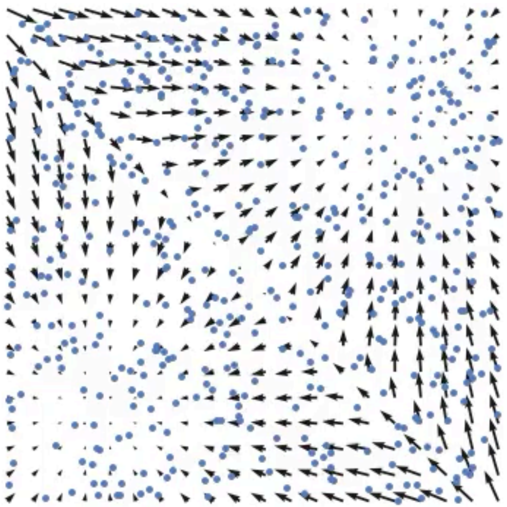
$$\tilde{\mathbf{x}}_{t+1} \leftarrow \tilde{\mathbf{x}}_t + \frac{\epsilon}{2}\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_t) + \sqrt{\epsilon}\,\mathbf{z}_t$$

From scores to samples: Langevin MCMC



Scores

$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})$



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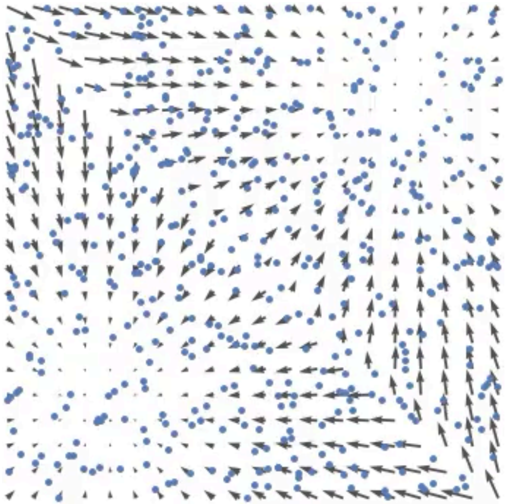

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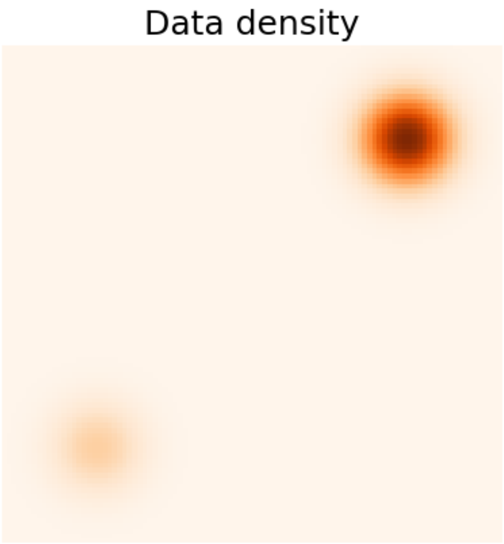
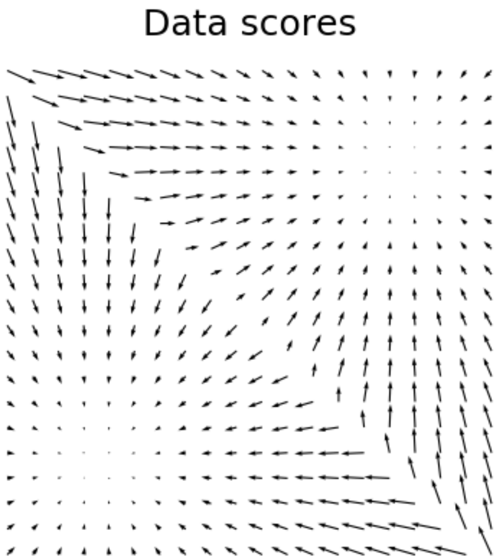
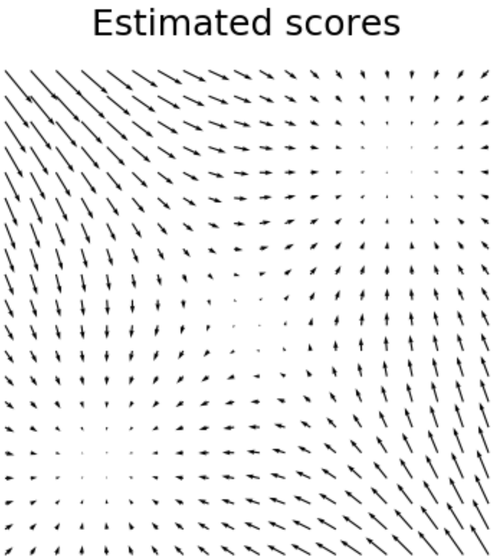
Challenge in low data density regions

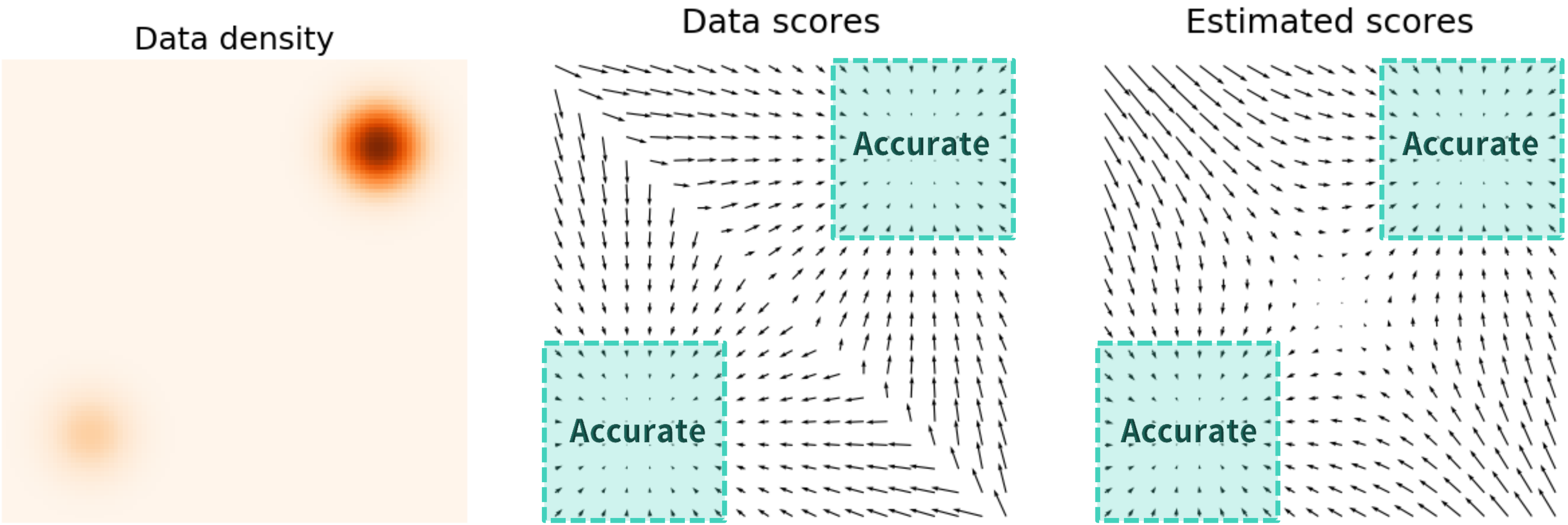






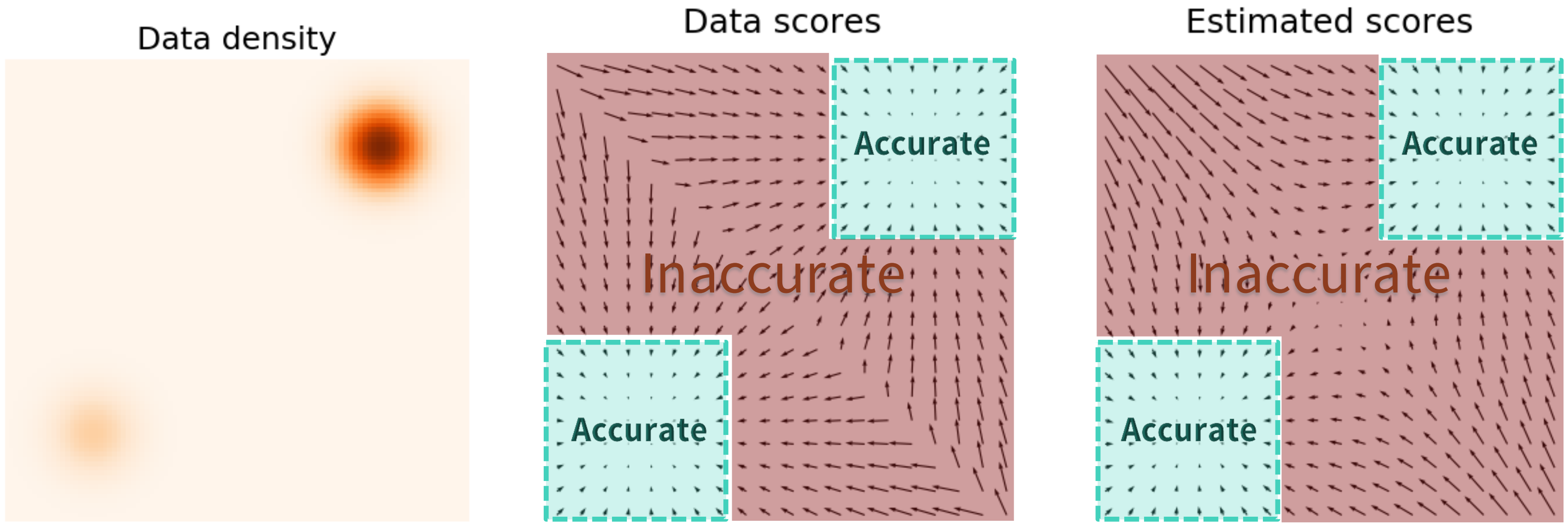
Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Challenge in low data density regions



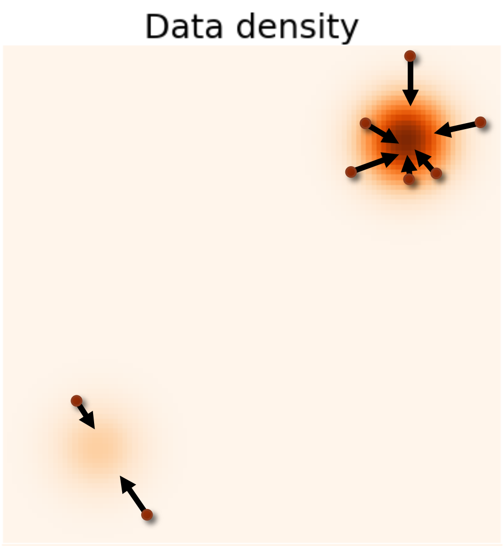
Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

Challenge in low data density regions

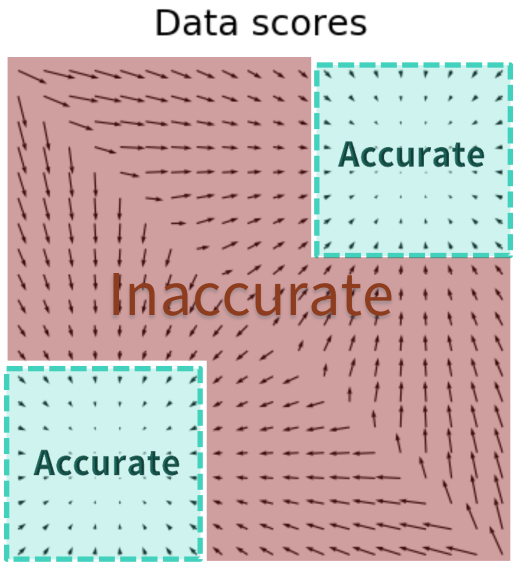


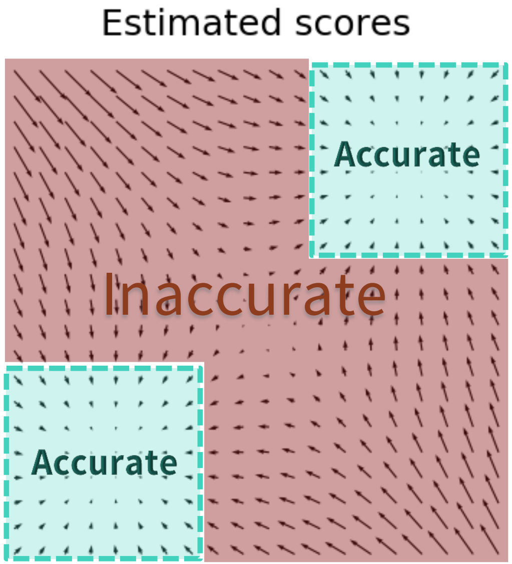
Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Challenge in low data density regions



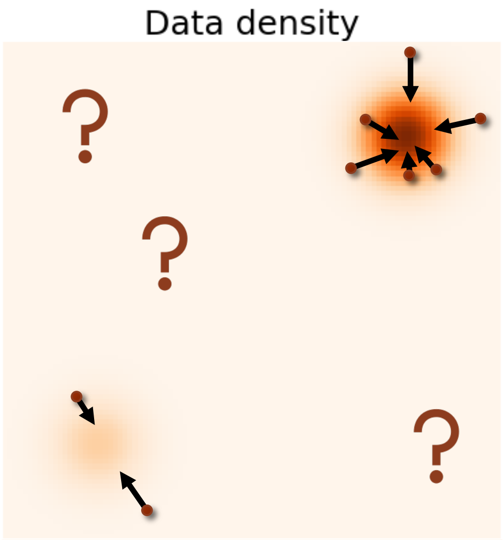
$$\frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2]$$



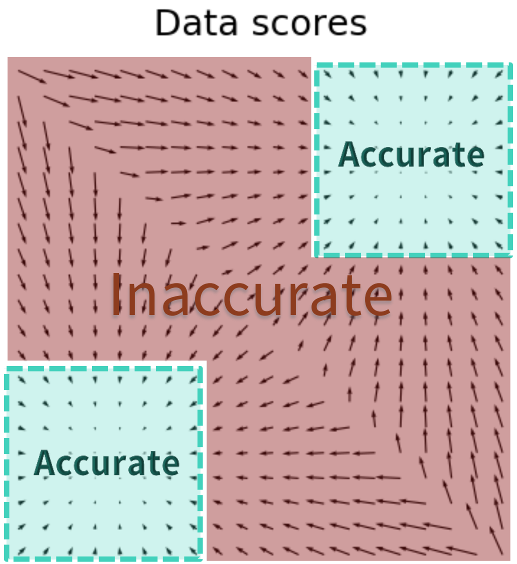


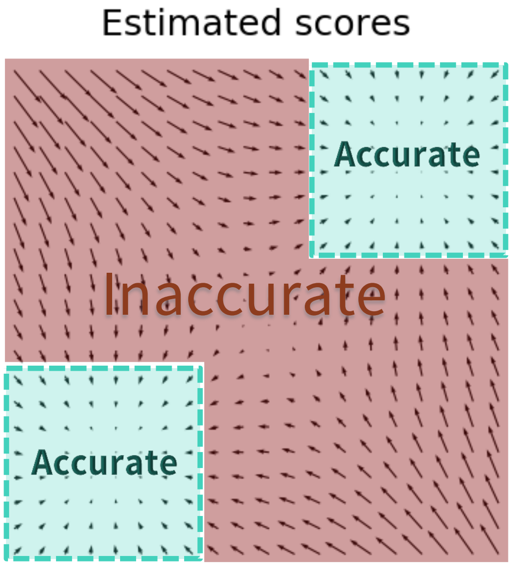
Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Challenge in low data density regions



$$\frac{1}{2}\mathbb{E}_{p_{\mathrm{data}}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\mathrm{data}}(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2]$$





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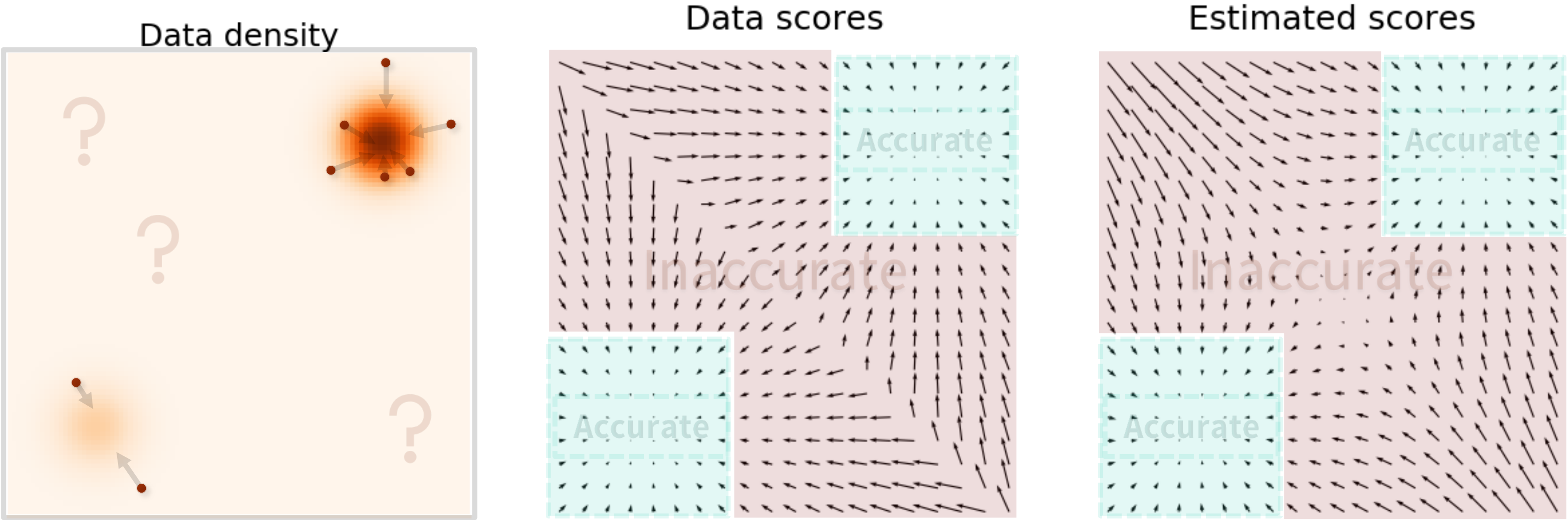
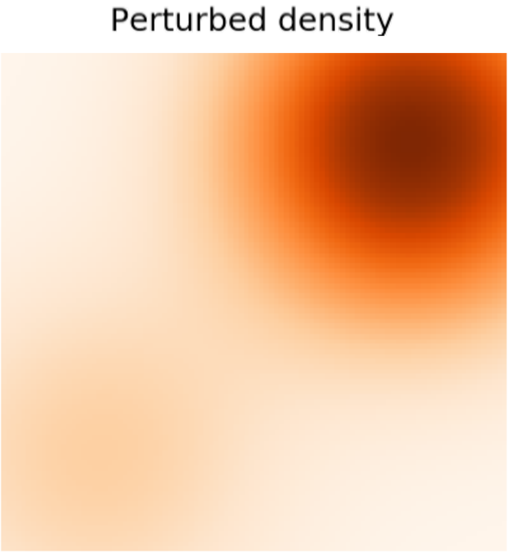


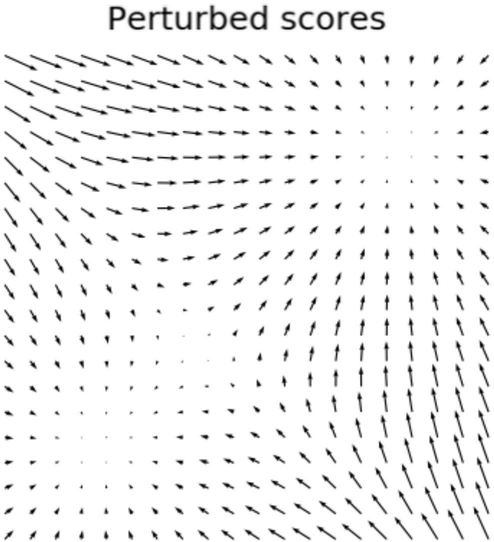
$$\frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2]$$

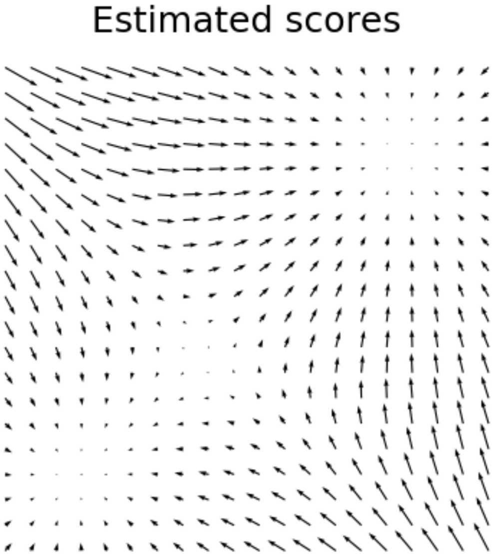
Langevin MCMC will have trouble exploring low density regions

Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Adding noise to data







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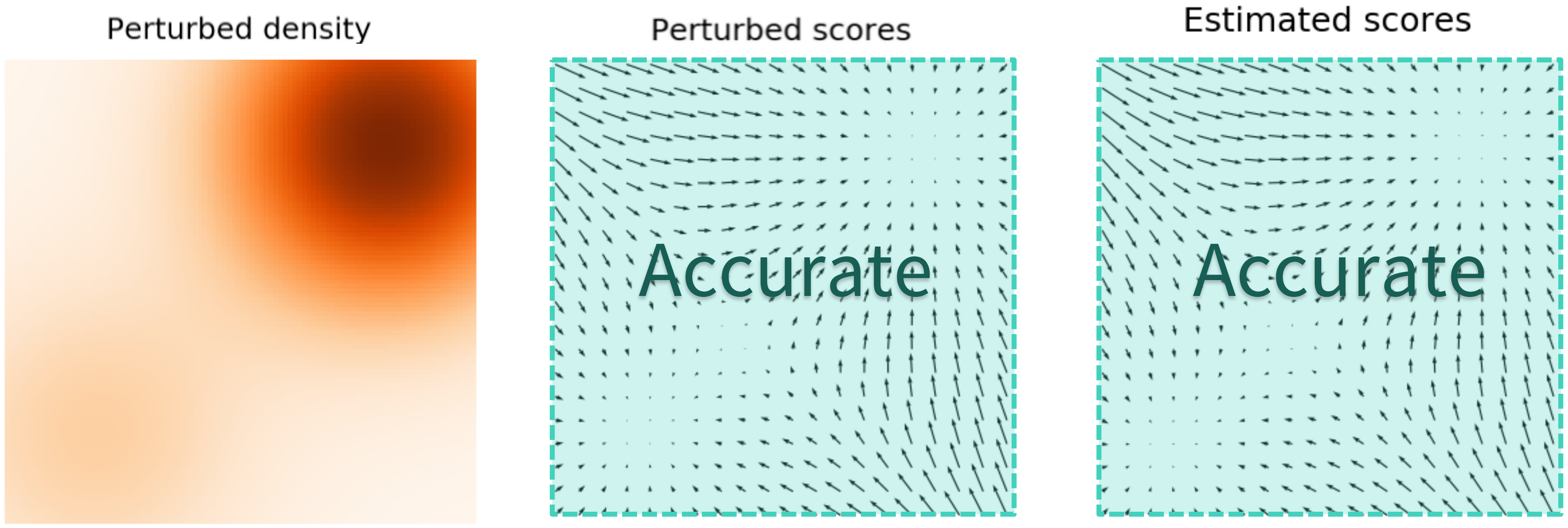

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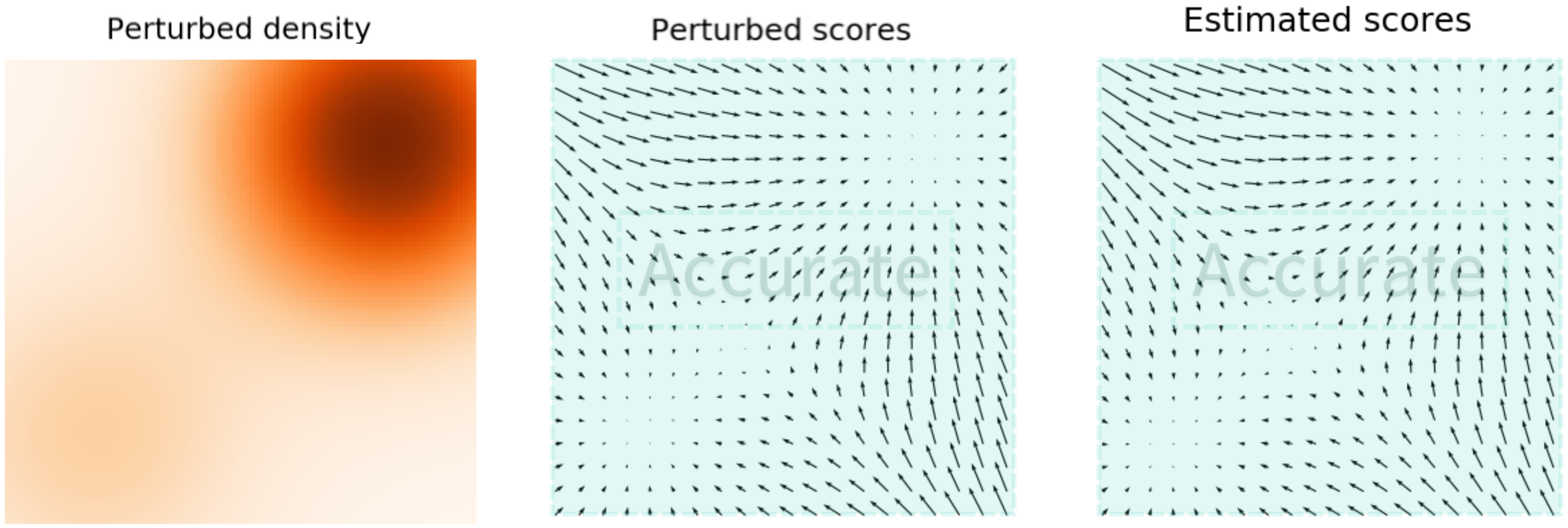
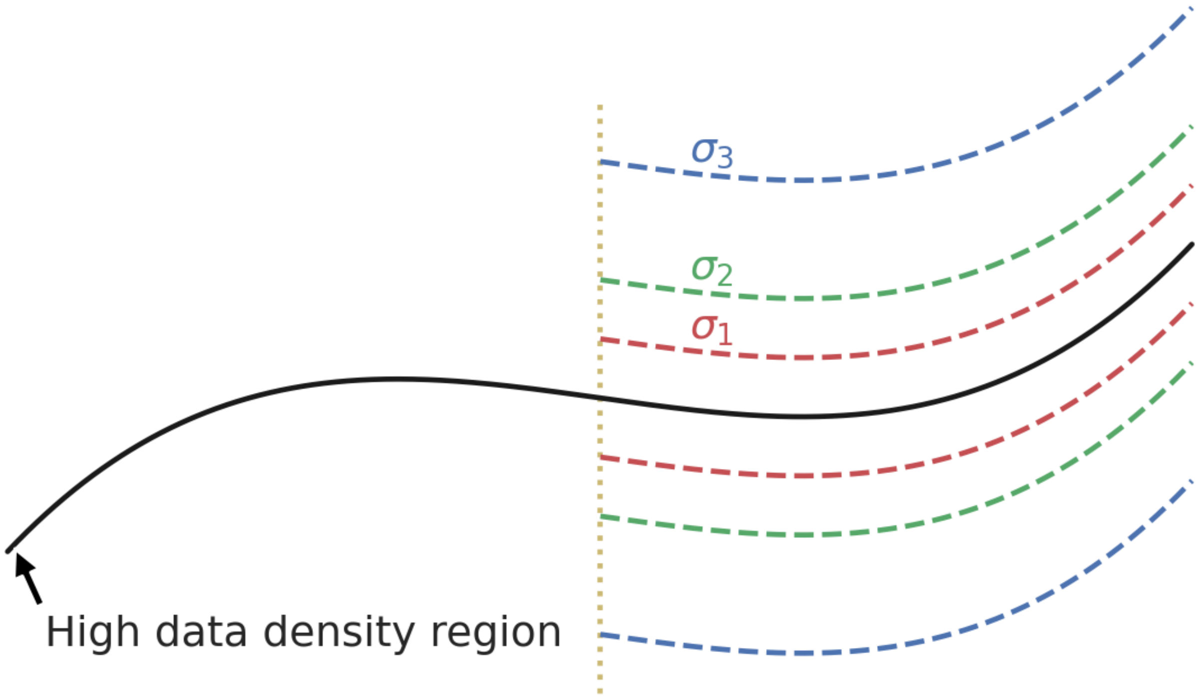


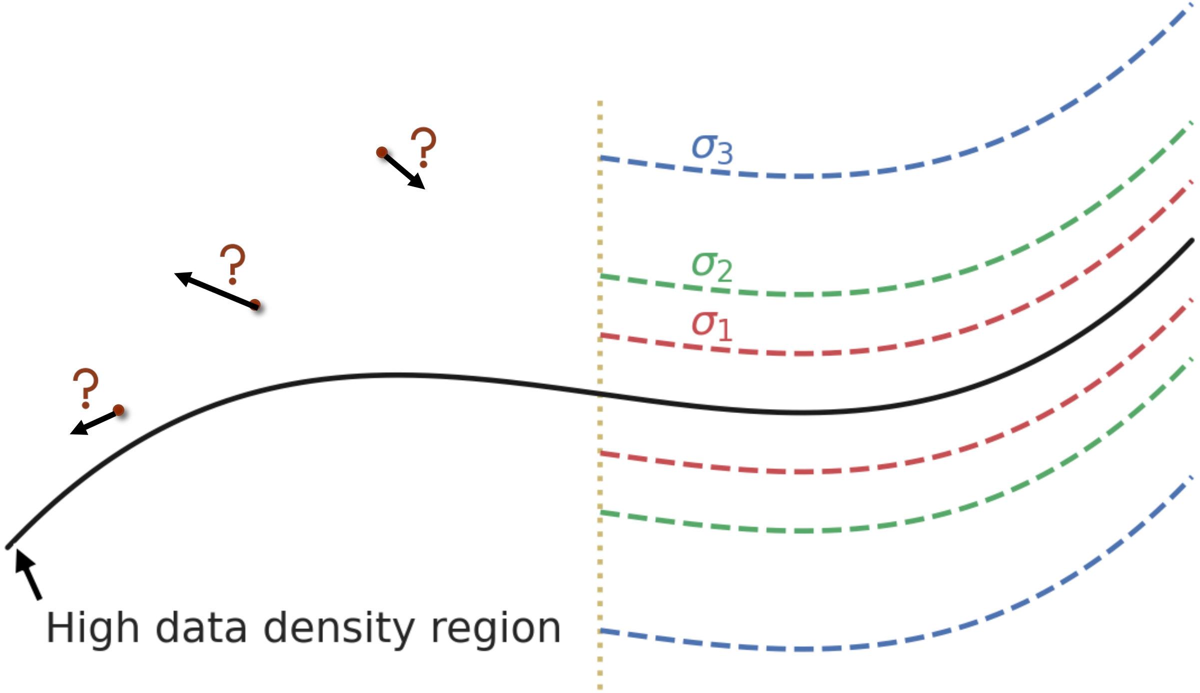
Provide useful directional information for Langevin MCMC.

Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

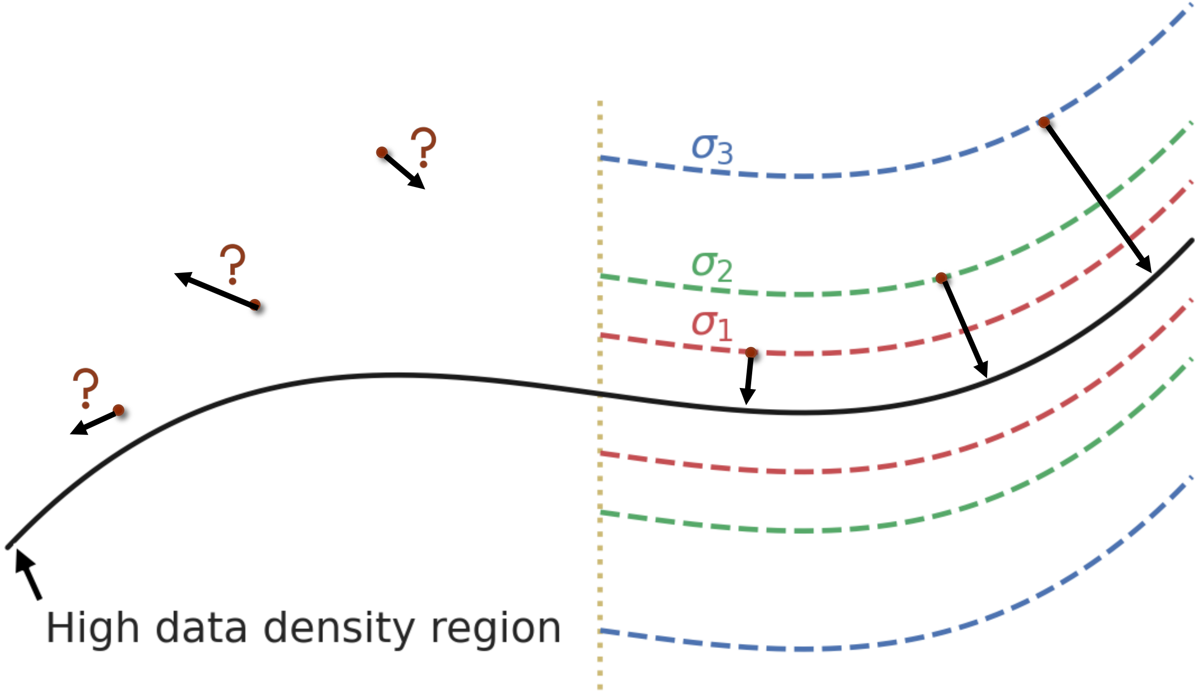
Using multiple noise scales



Using multiple noise scales



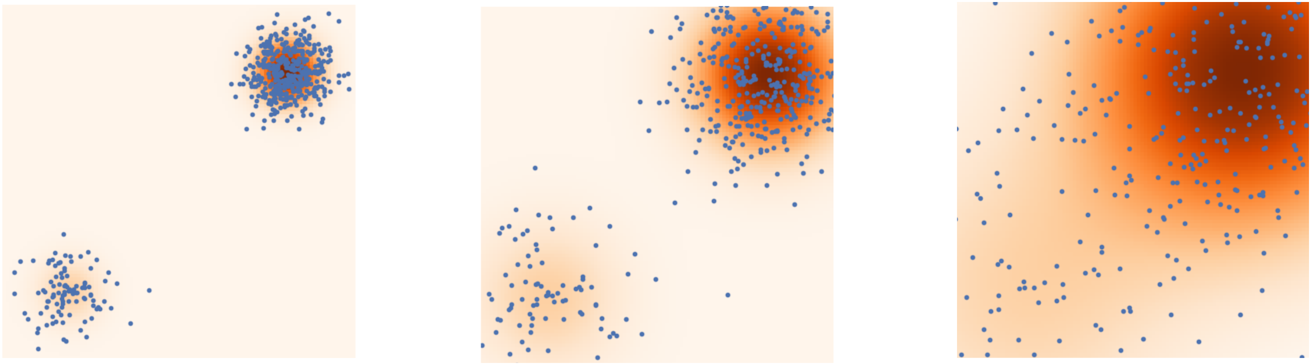
Using multiple noise scales



Using multiple noise scales

$\sigma_1 < \sigma_2 < \sigma_3$

Data



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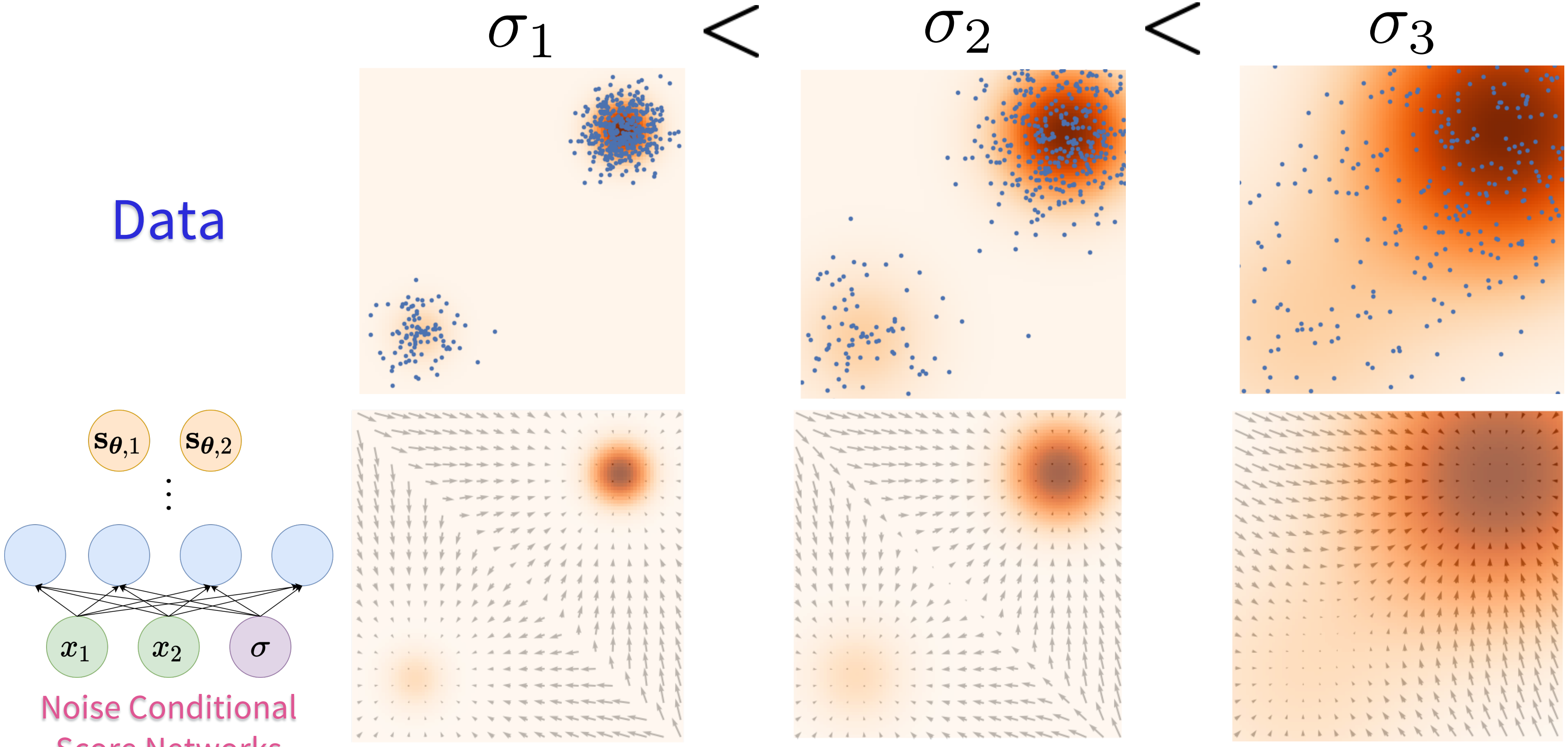
Using multiple noise scales



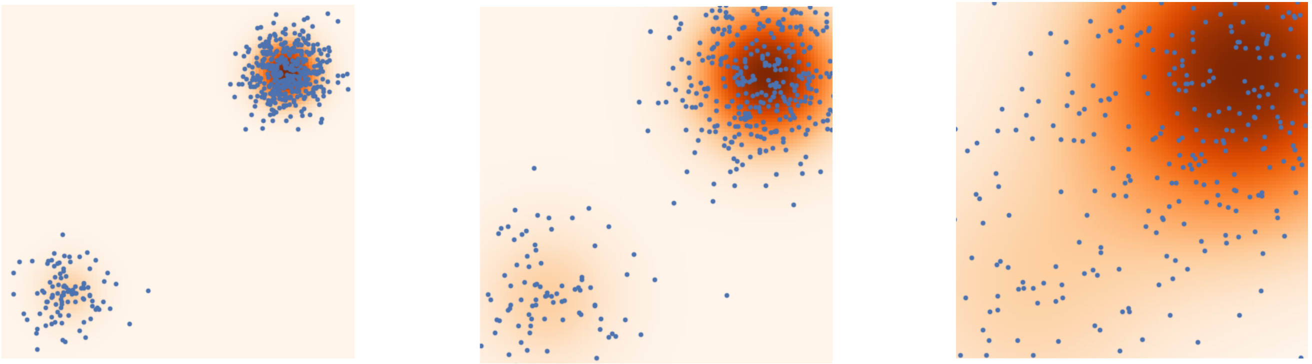
Noise Conditional Score Networks (NCSN)

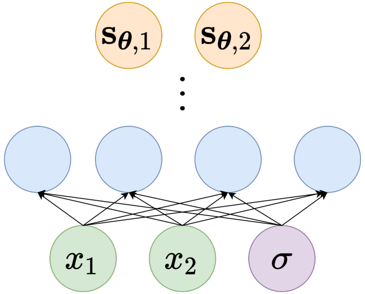
Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

Using multiple noise scales

$\sigma_1 < \sigma_2 < \sigma_3$

Data





Noise Conditional Score Networks (NCSN)

