# Statistical Models & Computing Methods

# Lecture 20: Energy-based and Score-based Generative Models

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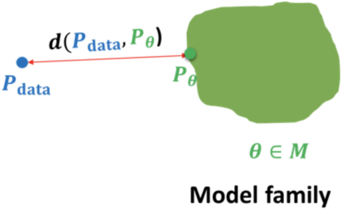
December 23, 2021

# Recap on Deep Generative Models



- Autoregressive Models: $p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_{<i})$
- Normalizing Flow Models:

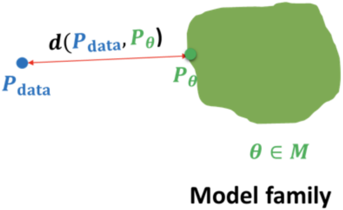
$$p_X(x;\theta) = p_Z(f_\theta^{-1}(x)) \left| \det \left( \frac{\partial f_\theta^{-1}(x)}{\partial x} \right) \right|$$

- Variational Autoencoders: $p_\theta(x) = \int_z p_\theta(x,z)dz$

Cons: Model architectures are restricted.

# Recap on Deep Generative Models

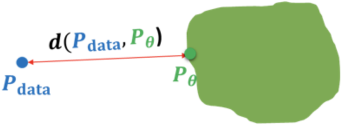
$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



- Generative Adversarial Networks (GANs).
  - $\min_\theta \max_\phi \mathbb{E}_{x \sim p_{\text{data}}} \log D_\phi(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_\phi(G_\theta(z)))$
  - Two sample tests. Can optimize $f$-divergences and the Wasserstein distance.
  - Very flexible model architectures. But likelihood is intractable, training is unstable, hard to evaluate, and has mode collapse issues.

# Recap on Deep Generative Models

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \dots, n$



$\theta \in M$

**Model family**

Energy-based Models (EBMs).

- Very flexible model architectures.
- Stable training.
- Relatively high sample quality.
- Flexible composition.

# How to Parameterize a Distribution?

Probability densities $p(x)$ need to satisfy

- non-negative: $p(x) \geq 0$.
- sum-to-one: $\sum_x p(x) = 1$ or $\int p(x) dx = 1$ for continuous variables

Coming up with a non-negative function $p_\theta(x)$ is not hard

- $p_\theta(x) = f_\theta(x)^2$
- $p_\theta(x) = \exp(f_\theta(x))$
- $p_\theta(x) = |f_\theta(x)|$

Sum to one is the key. Although many models allow analytical integration (e.g., autoregressive models, normalizing flows), what if the analytical integration is not available?

# Energy-based Model

$$p_\theta(x) = \frac{\exp(f_\theta(x))}{Z(\theta)}, \quad Z(\theta) = \int \exp(f_\theta(x))dx$$

The normalizing constant $Z(\theta)$ is also called the partition function. Why exponential (and not e.g. $f_\theta(x)^2$)?

- Want to capture very large variations in probability. log-probability is the nature scale we want to work with. Otherwise need highly non-smooth $f_\theta$.
- Exponential families. Many common distributions can be written in this form.
- These distributions arise under fairly general assumptions in statistical physics (maximum entropy, second law of thermodynamics).
  - $f_\theta(x)$ is called the energy, hence the name.
  - Intuitively, configurations $x$ with low energy (high $f_\theta(x)$) are more likely.

# Energy-based Model

$$p_\theta(x) = \frac{\exp(f_\theta(x))}{Z(\theta)}, \quad Z(\theta) = \int \exp(f_\theta(x))dx$$

Pros:

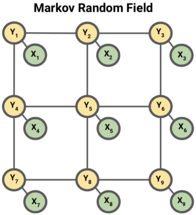
- extreme flexibility. pretty much any function $f_\theta(x)$ you want to use

Cons:

- Samping from $p_\theta(x)$ is hard
- Evaluating and optimizing likelihood $p_\theta(x)$ is hard (learning is hard)
- No feature learning (but can add latent variables)

**Curse of dimensionality**: The fundamental issue is that computing $Z(\theta)$ numerically (when no analytic solution is available) scales exponentially in the number of dimensions of $x$.

# Example: Ising Model



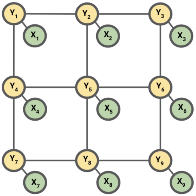
$X_i$: noisy pixels
$Y_i$: “true” pixels

- There is a true image $y \in \{0,1\}^{3\times 3}$, and a corrupted image $x \in \{0,1\}^{3\times 3}$. We know $x$, and want to somehow recover $y$.
- We model the joint probability distribution $p(y,x)$ as

$$p(y,x) \propto \exp\left(\sum_i \psi_i(x_i,y_i) + \sum_{i,j\in E} \psi_{i,j}(y_i,y_j)\right)$$

# Example: Ising Model

Markov Random Field



$X_i$: noisy pixels
$Y_i$: “true” pixels

The energy is $\sum_i \psi_i(x_i, y_i) + \sum_{i,j\in E} \psi_{i,j}(y_i, y_j)$

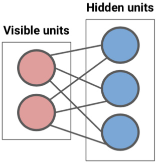
- $\psi_i(x_i, y_i)$: the $i$-th corrupted pixel depends on the $i$-th original pixel
- $\psi_{ij}(y_i, y_j)$: neighboring pixels tend to have the same value

How did the original image $y$ look like? Solution: maximize $p(y|x)$. Or equivalently, maximize $p(y, x)$.

# Example: Restricted Boltzmann Machine (RBM)

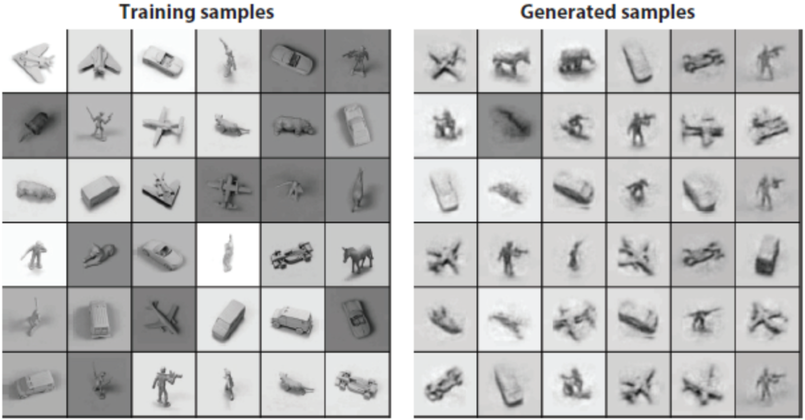
- RBM: energy-based model with latent variables
- Two types of variables:
  - $x \in \{0,1\}^n$ are visible variables (e.g., pixel values)
  - $z \in \{0,1\}^m$ are latent ones
- The joint distribution is

$$p_{W,b,c}(x,z) \propto \exp(x^T W z + b^T x + c^T z)$$



- Restricted as there are no within-class connections.
- Can be stacked together to make deep RBMs (one of the first generative models).

# Deep RBMs: Samples



Training samples

Generated samples

Adapted from Salakhutdinov and Hinton, 2009.

# Energy-based Models: Learning and Inference

- Learning by maximizing the likelihood function

$$\max_\theta \mathbb{E}_{x\sim p_{\text{data}}} \log p_\theta(x) = \max_\theta \left(\mathbb{E}_{x\sim p_{\text{data}}} f_\theta(x) - \log Z(\theta)\right)$$

- Gradient of log-likelihood:

$$\begin{aligned}\mathbb{E}_{x\sim p_{\text{data}}} \nabla_\theta f_\theta(x) - \nabla_\theta \log Z(\theta) &= \mathbb{E}_{x\sim p_{\text{data}}} \nabla_\theta f_\theta(x) - \frac{\nabla_\theta Z(\theta)}{Z(\theta)} \\ &= \mathbb{E}_{x\sim p_{\text{data}}} \nabla_\theta f_\theta(x) - \int \frac{\exp(f_\theta(x))}{Z(\theta)} \nabla_\theta f_\theta(x) dx \\ &= \mathbb{E}_{x\sim p_{\text{data}}} \nabla_\theta f_\theta(x) - \int p_\theta(x) \nabla_\theta f_\theta(x) dx \\ &= \mathbb{E}_{x\sim p_{\text{data}}} \nabla_\theta f_\theta(x) - \mathbb{E}_{x\sim p_\theta(x)} \nabla_\theta f_\theta(x)\end{aligned}$$

- **Contrastive Divergence**: sample $x_{\text{sample}} \sim p_\theta$, take gradient step on $\nabla_\theta f_\theta(x_{\text{train}}) - \nabla_\theta f_\theta(x_{\text{sample}})$.