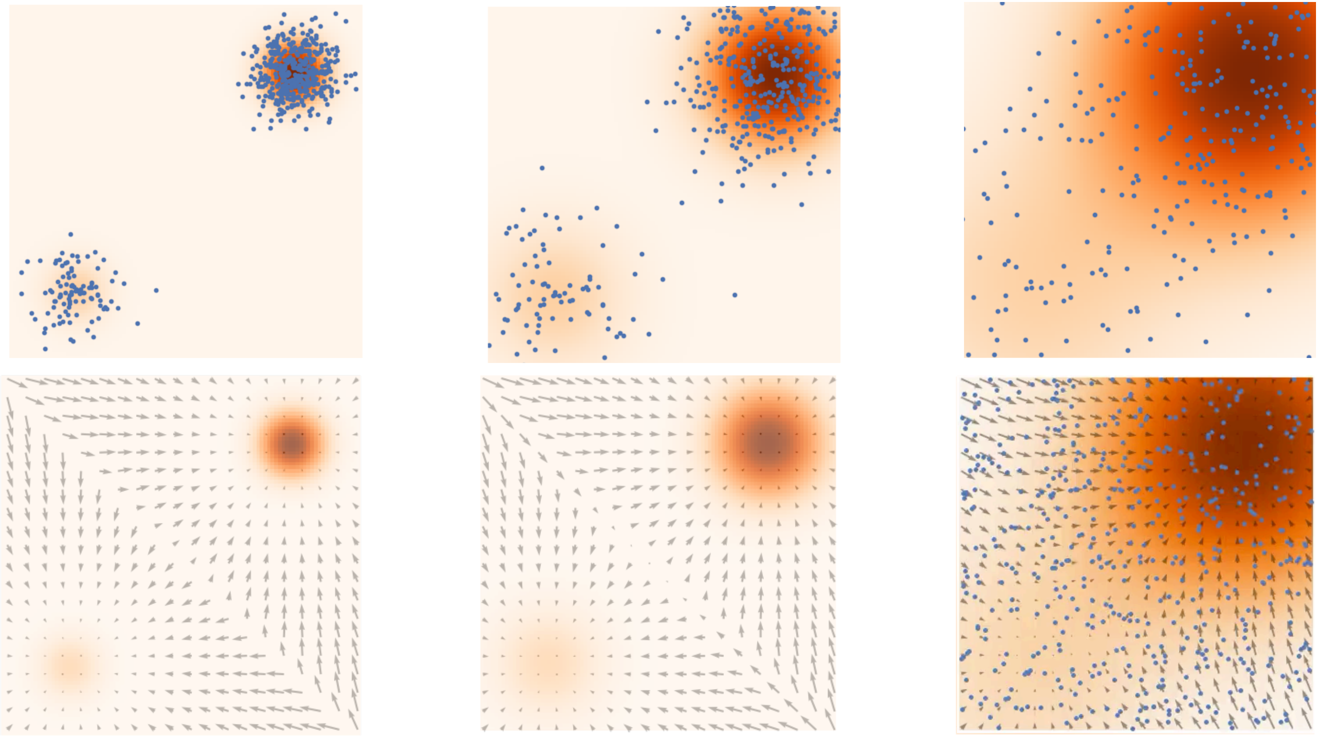
$$\sum_{i=1}^{N} \lambda(\sigma_i)\mathbb{E}_{p_{\sigma_i}(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p_{\sigma_i}(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, \sigma_i)\|_2^2]$$

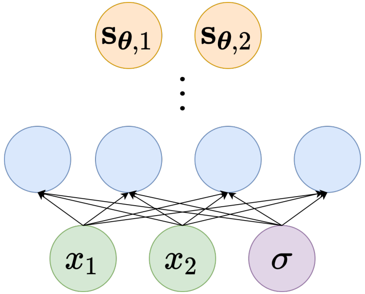
Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

Using multiple noise scales

$$\sigma_1 < \sigma_2 < \sigma_3$$

Data





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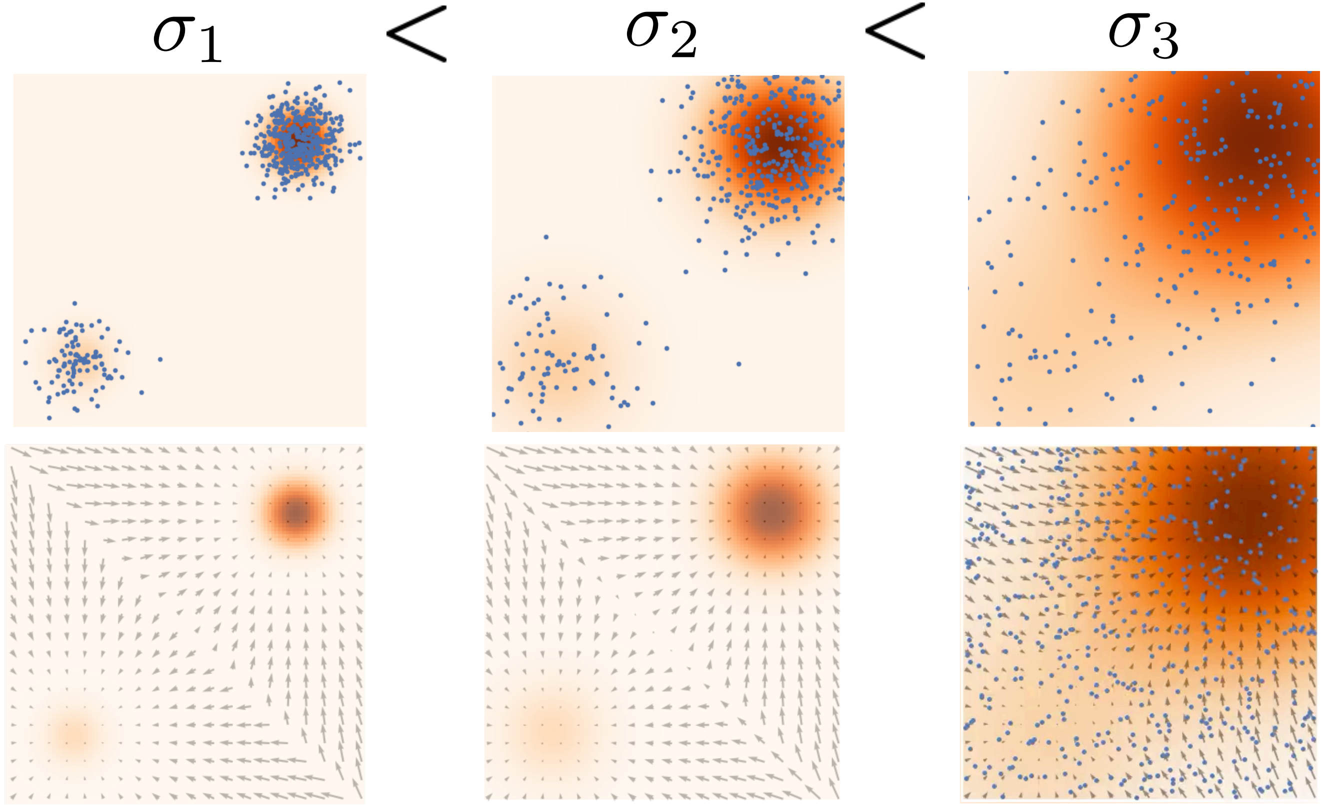
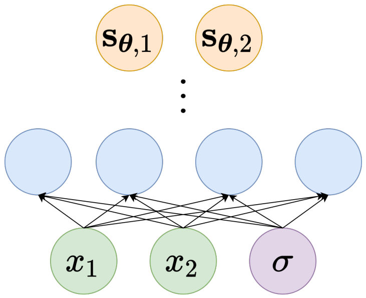
Using multiple noise scales





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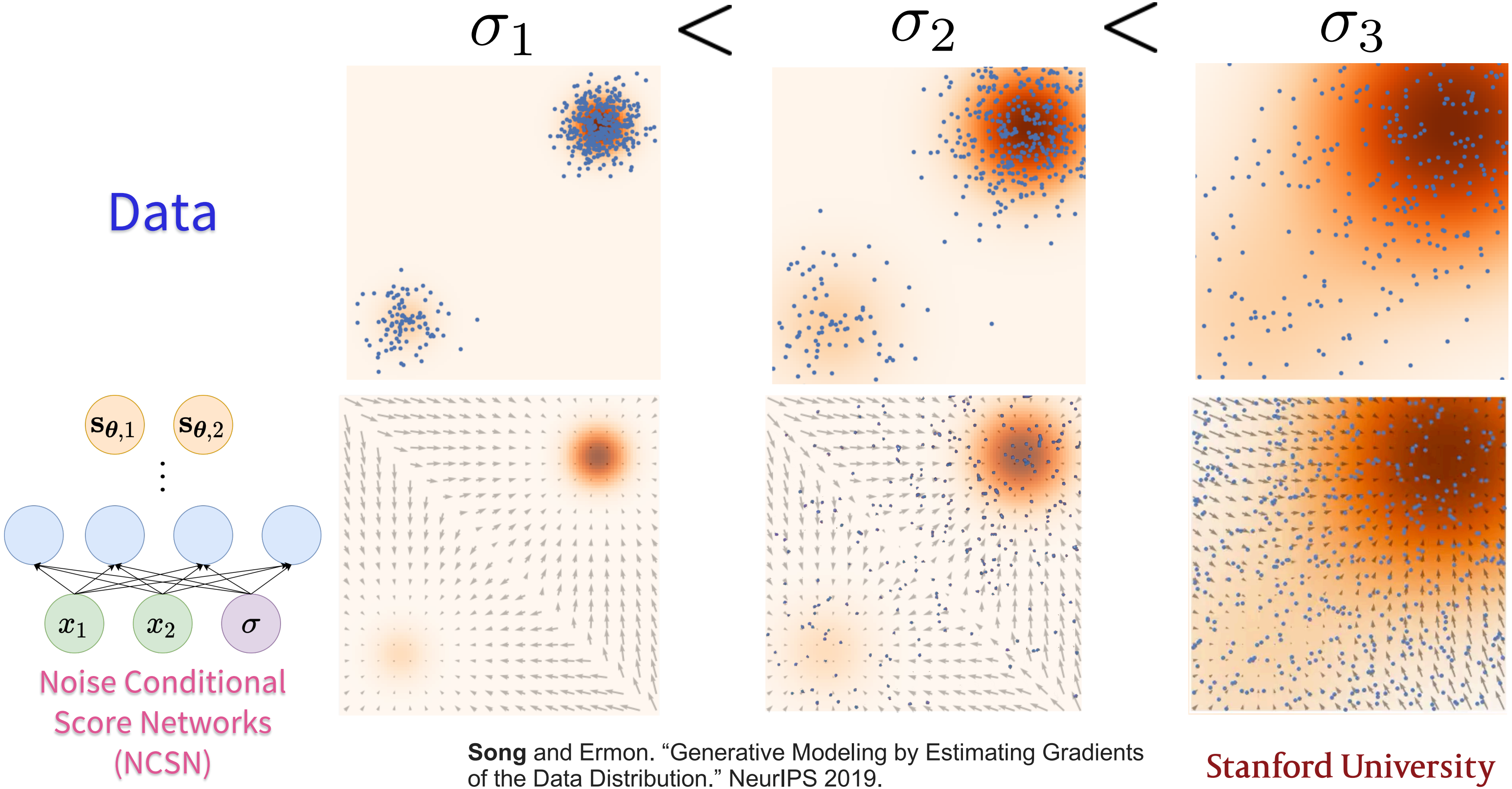
Using multiple noise scales

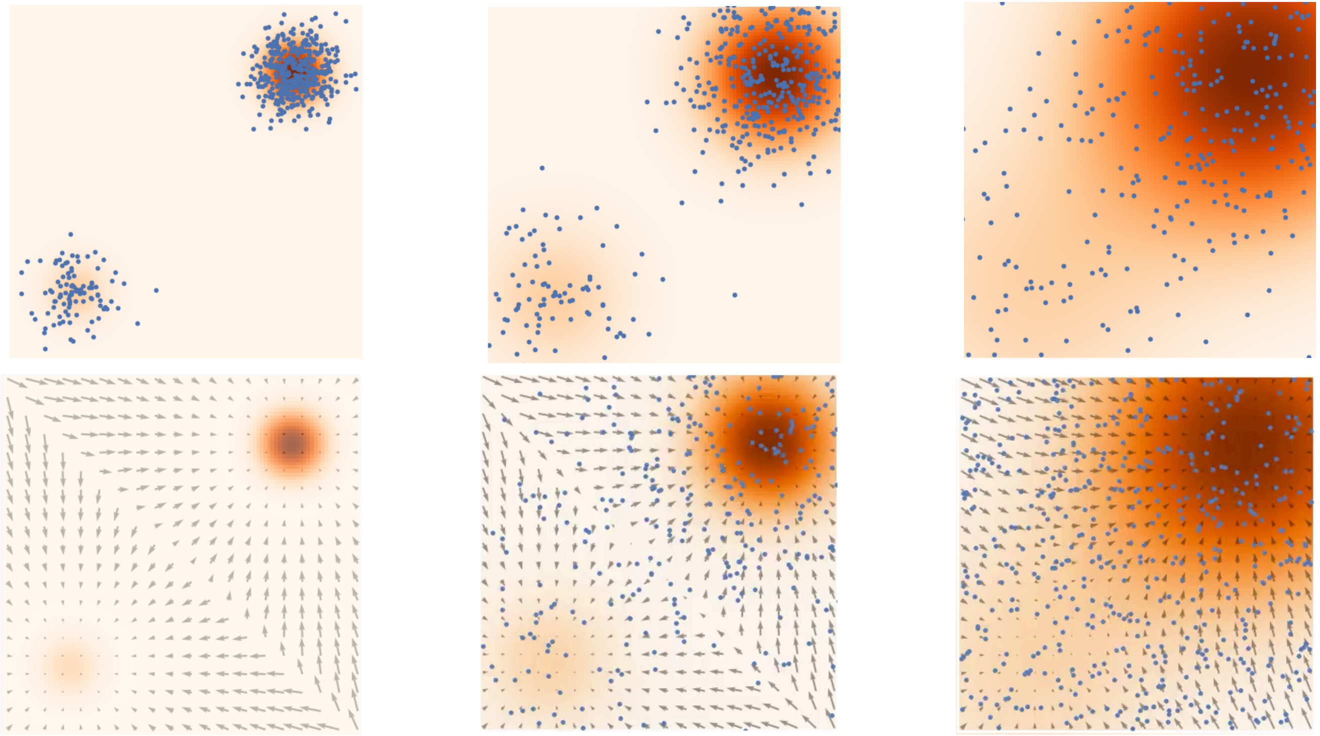


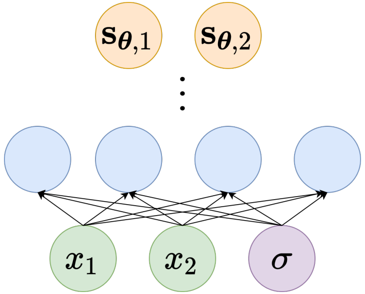
Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

Using multiple noise scales

$$\sigma_1 < \sigma_2 < \sigma_3$$

Data





Noise Conditional Score Networks (NCSN)

Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

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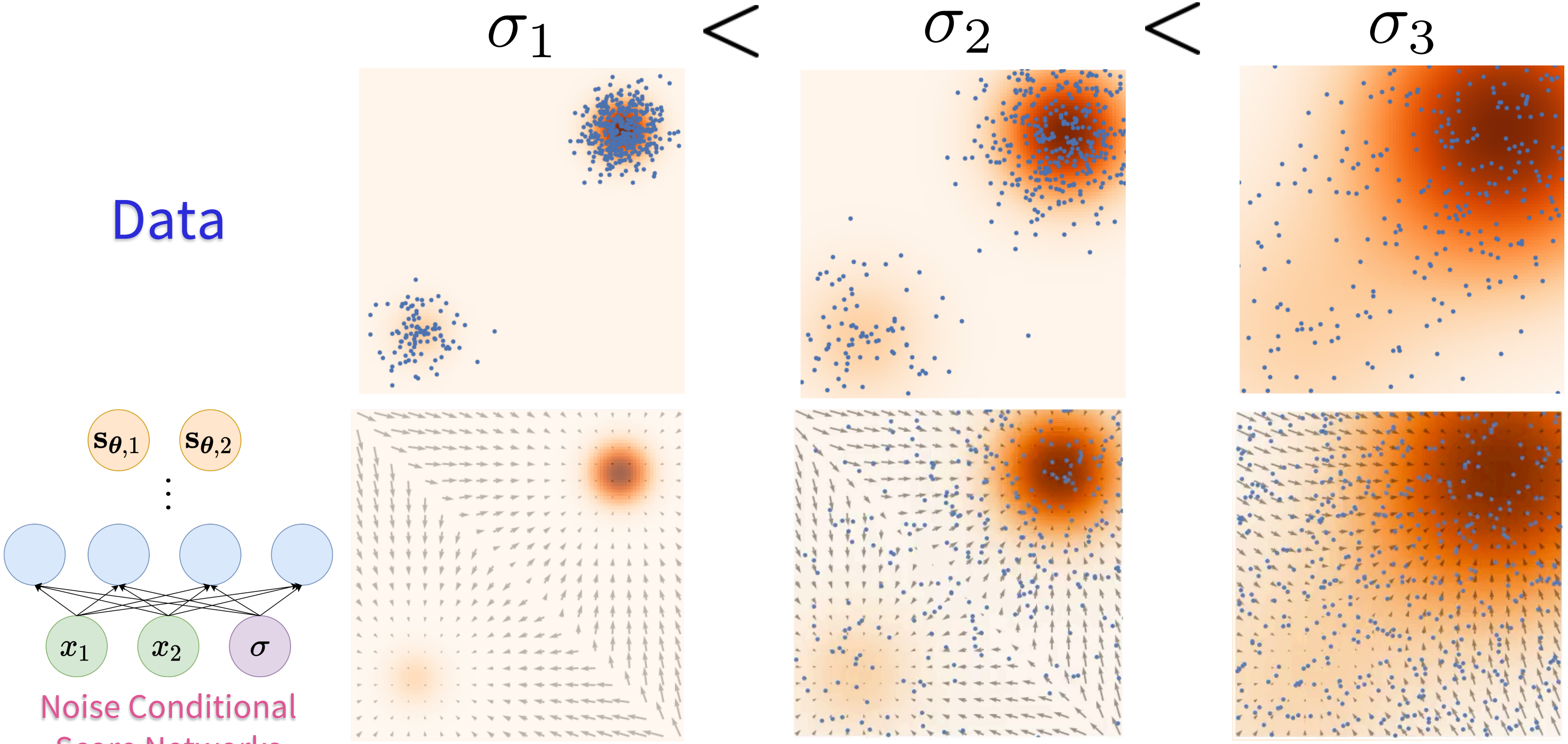

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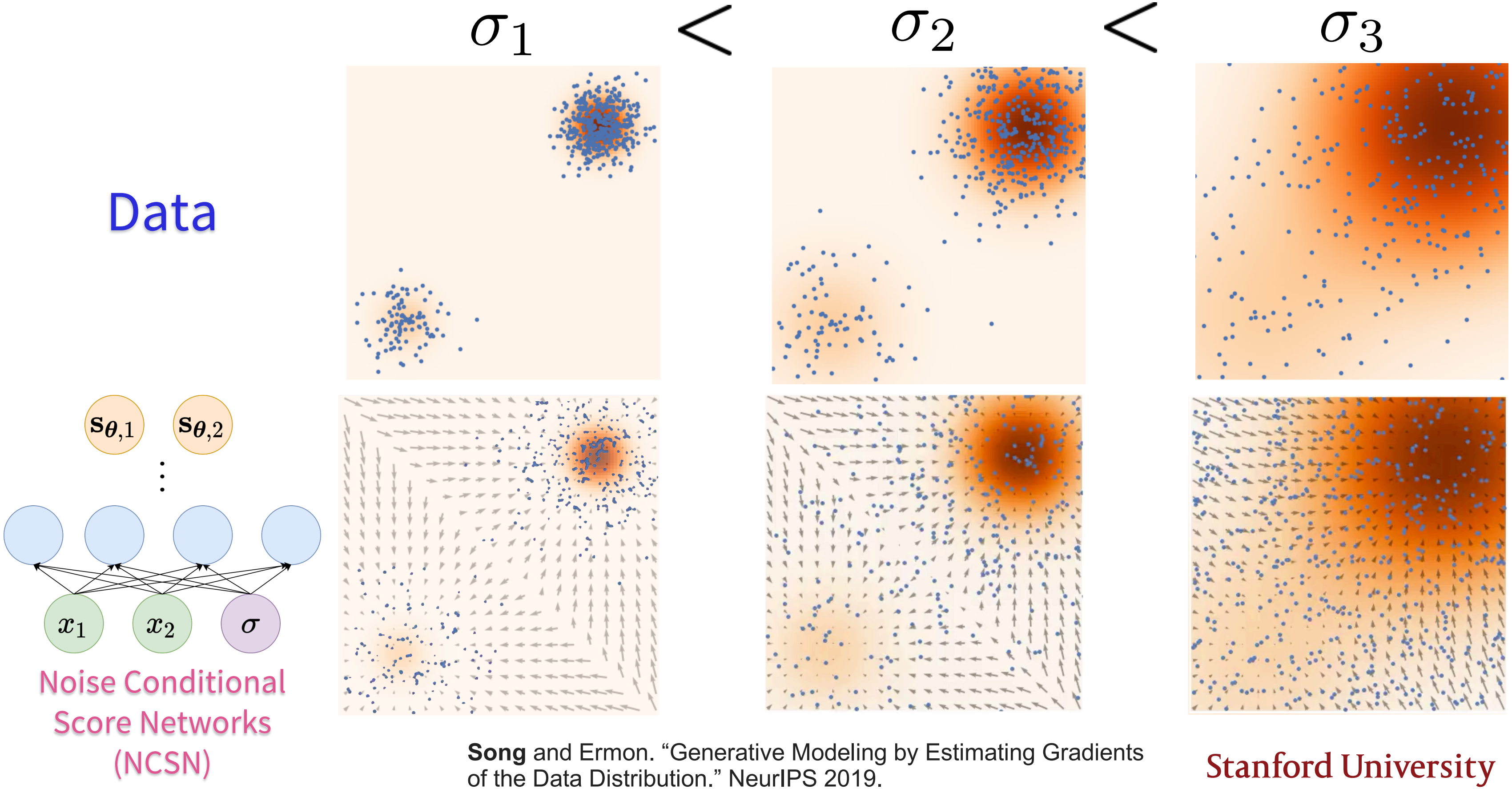

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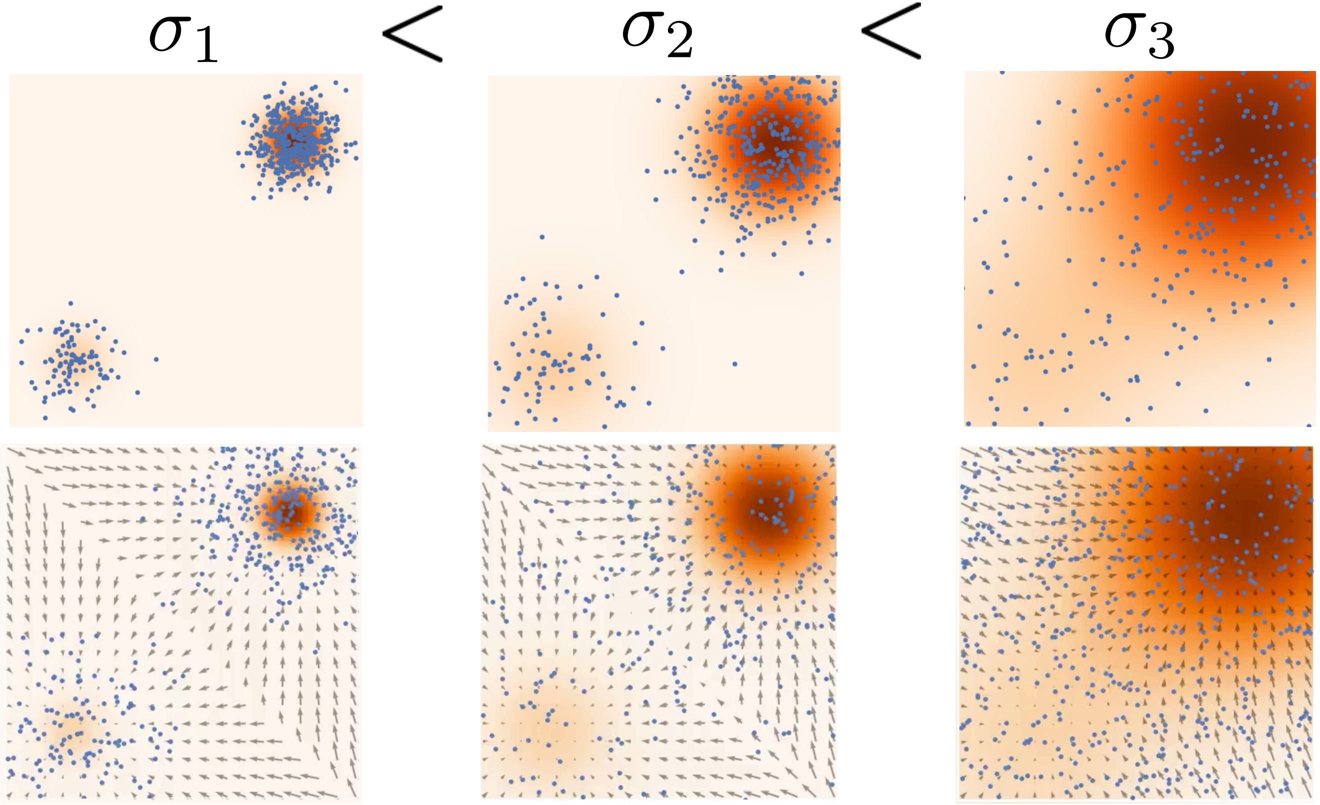
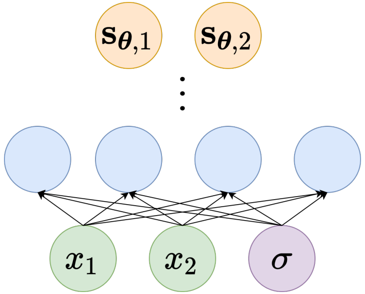
Using multiple noise scales



Data



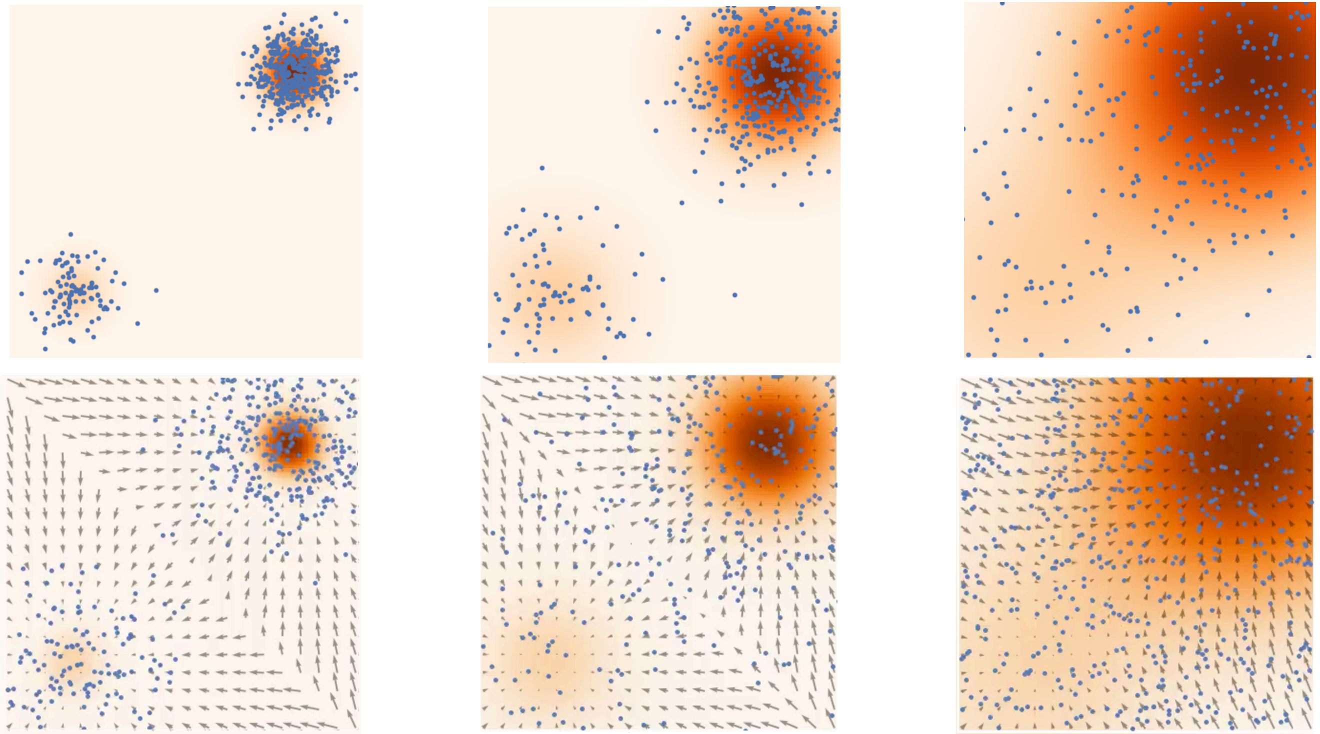
Noise Conditional Score Networks (NCSN)

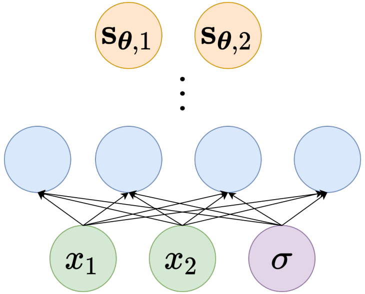
Song and Ermon. "Generative Modeling by Estimating Gradients of the Data Distribution." NeurIPS 2019.

Using multiple noise scales

$\sigma_1 < \sigma_2 < \sigma_3$

Data





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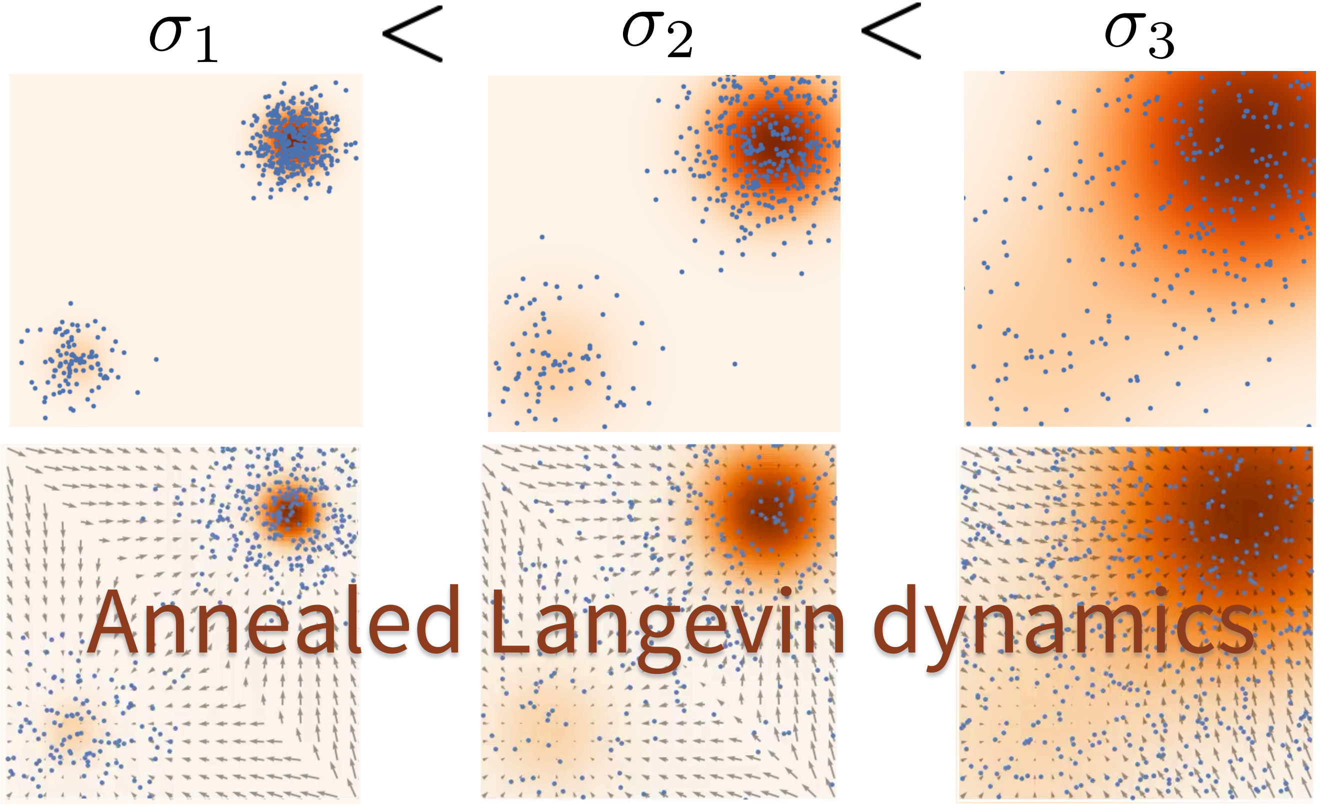
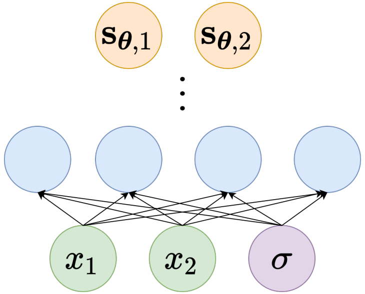
Using multiple noise scales

Data

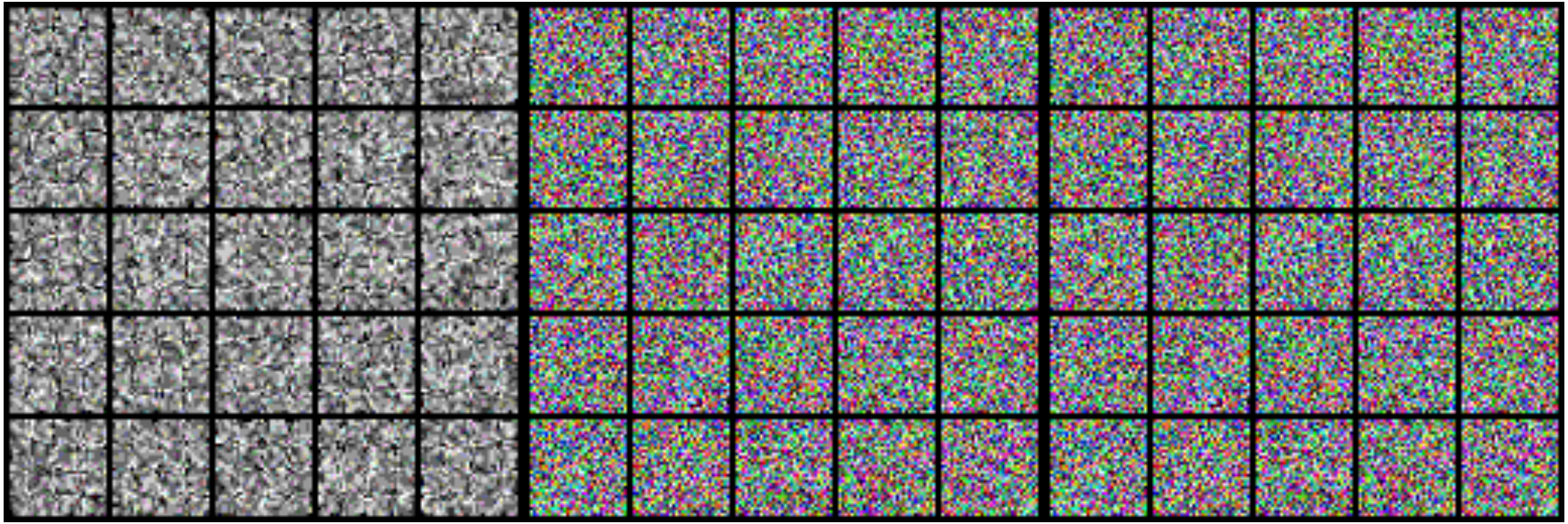




Noise Conditional Score Networks (NCSN)

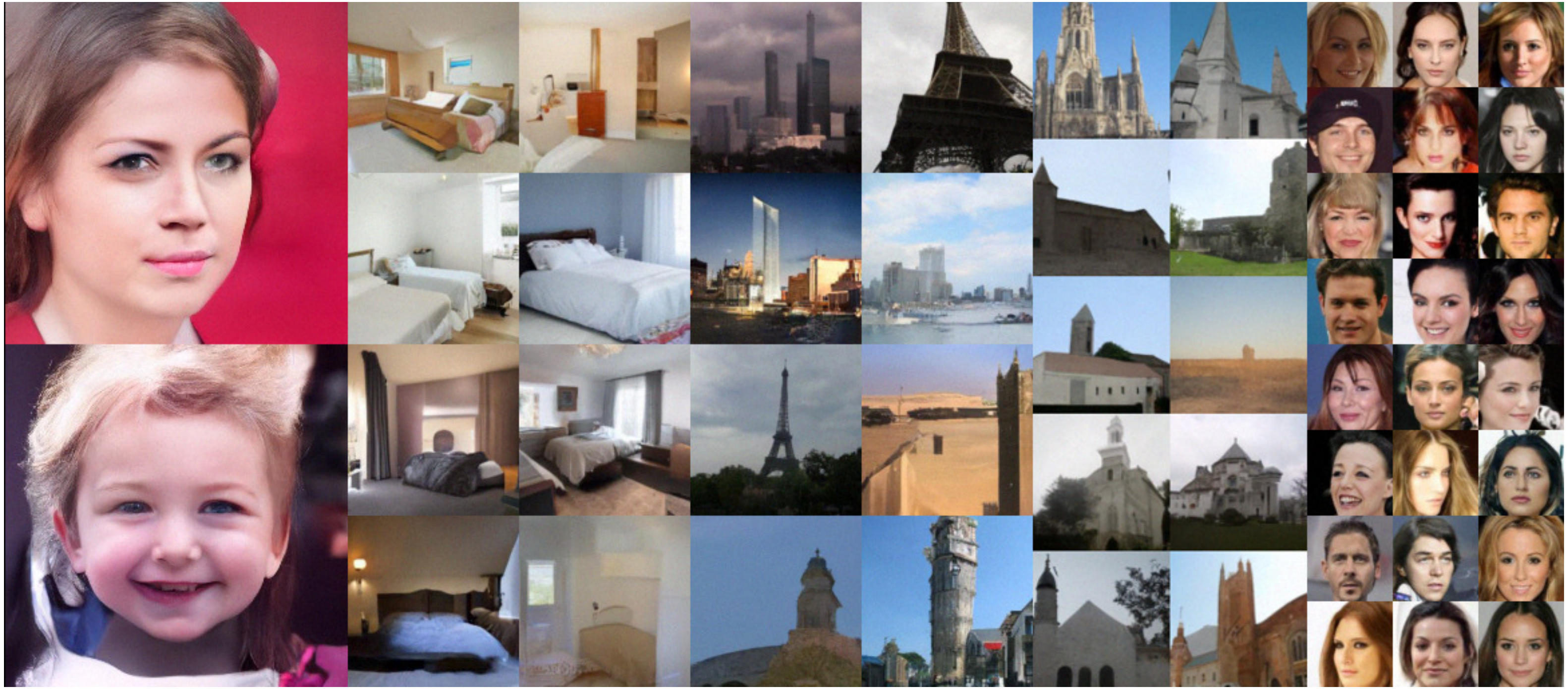
Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Sampling in the real world



Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

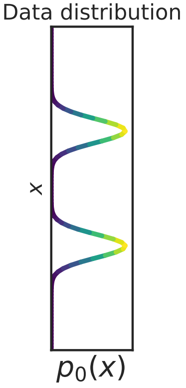
High resolution image generation



Song and Ermon. “Improved Techniques for Training Score-Based Generative Modles.” NeurIPS 2020.