# Sampling From EBMs

$$p_\theta(x) = \frac{\exp(f_\theta(x))}{Z(\theta)}, \quad Z(\theta) = \int \exp(f_\theta(x))dx$$

- No direct way to sample like in autoregressive or flow models.
- Can use gradient-based MCMC methods, e.g., SGLD

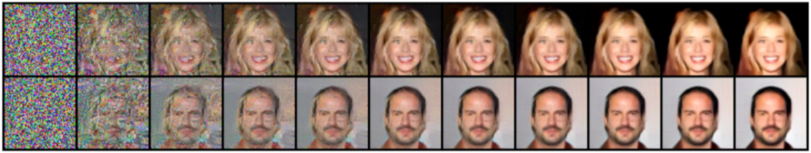
$$x^{t+1} = x^t + \epsilon \nabla_x \log p_\theta(x^t) + \sqrt{2\epsilon}\eta^t, \quad \eta^t \sim \mathcal{N}(0, I)$$

- Note that for energy-based models

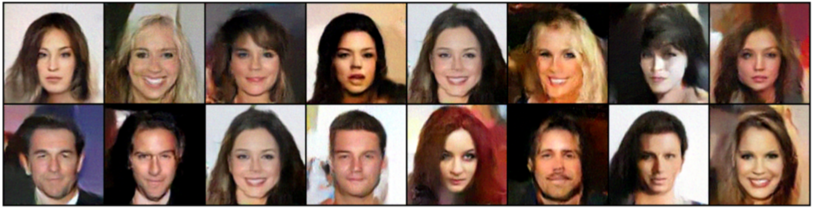
$$s_\theta(x) = \nabla_x \log p_\theta(x) = \nabla_x f_\theta(x) - \nabla_x \log Z(\theta) = \nabla_x f_\theta(x)$$

The score function does not depend on $Z(\theta)$!

# Modern EBMs



Langevin sampling



Face samples

Adapted from Nijkamp et al. 2019

# Training Without Sampling

$$x^{t+1} = x^t + \epsilon \nabla_x \log p_\theta(x^t) + \sqrt{2\epsilon}\eta^t, \quad \eta^t \sim \mathcal{N}(0, I)$$

- MCMC sampling converges slowly in high dimensional spaces, and repetitive sampling for each training iteration would be expensive.
- Can we train without sampling?
- Note that to generate samples from an EBM, we only need the score function $\nabla_x \log p_\theta(x)$.
- Can we properly train the score function without sampling?

# Score Matching

- A key observation: two distributions are identical iff their scores are the same

$$p(x) = q(x) \Leftrightarrow \nabla_x \log \tilde{p}(x) = \nabla_x \log \tilde{q}(x)$$

where $\tilde{p}, \tilde{q}$ are the unnormalized densities of $p, q$.

- Match the scores of the data distribution and EBMs by minimizing

$$\begin{aligned}&\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}}\|\nabla_x \log p_{\text{data}}(x) - s_\theta(x)\|^2\\ =&\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}}\|\nabla_x \log p_{\text{data}}(x) - \nabla_x f_\theta(x)\|^2\end{aligned}$$

This is also known as Fisher divergence.

# Score Matching

- Using integration by parts, we have

$$\begin{aligned}&\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}}\|\nabla_x \log p_{\text{data}}(x) - \nabla_x f_\theta(x)\|^2\\ =&\mathbb{E}_{x\sim p_{\text{data}}}\left(\operatorname{Tr}\left(\nabla_x^2 f_\theta(x)\right) + \frac{1}{2}\|\nabla_x f_\theta(x)\|^2\right) + \text{Const}\end{aligned}$$

- Sample a mini-batch of datapoints

$$\{x_1, x_2, \ldots, x_n\} \sim p_{\text{data}}(x)$$

- Estimate the score matching loss with the empirical mean

$$\frac{1}{n}\sum_{i=1}^{n}\left(\frac{1}{2}\|\nabla_x f_\theta(x_i)\|^2 + \operatorname{Tr}\left(\nabla_x^2 f_\theta(x_i)\right)\right)$$

# Score Matching

- Minimize the score matching loss via stochastic gradient descent.
- No need to sample from the EBM!
- Note that computing the trace of Hessian $\mathrm{Tr}\left(\nabla_x^2 f_\theta(x)\right)$ is in general very expensive for large models.
- Scalable score matching methods: denoising score matching (Vincent 2010) and sliced score matching (Song et al. 2019).