Using an infinite number of noise scales

Using an infinite number of noise scales



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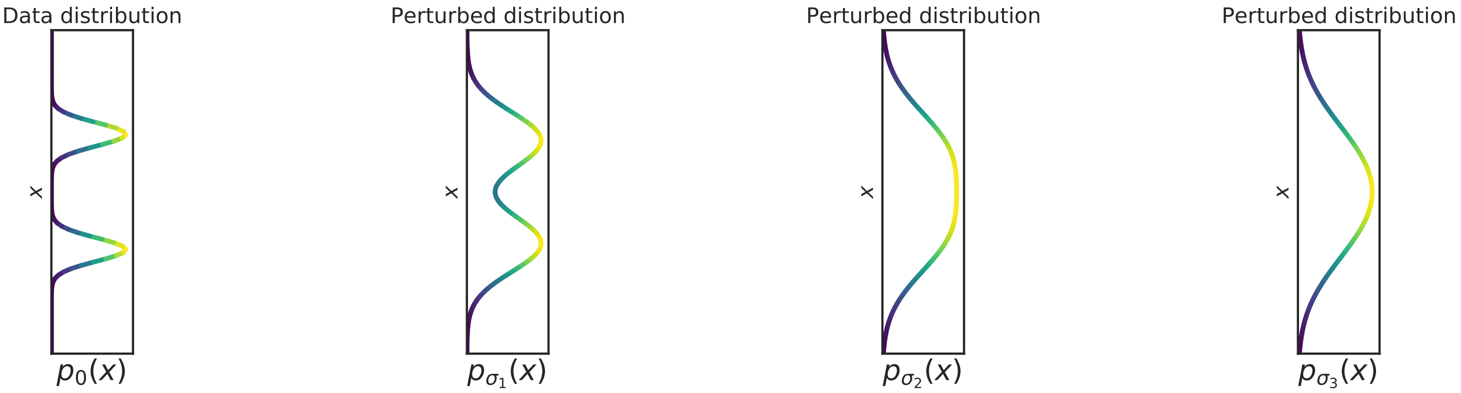

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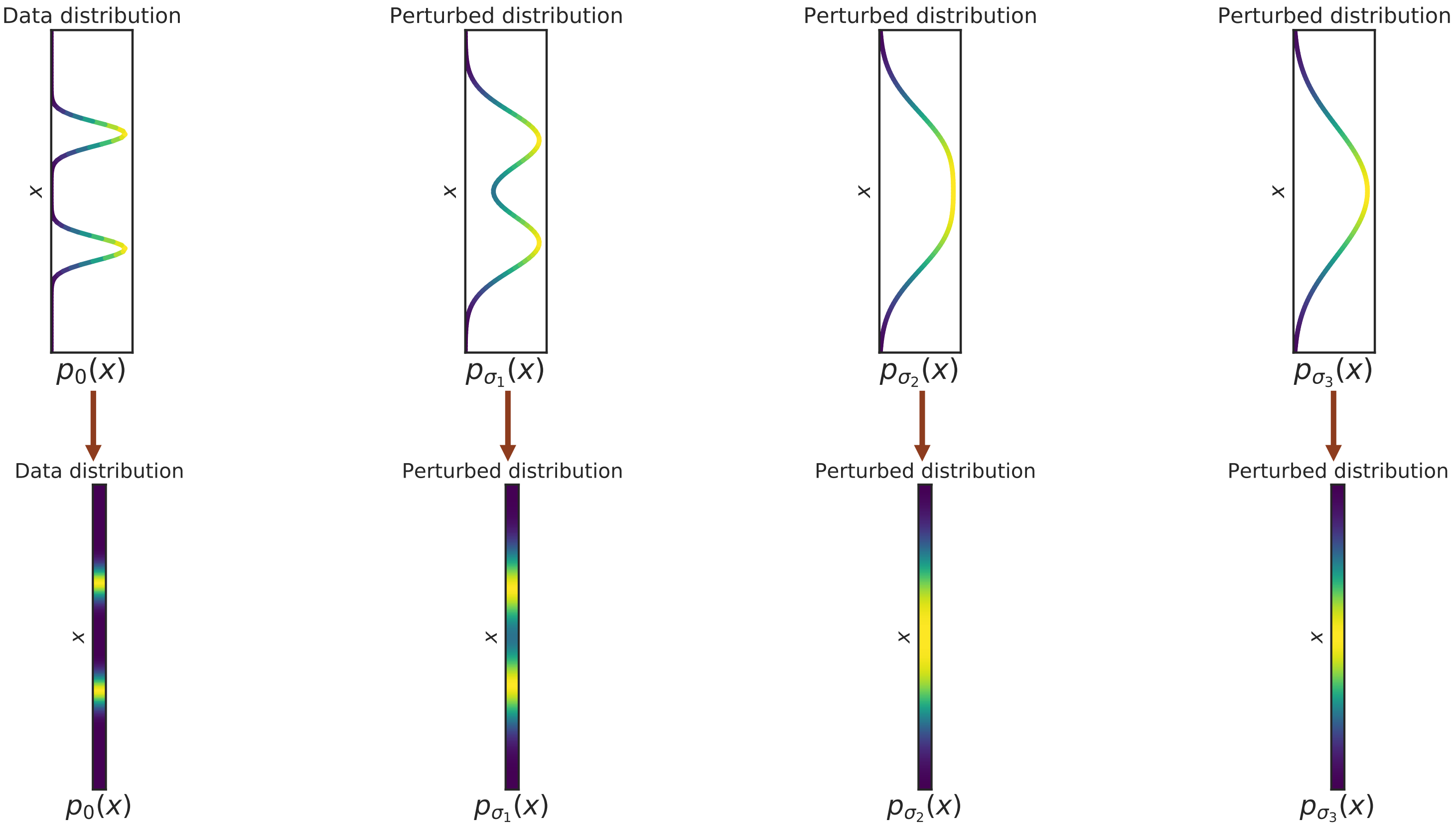
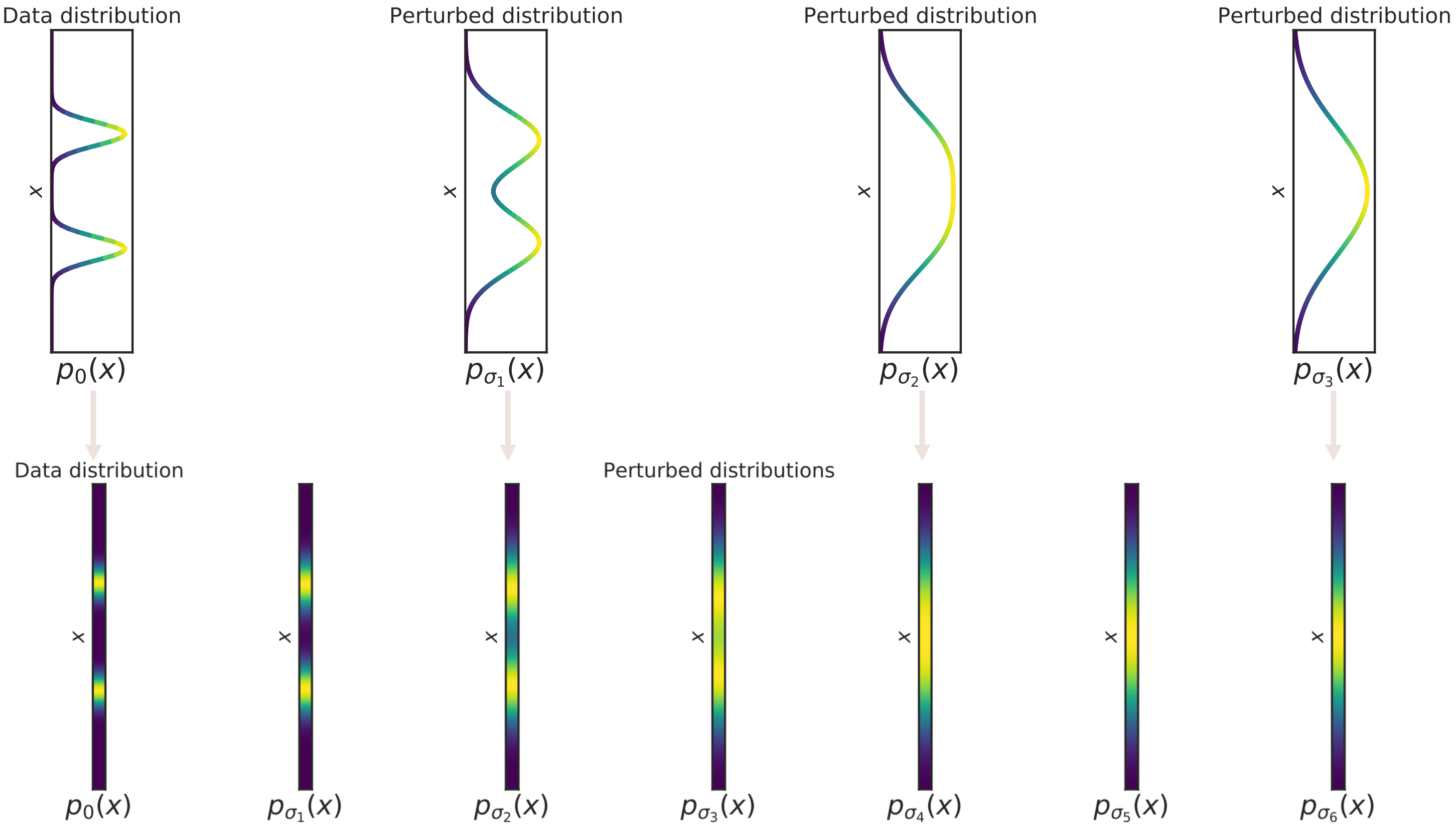


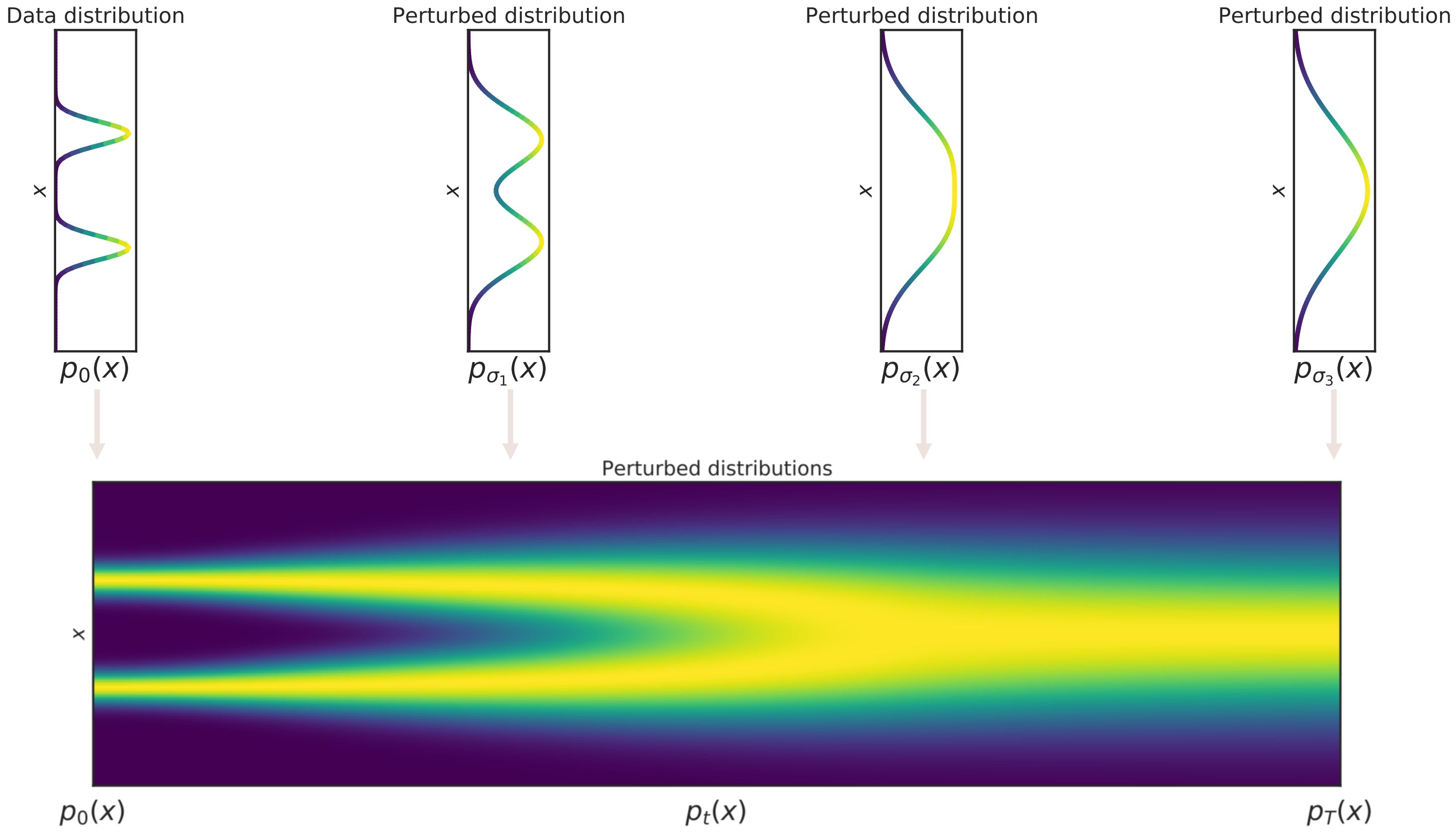
Stanford University

Using an infinite number of noise scales



Stanford University

Using an infinite number of noise scales



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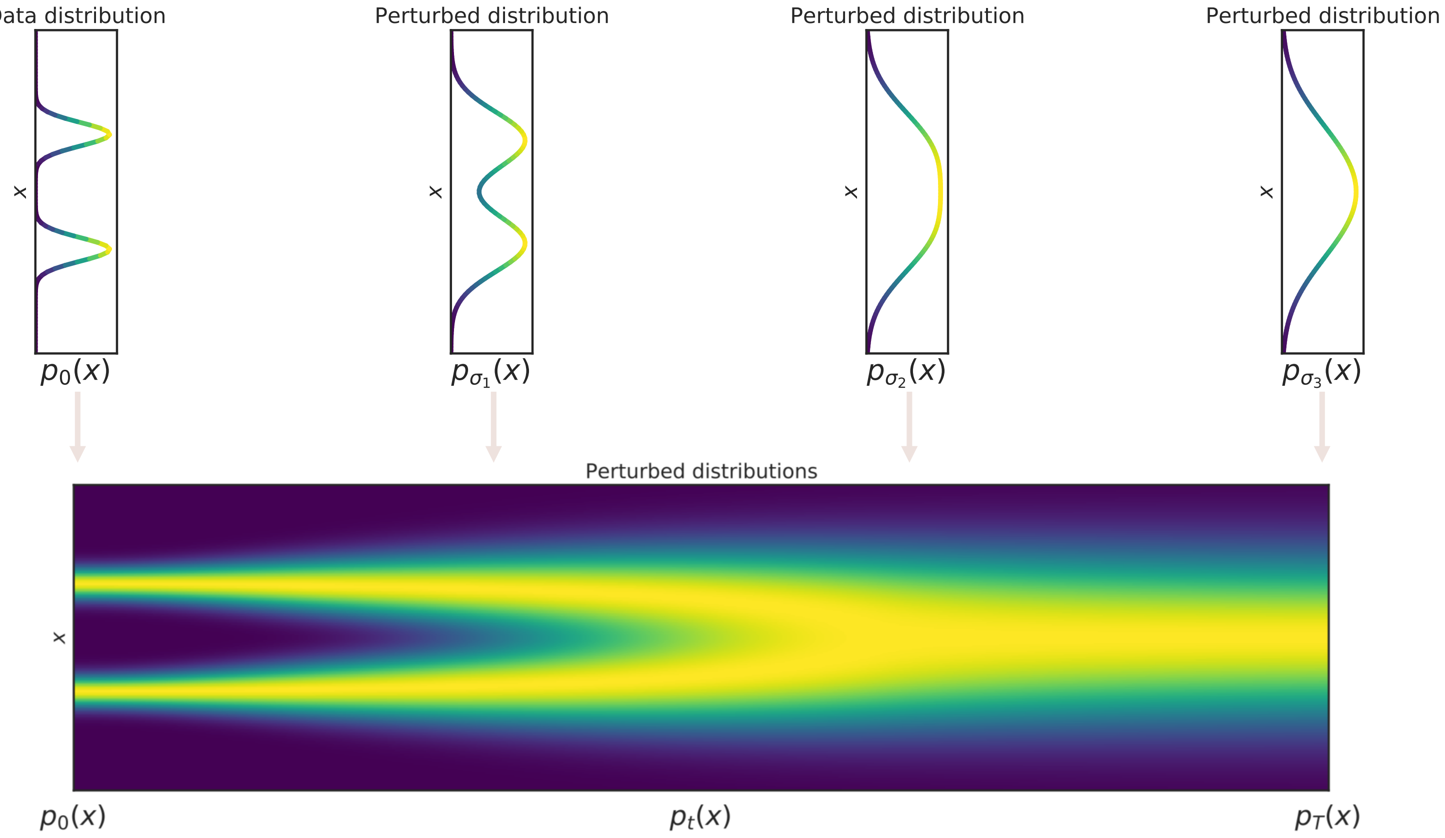
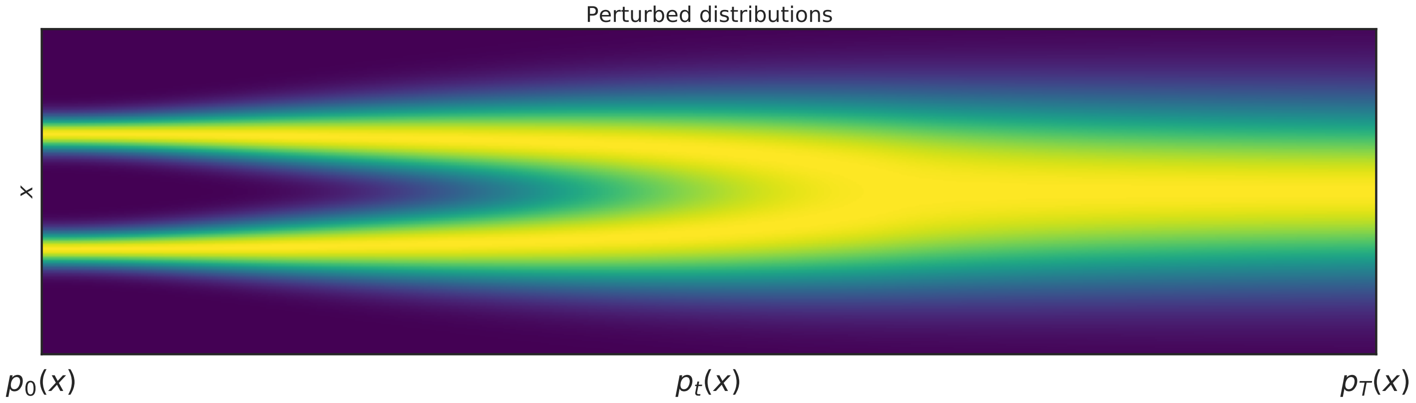


$t \in [0, T]$: continuous index of perturbed distributions

Compact representation of infinite distributions



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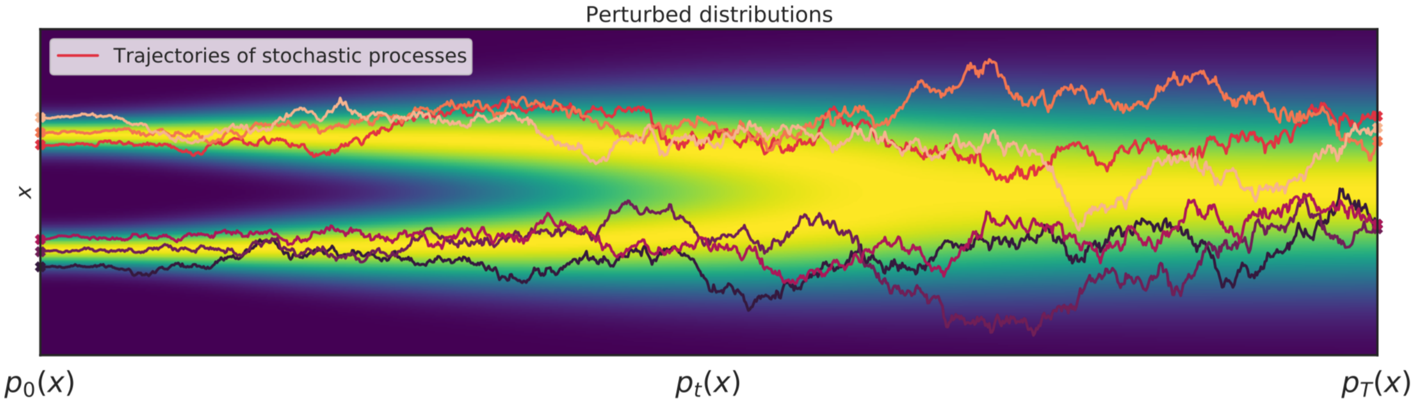

- Stochastic process $\{\mathbf{x}(t)\}_{t=0}^{T}$ → Marginal probability densities $\{p_t(\mathbf{x})\}_{t=0}^{T}$