# Noise Contrastive Estimation

Learning an energy-based model by constrasting it with a noise distribuiton.

- Data distribution: $p_{\text{data}}(x)$.
- Noise distribution: $p_n(x)$. Should be analytically tractable and easy to sample from.
- Training a discriminator $D_\theta(x) \in [0,1]$ to distinguish between data samples and noise samples.

$$\max_\theta \mathbb{E}_{x\sim p_{\text{data}}} \log D_\theta(x) + \mathbb{E}_{x\sim p_n} \log(1 - D_\theta(x))$$

- Optimal discriminator

$$D_\theta^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_n(x)}$$

# Noise Contrastive Estimation

- If the discriminator is parameterized as

$$D_\theta(x) = \frac{p_\theta(x)}{p_\theta(x) + p_n(x)}$$

- The optimal discriminator $D_\theta^*(x)$ satisfies

$$D_\theta^*(x) = \frac{p_\theta^*(x)}{p_\theta^*(x) + p_n(x)} = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_n(x)}$$

or equivalently,

$$p_\theta^*(x) = p_{\text{data}}(x)$$

# Noise Contrastive Estimation for Training EBMs

- EBMs require $Z(\theta)$ to be a normalizing constant, which is hard to satisfy.
- We can model $Z(\theta)$ with an additional trainable parameter $Z$ that relaxs the normalizing constraint

$$p_{\theta,Z}(x) = \frac{\exp(f_\theta(x))}{Z}$$

- With noise contrastive estimation (NCE), the optimal parameters $\theta^*, Z^*$ satisfy

$$p_{\theta^*,Z^*}(x) = \frac{\exp(f_{\theta^*}(x))}{Z^*} = p_{\text{data}}(x)$$

- The optimal parameter $Z^*$ hence automatically satifies the constraint as $p_{\theta^*,Z^*}$ is a valid density function.

# Noise Contrastive Estimation for Training EBMs

- Now we parameterize the discriminator $D_{\theta,Z}(x)$ as

$$D_{\theta,Z}(x) = \frac{\exp(f_\theta(x))/Z}{\exp(f_\theta(x))/Z + p_n(x)} = \frac{\exp(f_\theta(x))}{\exp(f_\theta(x)) + p_n(x)Z}$$

- The training objective in NCE becomes

$$\begin{aligned}
&\max_{\theta,Z} \mathbb{E}_{x\sim p_{\text{data}}} \log D_{\theta,Z}(x) + \mathbb{E}_{x\sim p_n} \log(1 - D_{\theta,Z}(x)) \\
=&\max_{\theta,Z} \mathbb{E}_{x\sim p_{\text{data}}} (f_\theta(x) - \log(\exp(f_\theta(x)) + Zp_n(x))) \\
&+ \mathbb{E}_{x\sim p_n} (\log(Zp_n(x)) - \log(\exp(f_\theta(x)) + Zp_n(x)))
\end{aligned}$$

- One can use the log-sum-exp trick for numerical stability.

# Noise Contrastive Estimation for Training EBMs

- Sample a mini-batch of datapoints $x_1, x_2, \ldots, x_n \sim p_{\text{data}}(x)$.
- Sample a mini-batch of noise samples $y_1, y_2, \ldots, y_n \sim p_n(y)$.
- Estimate the NCE loss

$$\frac{1}{n}\sum_{i=1}^{n}\big(f_\theta(x_i) - \log(\exp(f_\theta(x_i)) + Zp_n(x_i)) \\ + \log Z + \log p_n(y_i) - \log(\exp(f_\theta(y_i)) + Zp_n(y_i))\big)$$

- Stochastic gradient ascent.
- No need to sample from the EBM!

# Comparing NCE and GAN

Similarities:

- Both involve training a discriminator to perform binary classification with a cross-entropy loss.
- Both are likelihood-free.

Differences:

- GAN requires adversarial training or minimax optimization for training, while NCE does not.
- NCE requires the likelihood of the noise distribution for training, while GAN only requires efficient sampling from the prior.
- NCE trains an energy-based model, while GAN trains a deterministic sample generator.

# Flow Contrastive Estimation

Intuition:

- We need to both evaluate the probability of $p_n(x)$, and sample from it efficiently.
- We hope to make the classification task as hard as possible, i.e., $p_n(x)$ should be close to $p_{\text{data}}(x)$.