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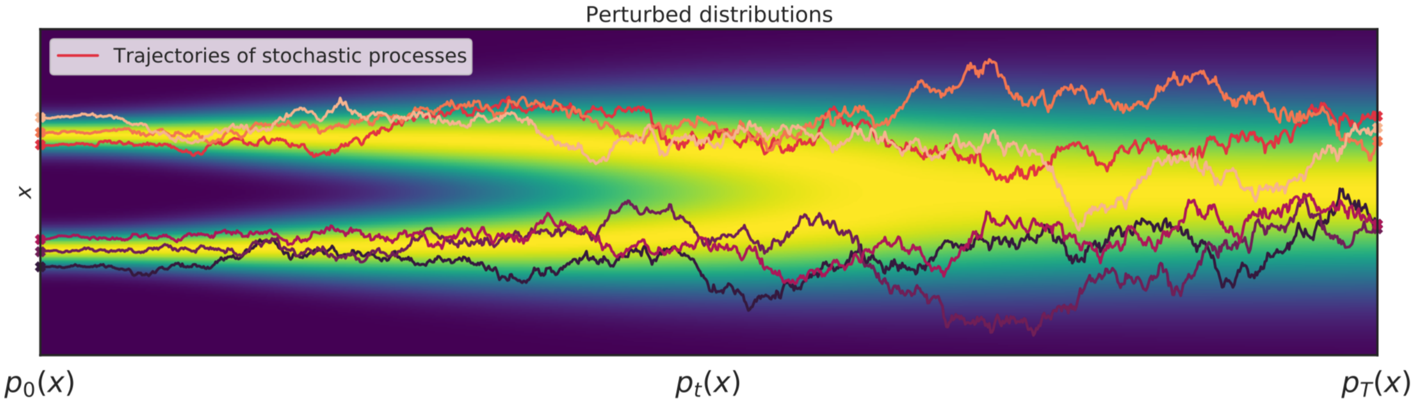

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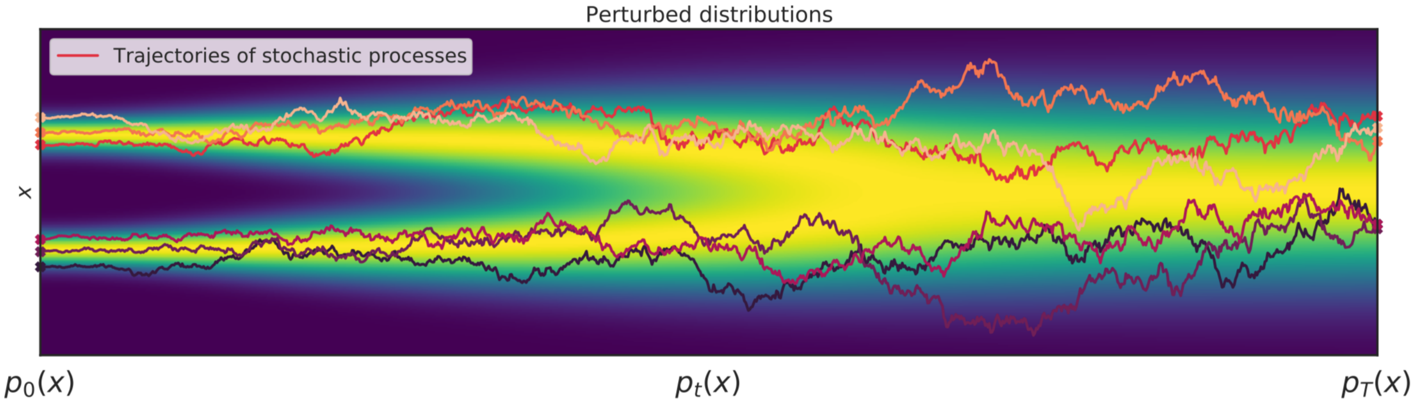

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Deterministic drift

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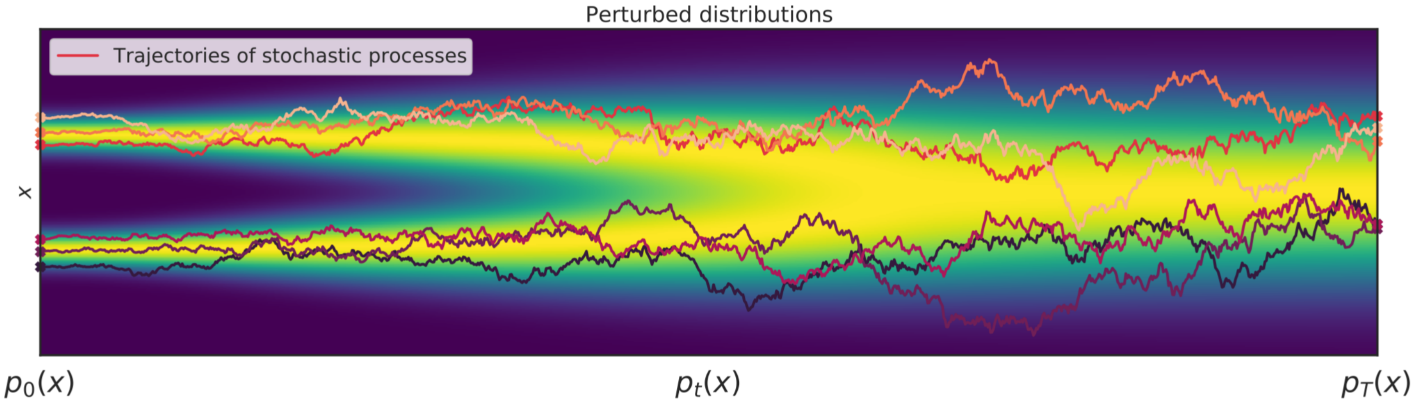

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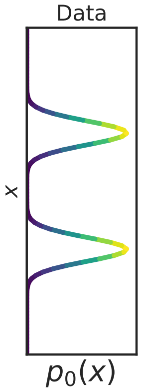
Deterministic drift

Infinitesimal white noise

Score-based generative modeling via SDEs



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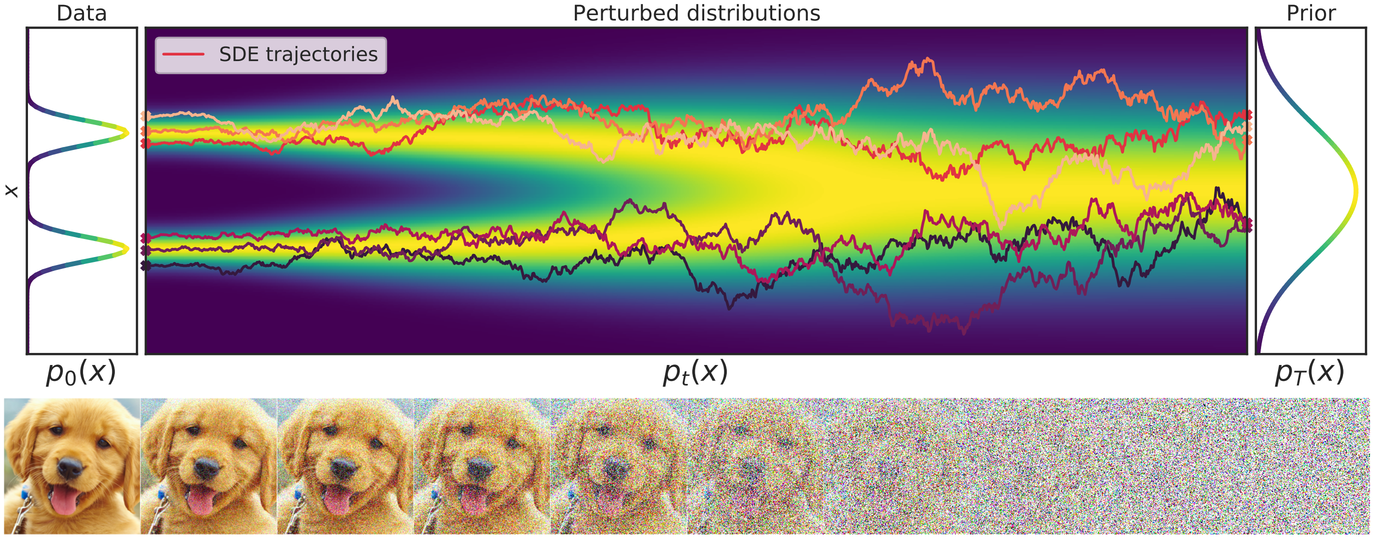

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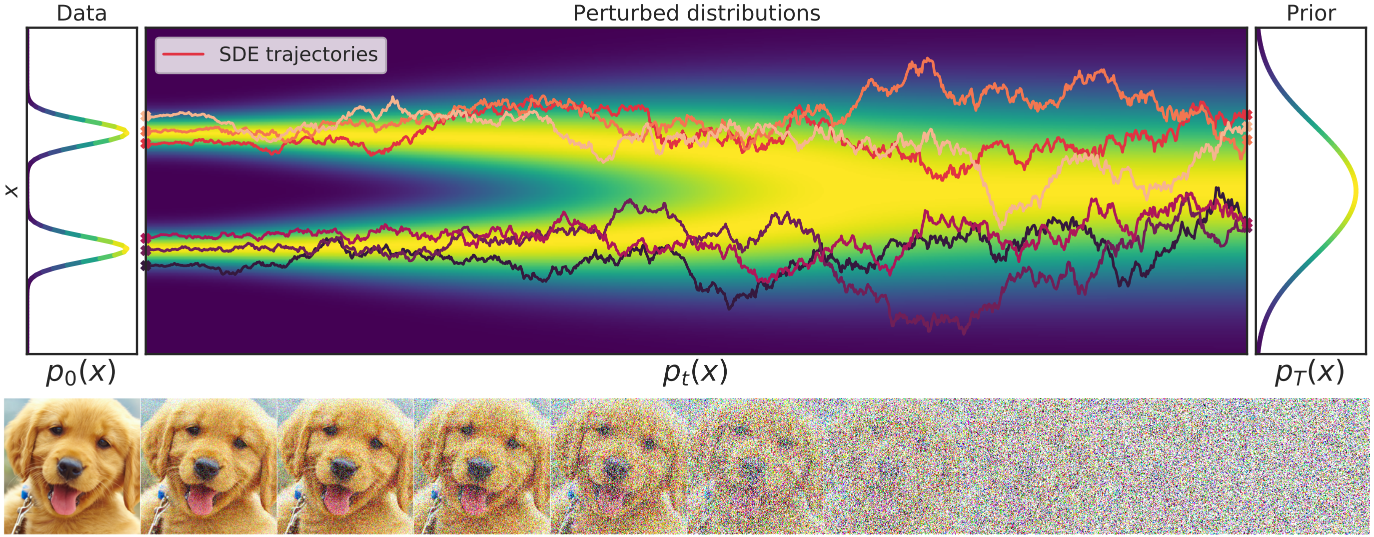

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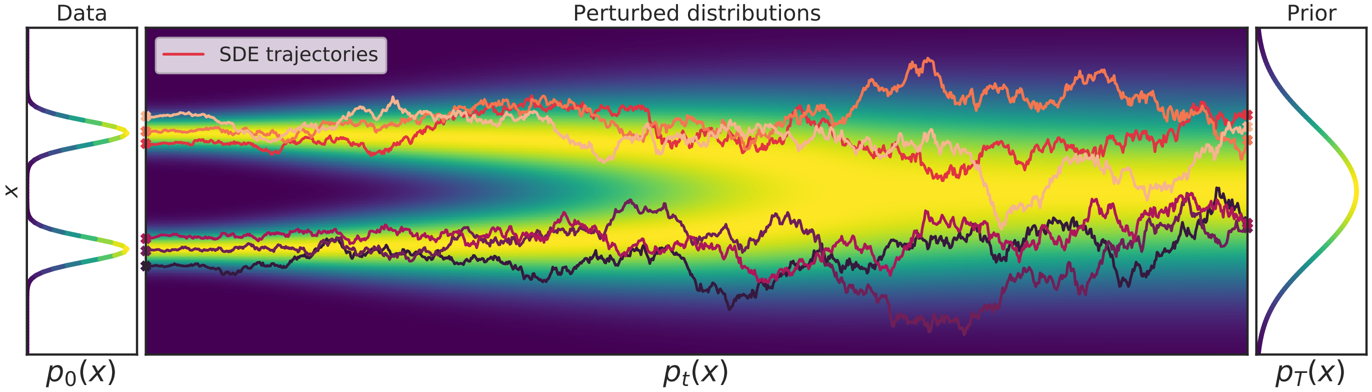

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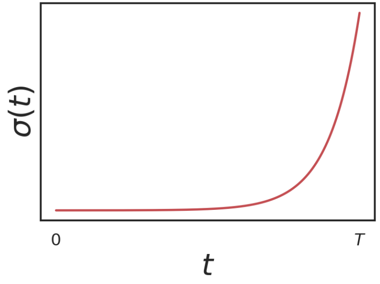

Stanford University

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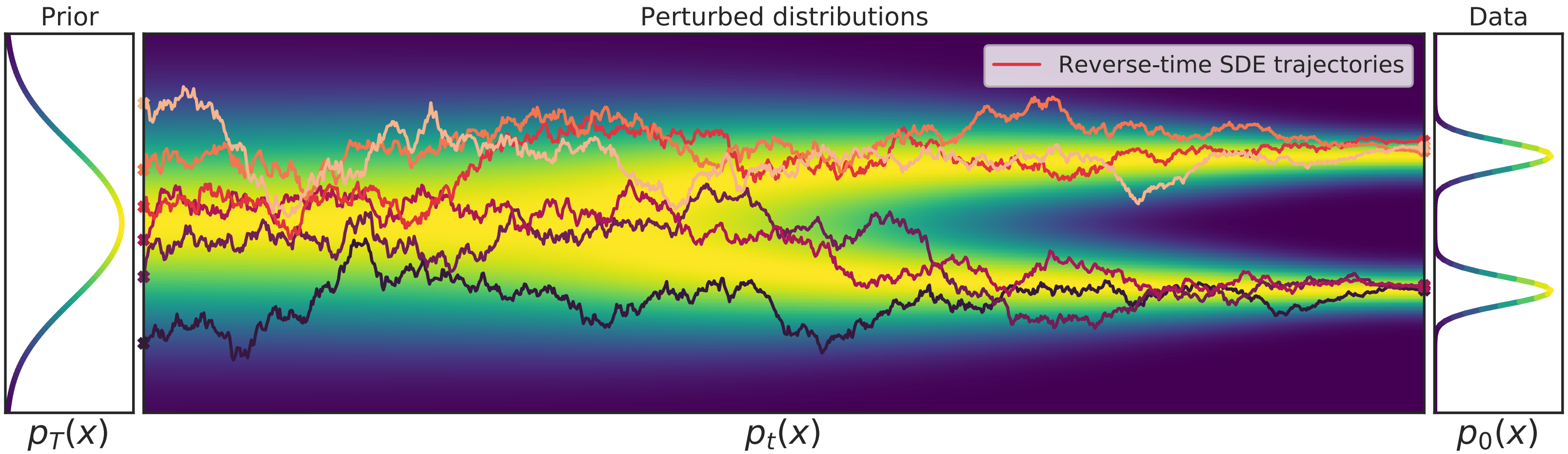

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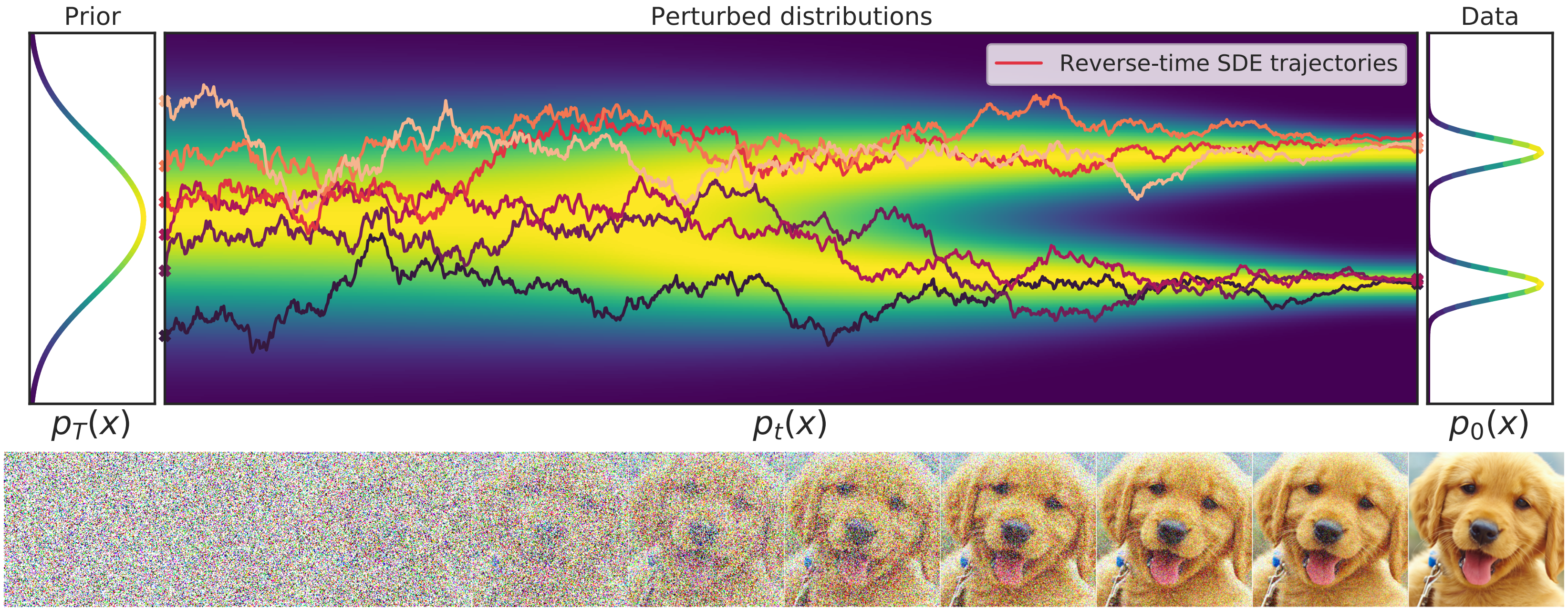

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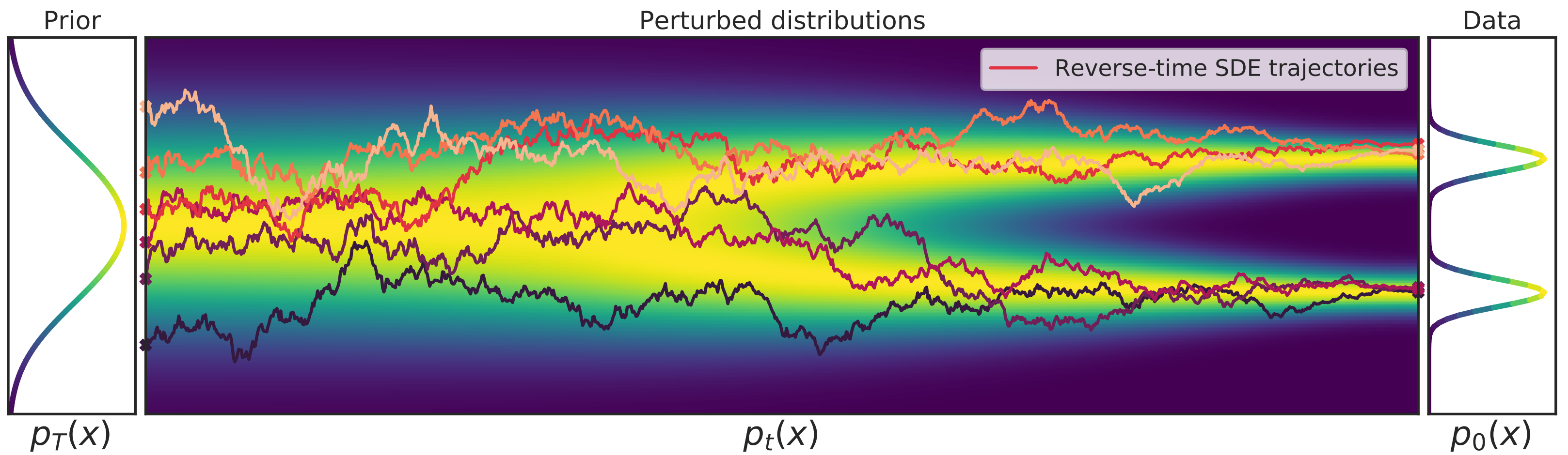

$$\mathrm{d}\mathbf{x} = \sigma(t)\mathrm{d}\mathbf{w}$$

Time reversal

$\{p_t(\mathbf{x})\}_{t=0}^{T}$

$$\mathrm{d}\mathbf{x} = -\sigma^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x})\mathrm{d}t + \sigma(t)\mathrm{d}\bar{\mathbf{w}}$$

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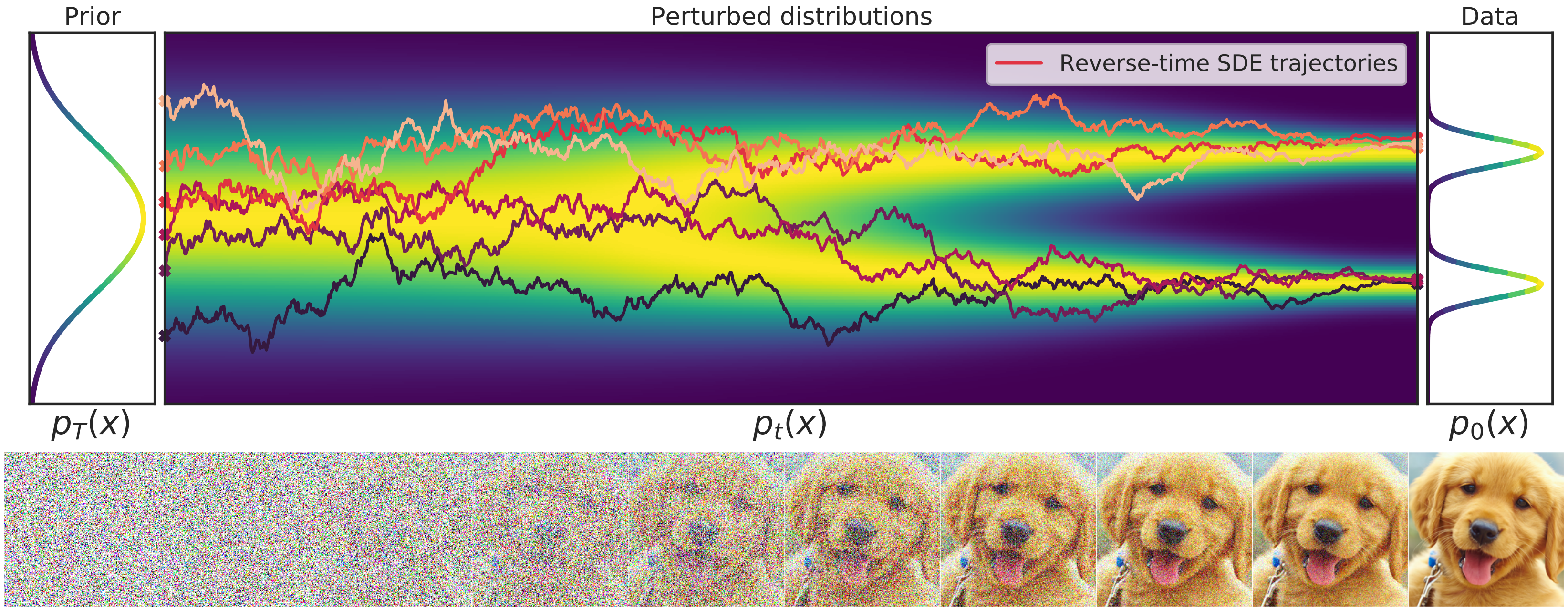

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Score function!

Score-based generative modeling via SDEs

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

Score-based generative modeling via SDEs

- Time-dependent score-based model

$$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t) \approx \nabla_{\mathbf{x}} \log p_t(\mathbf{x})$$

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$$\mathbb{E}_{t \in \mathcal{U}(0,T)}[\lambda(t)\mathbb{E}_{p_t(\mathbf{x})}[||\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)||_2^2]]$$

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- Reverse-time SDE

$$\mathrm{d}\mathbf{x} = -\sigma^2(t)\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)\mathrm{d}t + \sigma(t)\mathrm{d}\bar{\mathbf{w}}$$

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- Euler-Maruyama (analgous to Euler for ODEs)

$$\mathbf{x} \leftarrow \mathbf{x} - \sigma(t)^2\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)\Delta t + \sigma(t)\ \mathbf{z} \quad (\mathbf{z} \sim \mathcal{N}(\mathbf{0}, |\Delta t|\ \mathbf{I}))$$

$$t \leftarrow t + \Delta t$$

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Mixture of score matching subsumes MLE

$$\mathbb{E}_{t\in\mathcal{U}(0,T)}[\lambda(t)\mathbb{E}_{p_t(\mathbf{x})}[\|\nabla_{\mathbf{x}}\log p_t(\mathbf{x}) - \nabla_{\mathbf{x}}\log q_{t,\boldsymbol{\theta}}(\mathbf{x},t)\|_2^2]]$$

$$=$$

$$\frac{2}{T}\mathrm{KL}(p_0(\mathbf{x}) \parallel q_{0,\boldsymbol{\theta}}(\mathbf{x}))$$

For certain choice of the weighting function $\lambda(t)$

Durkan* and **Song***, “On Maximum Likelihood Training of Score-Based Generative Models”, arXiv 2101.09258

Predictor-Corrector sampling methods

- Predictor-Corrector sampling.
  - **Predictor:** Numerical SDE solver
  - **Corrector:** Score-based MCMC

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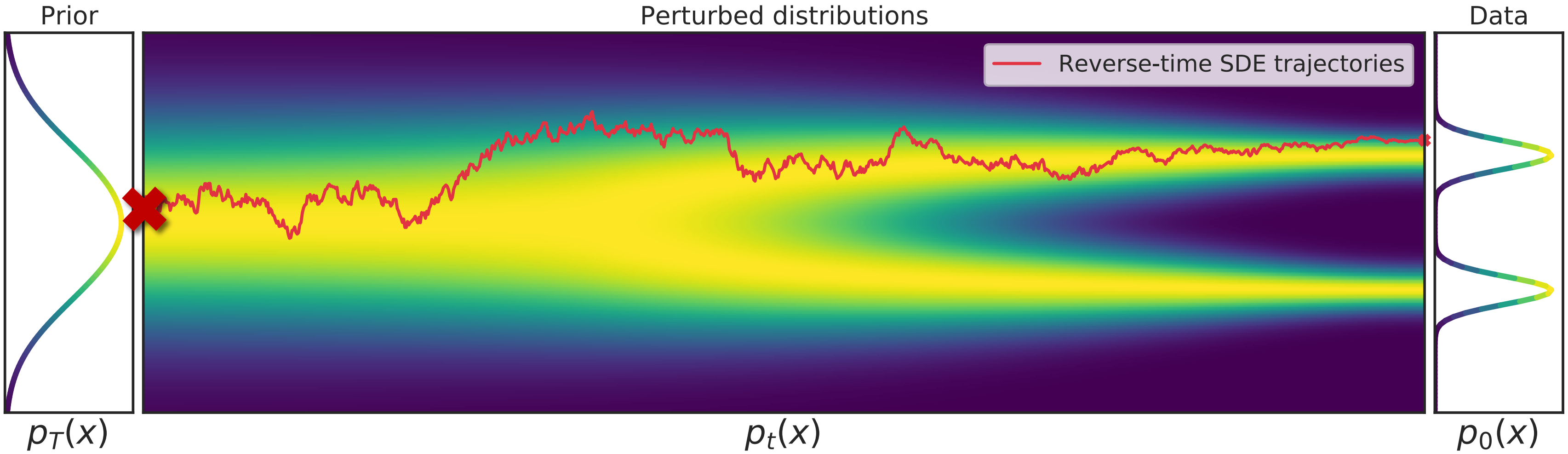

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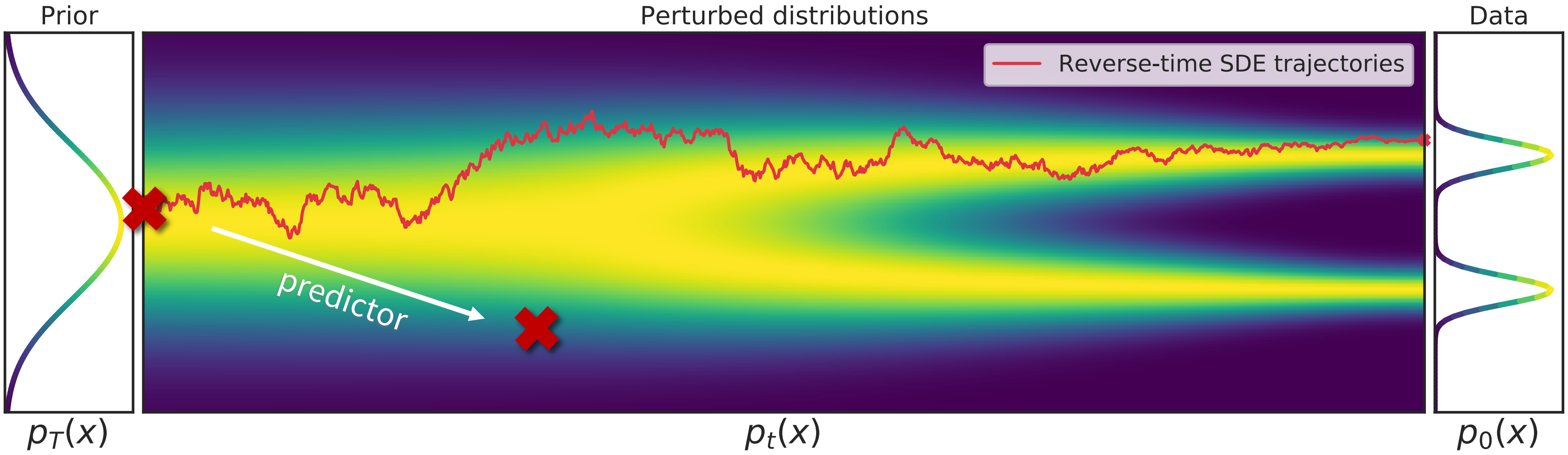

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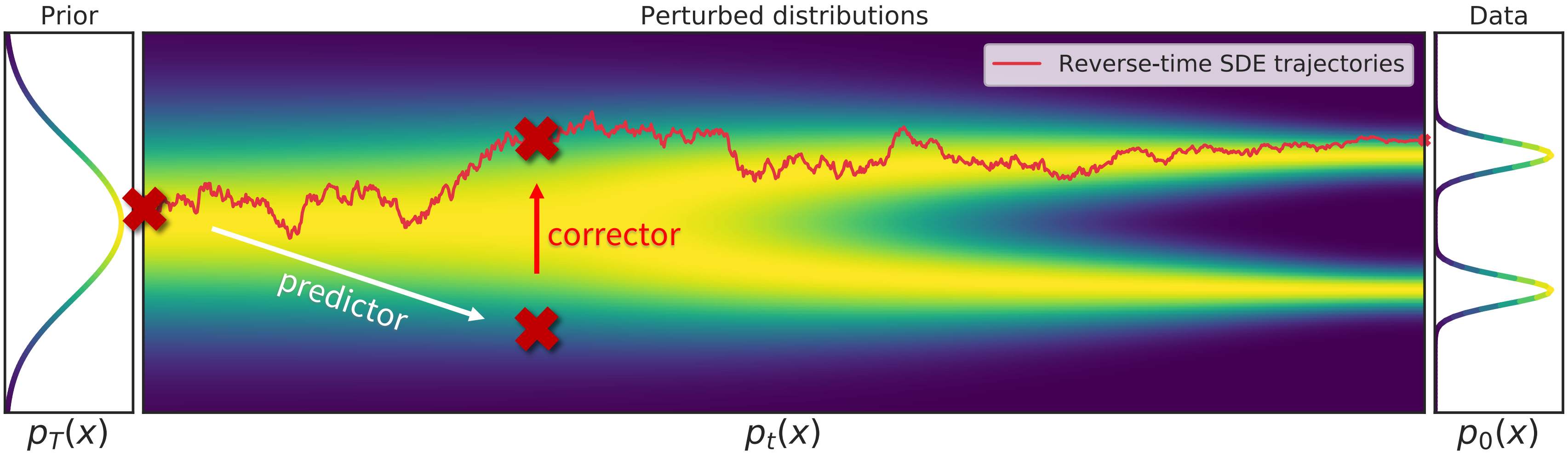

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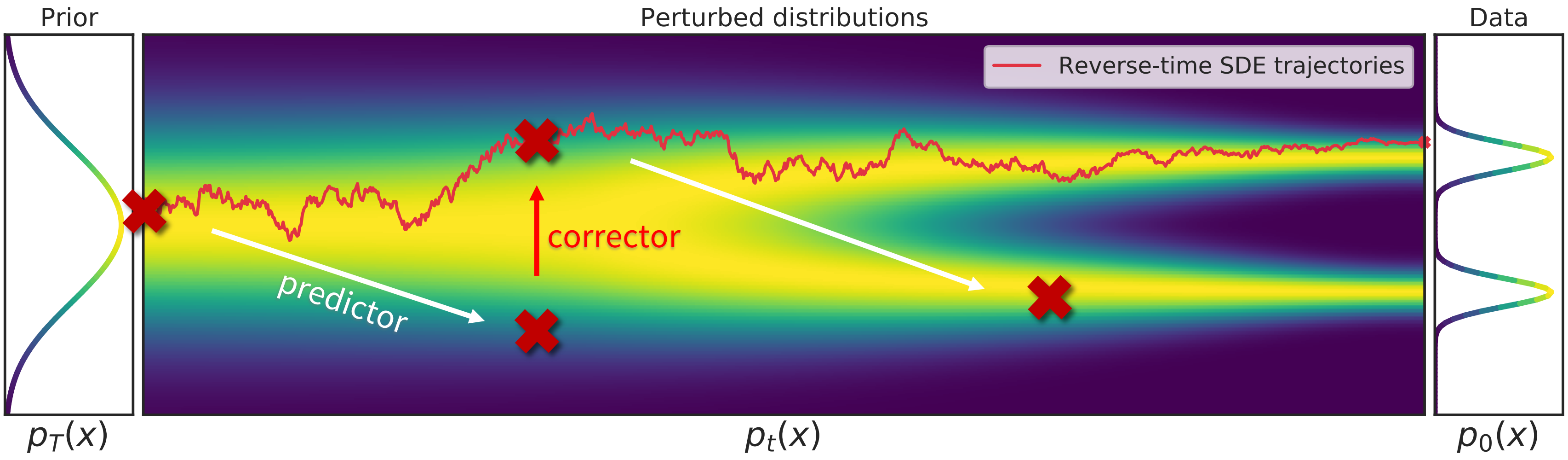

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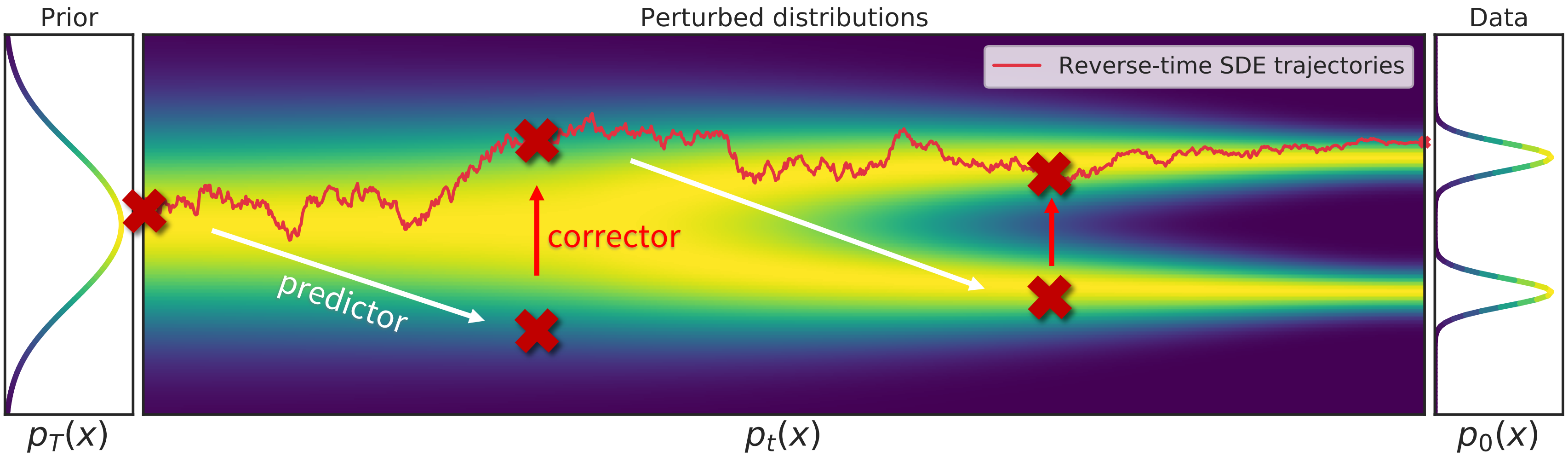

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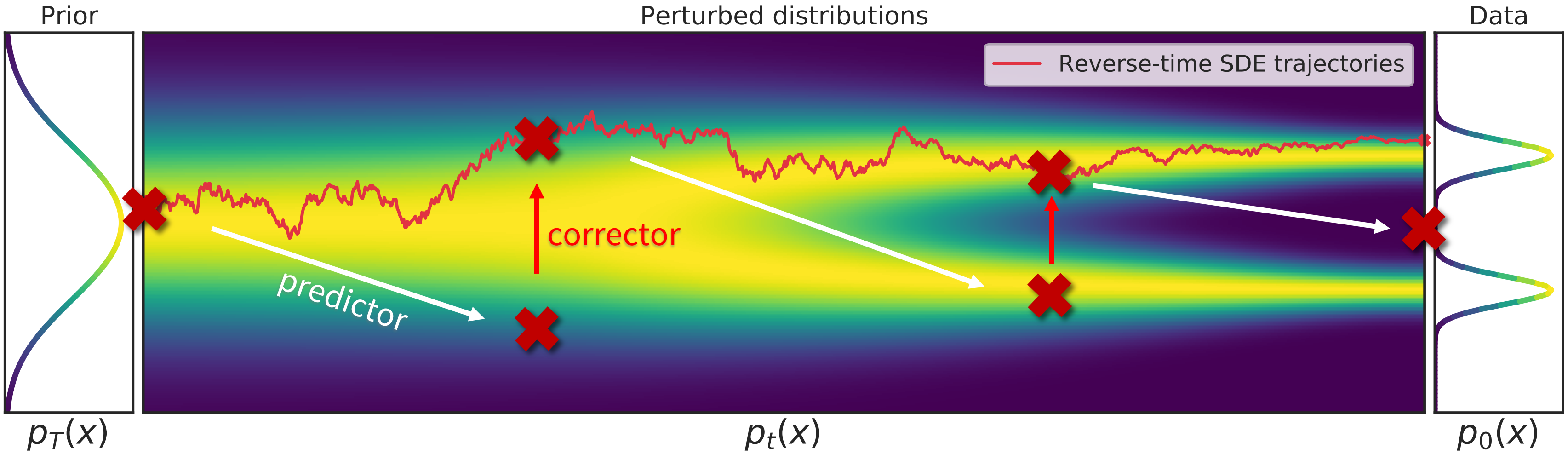

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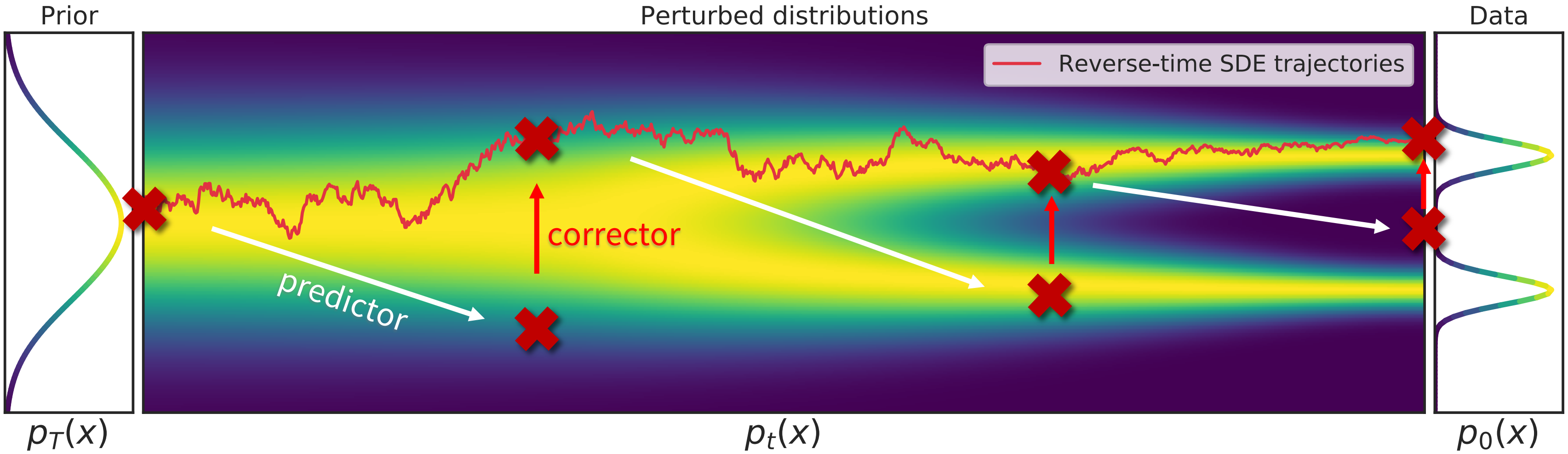

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Results on predictor-corrector sampling