Flow contrastive estimation:

- Parameterize the noise distribution with a normalizing flow model $p_{n,\phi}(x)$.
- Parameterize the discriminator $D_{\theta,Z,\phi}(x)$ as

$$D_{\theta,Z,\phi}(x) = \frac{\exp(f_\theta(x))/Z}{\exp(f_\theta(x))/Z + p_{n,\phi}(x)} = \frac{\exp(f_\theta(x))}{\exp(f_\theta(x)) + Zp_{n,\phi}(x)}$$

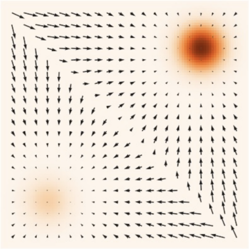
- Train the flow model to minimize $D_{JS}(p_{\text{data}}, p_{n,\phi})$:

$$\min_{\phi} \max_{\theta,Z} \mathbb{E}_{x\sim p_{\text{data}}} \log D_{\theta,Z,\phi}(x) + \mathbb{E}_{x\sim p_{n,\phi}} \log(1 - D_{\theta,Z,\phi}(x))$$

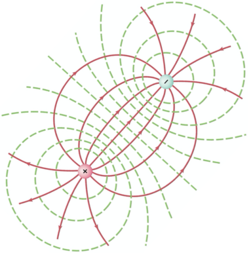
# Score-based Models

- When the pdf is differentiable, we can compute the gradient of a probability density, and use it to represent the distribution.

Score function $\nabla_x \log p(x)$



(pdf and score)



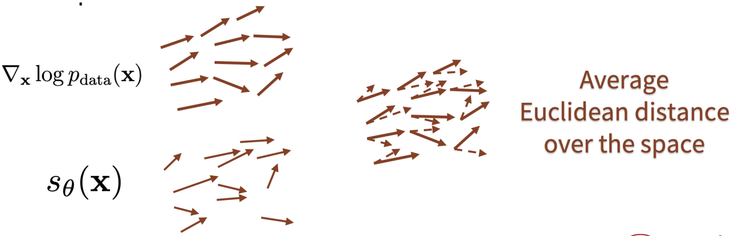
(Electrical potentials and fields)

# How to Train Score-based Models

- Given i.i.d. samples $\{x_1, \ldots, x_N\} \sim p(x)$
- We want to estimate the score $\nabla_x \log p_{\text{data}}(x)$
- Score model: a learnable vector-valued function

$$s_\theta(x) : \mathbb{R}^D \to \mathbb{R}$$

- Goal: $s_\theta(x) \approx \nabla_x \log p_{\text{data}}(x)$
- How to compare two vector fields of scores?



$\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$

$s_\theta(\mathbf{x})$

Average
Euclidean distance
over the space

# How to Train Score-based Models

- Objective: Average Euclidean distance over the whole space.

$$\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}}\|\nabla_x \log p_{\text{data}}(x) - s_\theta(x)\|^2$$

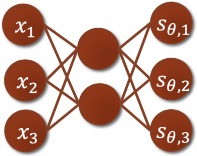
- **Score matching**:

$$\mathbb{E}_{x\sim p_{\text{data}}}\left(\frac{1}{2}\|s_\theta(x)\|^2 + \text{Tr}(\nabla_x s_\theta(x))\right)$$

- Requirements:
  - The score model must be efficient to evaluated.
  - Do we need the score model to be a proper score function?

# Score Matching is Not Scalable

- We can use deep neural networks for more expressive score models



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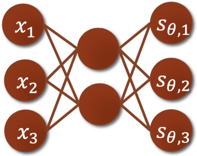

- However, $\mathrm{Tr}(\nabla_x s_\theta(x))$ can be a problem.

$O(D)$ Backprops!

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

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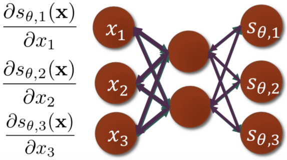
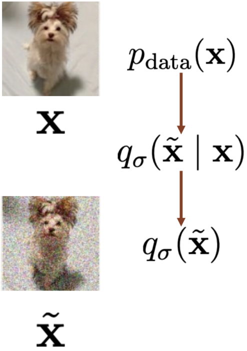

$\frac{\partial s_{\theta,1}(\mathbf{x})}{\partial x_1}$
$\frac{\partial s_{\theta,2}(\mathbf{x})}{\partial x_2}$
$\frac{\partial s_{\theta,3}(\mathbf{x})}{\partial x_3}$
$x_1$
$x_2$
$x_3$
$s_{\theta,1}$
$s_{\theta,2}$
$s_{\theta,3}$

- However, $\mathrm{Tr}(\nabla_x s_\theta(x))$ can be a problem.

$O(D)$ Backprops!

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

# Denoising Score Matching


$p_{\text{data}}(\mathbf{x})$
$\mathbf{x}$
$q_\sigma(\tilde{\mathbf{x}} \mid \mathbf{x})$
$q_\sigma(\tilde{\mathbf{x}})$
$\tilde{\mathbf{x}}$

- Denoising score matching (Vincent 2011) used a noise-perturbed data distribution

$$
\begin{aligned}
&\frac{1}{2}\mathbb{E}_{\tilde{x}\sim q_\sigma}\|\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}) - s_\theta(\tilde{x})\|^2 \\
=&\frac{1}{2}\int q_\sigma(\tilde{x})\|\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}) - s_\theta(\tilde{x})\|^2 d\tilde{x} \\
=&\frac{1}{2}\int q_\sigma(\tilde{x})\|s_\theta(\tilde{x})\|^2 d\tilde{x} \\
&-\int q_\sigma(\tilde{x})\nabla_{\tilde{x}}\log q_\sigma(\tilde{x})^T s_\theta(\tilde{x})d\tilde{x} + \text{Const}
\end{aligned}
$$

# Denoising Score Matching

- The second term can be rewritten as

$$
\begin{aligned}
-\int q_\sigma(\tilde{x})\nabla_{\tilde{x}}\log q_\sigma(\tilde{x})^T s_\theta(\tilde{x})d\tilde{x} &= -\int \nabla_{\tilde{x}} q_\sigma(\tilde{x})^T s_\theta(\tilde{x})d\tilde{x} \\
&= -\int \nabla_{\tilde{x}}\left(\int p_{\text{data}}(x)q_\sigma(\tilde{x}|x)dx\right)^T s_\theta(\tilde{x})d\tilde{x} \\
&= -\int \left(\int p_{\text{data}}(x)\nabla_{\tilde{x}} q_\sigma(\tilde{x}|x)dx\right)^T s_\theta(\tilde{x})d\tilde{x} \\
&= -\int\int p_{\text{data}}(x)q_\sigma(\tilde{x}|x)\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}|x)^T s_\theta(\tilde{x})dxd\tilde{x} \\
&= -\mathbb{E}_{x\sim p_{\text{data}}(x),\tilde{x}\sim q_\sigma(\tilde{x}|x)}\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}|x)^T s_\theta(\tilde{x})
\end{aligned}
$$

# Denoising Score Matching

- Plug it back we have

$$
\begin{aligned}
&\frac{1}{2}\mathbb{E}_{\tilde{x}\sim q_\sigma}\|\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}) - s_\theta(\tilde{x})\|^2 \\
=&\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}(x),\tilde{x}\sim q_\sigma(\tilde{x}|x)}\|s_\theta(\tilde{x}) - \nabla_{\tilde{x}}\log q_\sigma(\tilde{x}|x)\|^2 + \text{Const}
\end{aligned}
$$

- The noise score $\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}|x)$ is easy to compute. For example, when use Gaussian noise $q_\sigma(\tilde{x}|x) = \mathcal{N}(\tilde{x}|x,\sigma^2 I)$, the score is

$$\nabla_{\tilde{x}}\log q_\sigma(\tilde{x}|x) = -\frac{\tilde{x}-x}{\sigma^2}$$

- Pros: efficient to optimize even for very high dimensional data, and useful for optimal denoising.
- Cons: cannot estimate the score of clean data (noise-free)

# Denoising Score Matching

- Sample a minibatch of datapoints $\{x_1, \ldots, x_n\} \sim p_{\text{data}}(x)$.
- Sample a minibatch of perturbed datapoints

$$\tilde{x}_i \sim q_\sigma(\tilde{x}_i | x_i), \quad i = 1, 2, \ldots, n$$

- Estimate the denoising score matching loss with empirical means

$$\frac{1}{2n} \sum_{i=1}^{n} \| s_\theta(\tilde{x}) - \nabla_{\tilde{x}} \log q_\sigma(\tilde{x}_i | x) \|^2$$

- Stochastic gradient descent
- Need to choose a very small $\sigma$! However, the loss variance would also increase drastically as $\sigma \to 0$!