Model	FID↓	IS↑
Conditional		
BigGAN (Brock et al., 2018)	14.73	9.22
StyleGAN2-ADA (Karras et al., 2020a)	**2.42**	**10.14**
Unconditional		
StyleGAN2-ADA (Karras et al., 2020a)	2.92	9.83
NCSN (Song & Ermon, 2019)	25.32	8.87 ± .12
NCSNv2 (Song & Ermon, 2020)	10.87	8.40 ± .07
DDPM (Ho et al., 2020)	3.17	9.46 ± .11
DDPM++	2.78	9.64
DDPM++ cont. (VP)	2.55	9.58
DDPM++ cont. (sub-VP)	2.61	9.56
DDPM++ cont. (deep, VP)	2.41	9.68
DDPM++ cont. (deep, sub-VP)	2.41	9.57
NCSN++	2.45	9.73
NCSN++ cont. (VE)	2.38	9.83
NCSN++ cont. (deep, VE)	**2.20**	**9.89**

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

High-Fidelity Generation for 1024x1024 Images

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Probability flow ODE: turning the SDE to ODE

- Probability flow ODE (ordinary differential equation)

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

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$$\mathrm{d}\mathbf{x} = \sigma(t)\mathrm{d}\mathbf{w}$$

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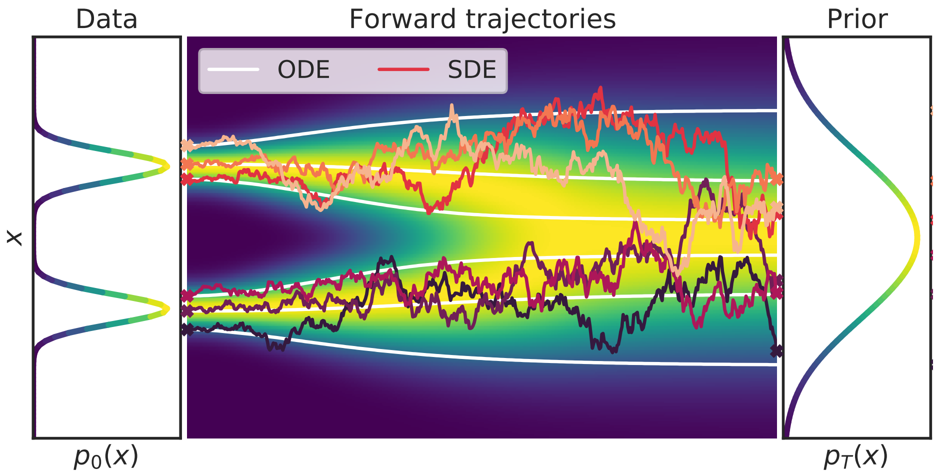
Score function

$\approx \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)$



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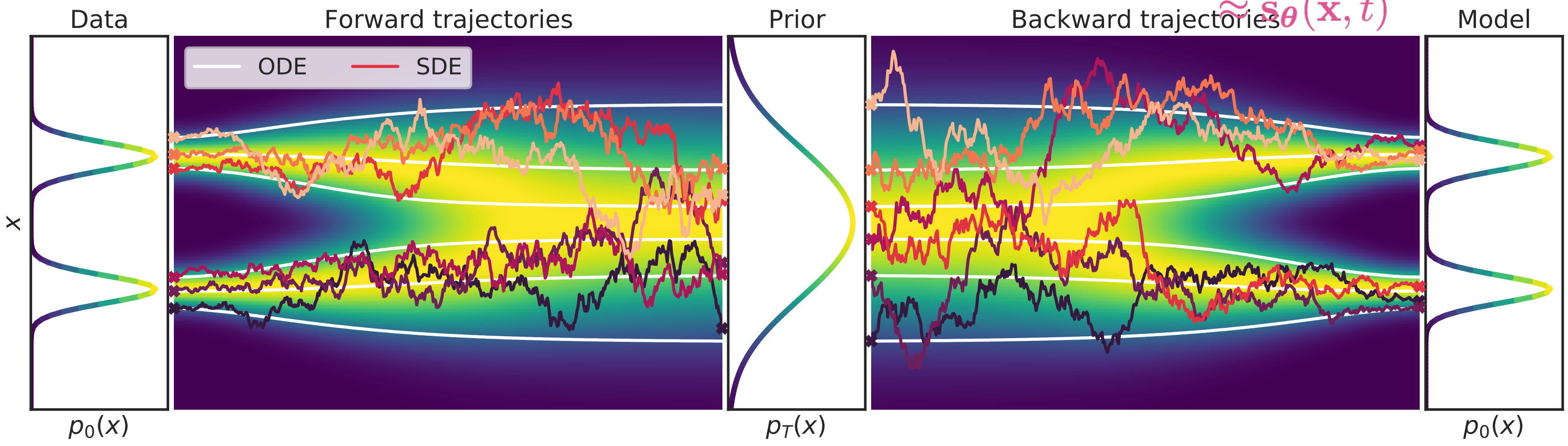
Score function $\approx \mathbf{s}_\theta(\mathbf{x}, t)$



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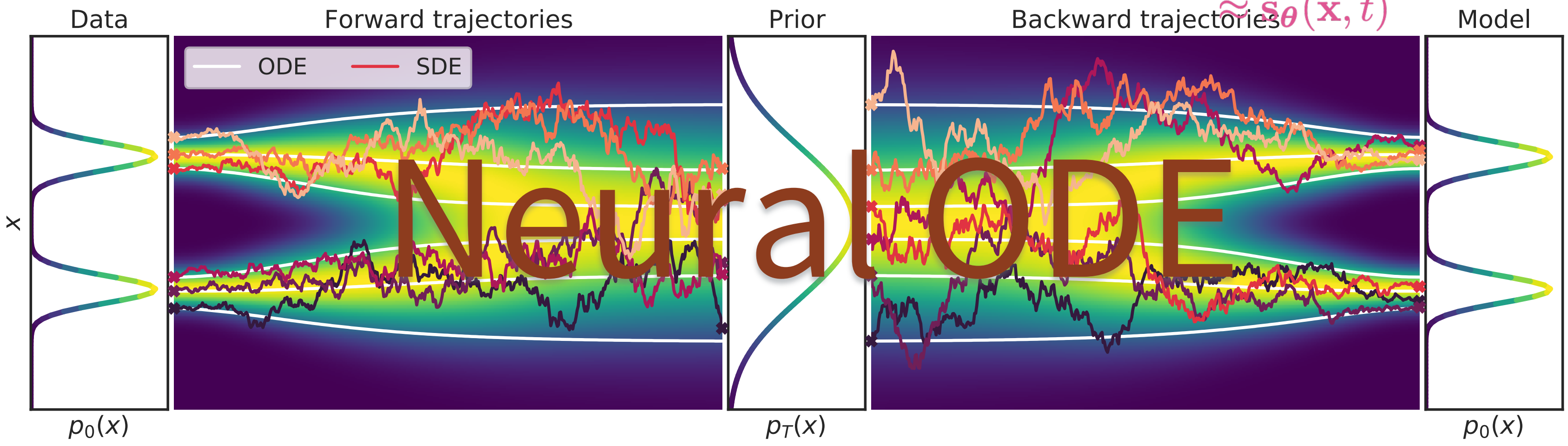

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

Solving Reverse-ODE for Sampling

- **More efficient samplers** via black-box ODE solvers

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

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- **More efficient samplers** via black-box ODE solvers

NFE = Number of score Function Evaluations

- Predictor-corrector:
  - $>$ 1000 NFE
- ODE
  - $\approx$100 NFE

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- ODE
  - $\approx$100 NFE

- **Exact likelihood** though models are trained with score matching.

$$\log p_0(\mathbf{x}) = \log p_T(\mathbf{x}) - \frac{1}{2}\int_0^T \sigma(t)^2 \mathrm{trace}(\nabla_{\mathbf{x}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t))\mathrm{d}t$$

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Solving Reverse-ODE for Sampling

Model	NLL Test ↓	FID ↓
RealNVP (Dinh et al., 2016)	3.49	-
iResNet (Behrmann et al., 2019)	3.45	-
Glow (Kingma & Dhariwal, 2018)	3.35	-
MintNet (Song et al., 2019b)	3.32	-
Residual Flow (Chen et al., 2019)	3.28	46.37
FFJORD (Grathwohl et al., 2018)	3.40	-
Flow++ (Ho et al., 2019)	3.29	-
DDPM (L) (Ho et al., 2020)	$\leqslant 3.70^{*}$	13.51
DDPM (L_{simple}) (Ho et al., 2020)	$\leqslant 3.75^{*}$	3.17
DDPM	3.28	3.37
DDPM cont. (VP)	3.21	3.69
DDPM cont. (sub-VP)	3.05	3.56
DDPM++ cont. (VP)	3.16	3.93
DDPM++ cont. (sub-VP)	3.02	3.16
DDPM++ cont. (deep, VP)	3.13	3.08
DDPM++ cont. (deep, sub-VP)	**2.99**	**2.92**

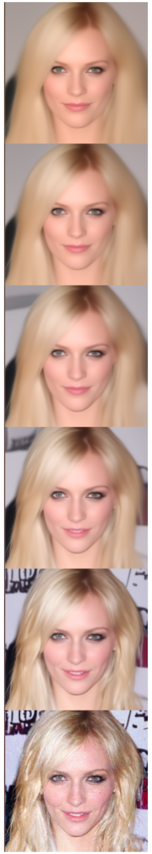
models trained
with score matching

black-box ODE
Solvers for sampling

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Probability flow ODE: latent space manipulation

Interpolation

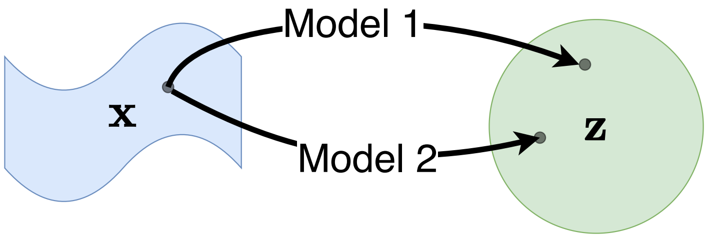


Temperature scaling

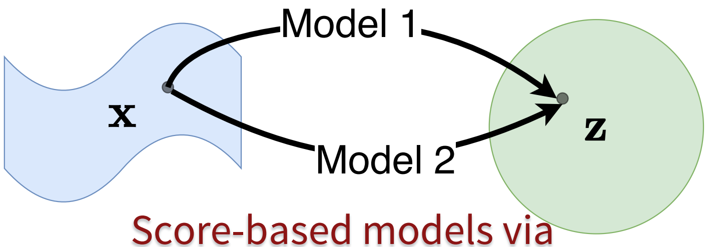
Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Probability flow ODE: uniquely identifiable encoding

- Uniquely **identifiable** encoding



Flow models, VAE, etc

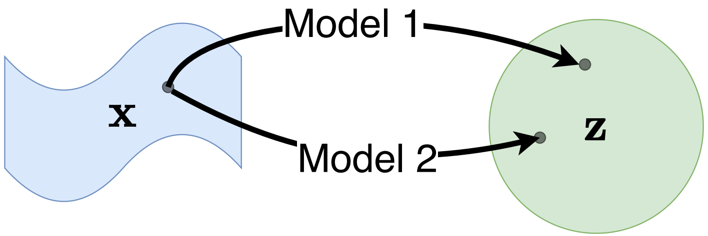


Score-based models via probability flow ODE

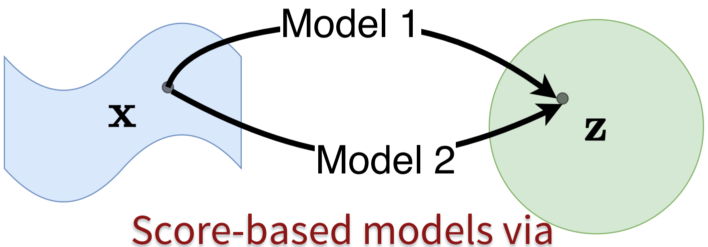
Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Probability flow ODE: uniquely identifiable encoding

- Uniquely **identifiable** encoding



Flow models, VAE, etc



Score-based models via probability flow ODE

- No trainable parameters in the probability flow ODE!

$$\mathrm{d}\mathbf{x} = -\frac{1}{2}\sigma(t)^2 \nabla_{\mathbf{x}} \log p_t(\mathbf{x}) \mathrm{d}t$$

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

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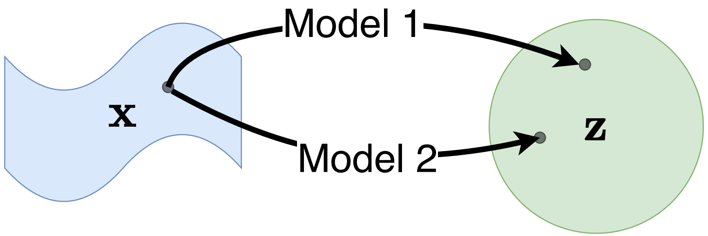

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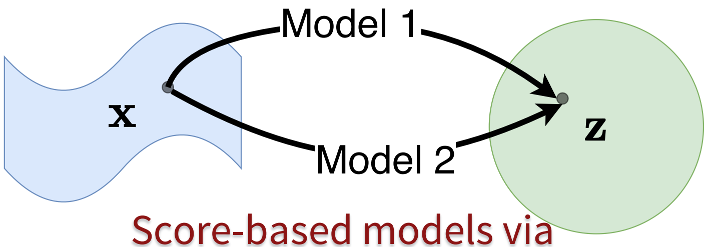

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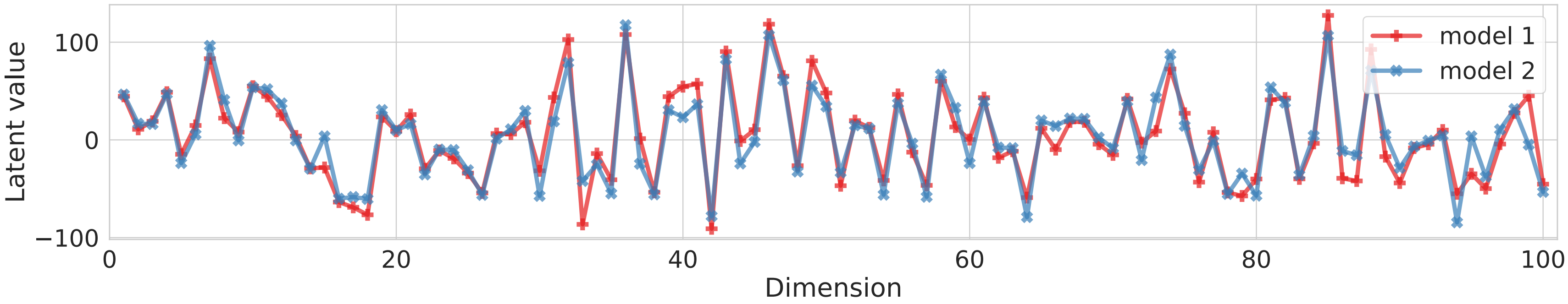

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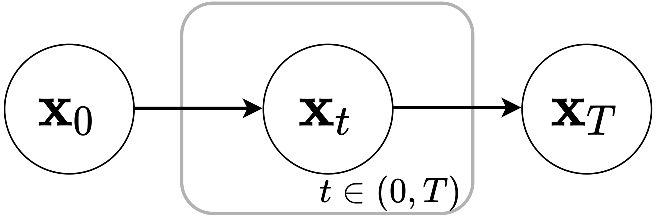
Controllable Generation



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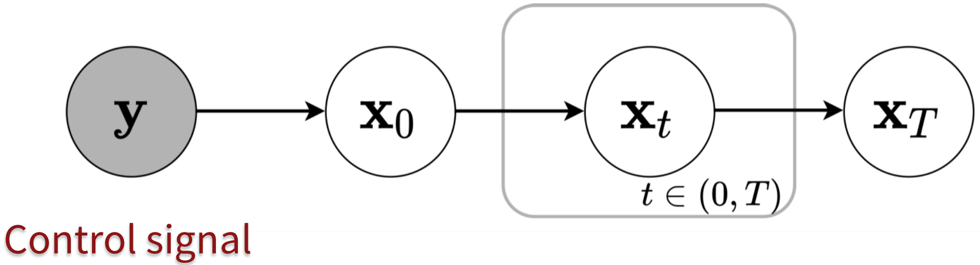

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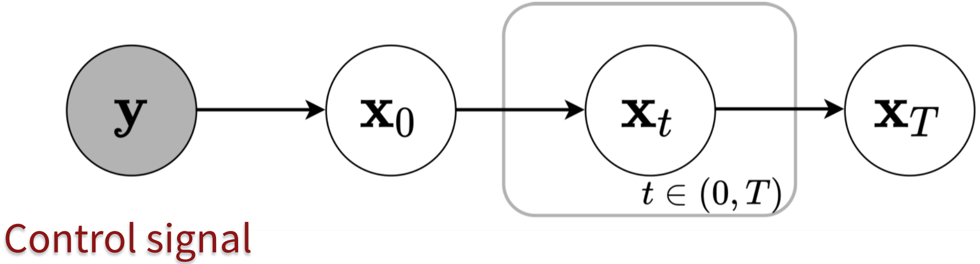

- Conditional reverse-time SDE via unconditional scores

$$\mathrm{d}\mathbf{x} = -\sigma^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x} \mid \mathbf{y})\mathrm{d}t + \sigma(t)\mathrm{d}\bar{\mathbf{w}}$$

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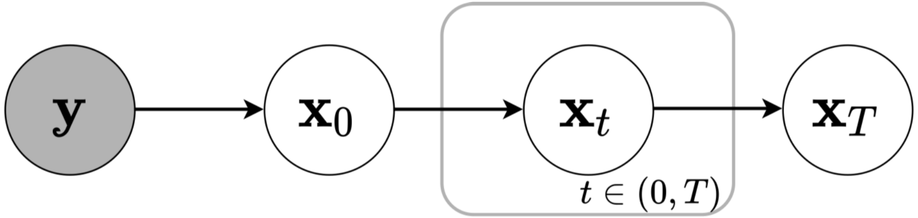

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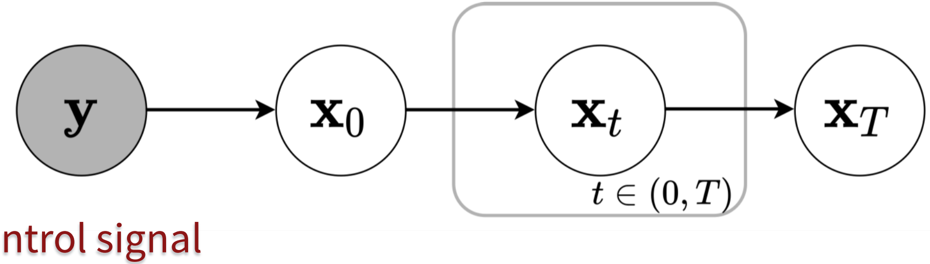

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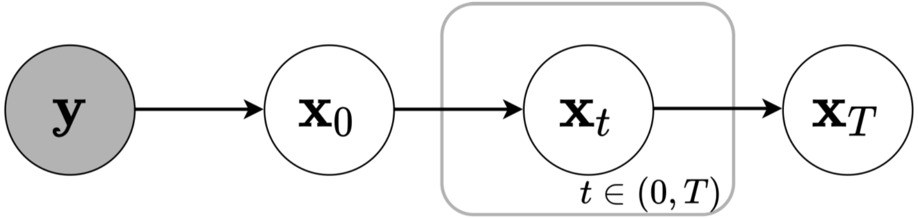

Control signal

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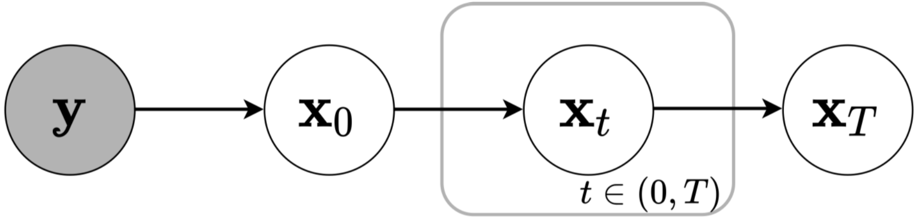

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Trained separately or
specified with domain knowledge

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Controllable Generation: class-conditional generation

- $\mathbf{y}$ is the **class label**
- $p_t(\mathbf{y} \mid \mathbf{x})$ is a time-dependent classifier

class: bird

class: deer

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Controllable Generation: inpainting

- $\mathbf{y}$ is the **masked image**
- $p_t(\mathbf{y} \mid \mathbf{x})$ can be approximated without training

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Controllable Generation: colorization

- $\mathbf{y}$ is the **gray-scale image**
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Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. "Score-Based Generative Modeling through Stochastic Differential Equations." ICLR 2021.

Future directions

- Discrete data, such as text generation
- Theoretical understanding on sample quality
- Faster sampling

Improvements

- Semi-supervised learning
- Inverse problems
- Unrestricted adversarial attacks
- Outlier detection

Applications

Conclusion

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  - Competitive likelihood on CIFAR-10
  - Equivalence to Neural ODEs, plus uniquely identifiable encoding

Collaborators

Stefano Ermon

Ben Poole

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Sahaj Garg

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Abhishek Kumar