# Tweedie's Formula and Denoising Score Matching

- Denoising score matching is suitable for optimal denoising
- Given $p(x)$, $q_\sigma(\tilde{x}|x) = \mathcal{N}(\tilde{x}|x, \sigma^2 I)$, we can define the posterior $p(x|\tilde{x})$ with Bayes' rule

$$p(x|\tilde{x}) = \frac{p(x)q_\sigma(\tilde{x}|x)}{q_\sigma(\tilde{x})}$$

  where

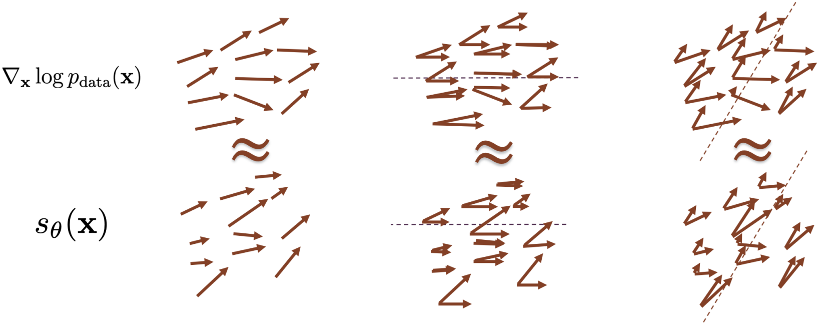
$$q_\sigma(\tilde{x}) = \int p(x)q_\sigma(\tilde{x}|x)dx$$

- Tweedie's formula:

$$\begin{aligned}\mathbb{E}_{x\sim p(x|\tilde{x})}[x] &= \tilde{x} + \sigma^2 \nabla_{\tilde{x}} \log q_\sigma(\tilde{x}) \\ &\approx \tilde{x} + \sigma^2 s_\theta(\tilde{x})\end{aligned}$$

# Sliced Score Matching

- One dimensional problems should be easier.
- Consider projections onto random directions.
- Sliced score matching (Song et al 2019).



# Sliced Score Matching

- Objective: Sliced Fisher Divergence

$$\frac{1}{2}\mathbb{E}_{v\sim p_v}\mathbb{E}_{x\sim p_{\text{data}}}\left(v^T\nabla_x \log p_{\text{data}}(x) - v^T s_\theta(x)\right)^2$$

- Similarly, we can do integration by parts

$$\mathbb{E}_{v\sim p_v}\mathbb{E}_{x\sim p_{\text{data}}}\left(v^T\nabla_x s_\theta(x)v + \frac{1}{2}(v^T s_\theta(x))^2\right)$$

- Computing Jacobian-vector products is scalable

$$v^T\nabla_x s_\theta(x)v = v^T\nabla_x(s_\theta(x)^T v)$$

This only requires one backpropagation!

# Sliced Score Matching

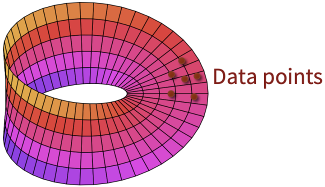
- Sample a minibatch of datapoints $\{x_1, \ldots, x_n\} \sim p_{\text{data}}(x)$
- Sample a minibatch of projection directions $\{v_i \sim p_v\}_{i=1}^n$
- Estimate the sliced score matching loss with empirical means

$$\frac{1}{n}\sum_{i=1}^{n}\left(v_i^T \nabla_x s_\theta(x_i) v_i + \frac{1}{2}(v_i^T s_\theta(x_i))^2\right)$$

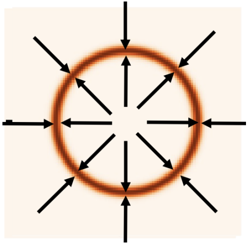
- The perturbation distribution is typically Gaussian or Rademacher. When $\mathbb{E}vv^T = I$, this is equivalent to the Hutchinson's trick.
- Can use $\|s_\theta(x)\|^2$ instead of $(v^T s_\theta(x))^2$ to reduce variance.
- Can use more projections per datapoint to boost performance.

# Pitfalls: Manifold Hypothesis

- Datapoints would lie on a lower dimensional manifold.

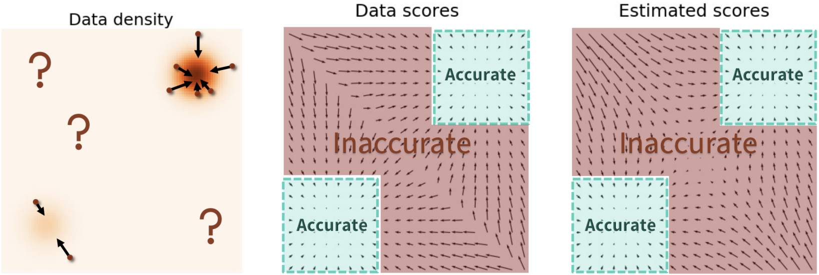


- Data score hence would be undefined.



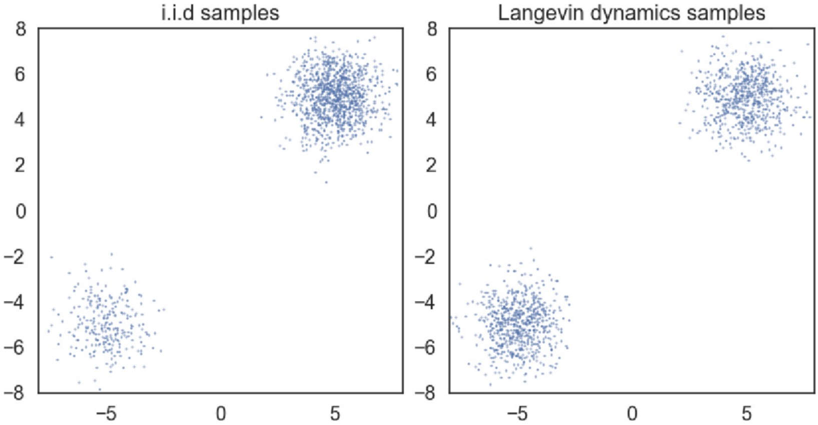
# Pitfalls: Challenges in Low Data Density Region

$$\frac{1}{2}\mathbb{E}_{x\sim p_{\text{data}}}\|\nabla_x \log p_{\text{data}}(x) - s_\theta(x)\|^2$$



- Poor score estimation in low data density regions.
- Langevin MCMC will also have trouble exploring low density regions.

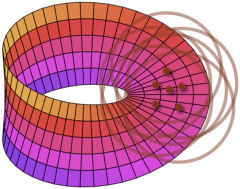
# Pitfalls: Slow Mixing Between Data Modes



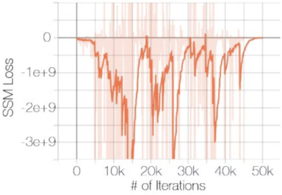
Adapted from Song et al 2019.

# Gaussian Perturbation

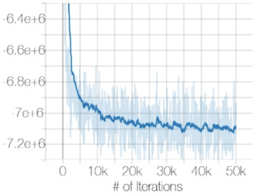
- The solution to all pitfalls: Gaussian perturbation!
- Inflate the flat manifold with noise.



- Score matching on noise data



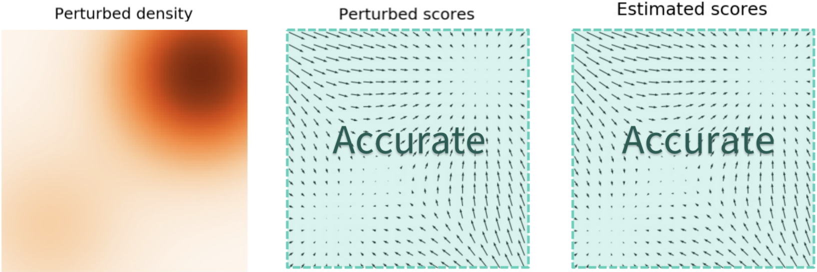
CIFAR-10



Noisy CIFAR-10

# Noisy Data Score Estimation

$$\frac{1}{2}\mathbb{E}_{\tilde{x}\sim q_\sigma}\|\nabla_{\tilde{x}}\log q_\sigma(\tilde{x})-s_\theta(\tilde{x})\|^2$$

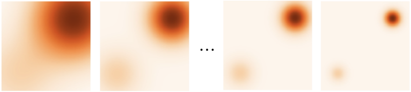


- Noisy score can provide useful directional information for Langevin MCMC.

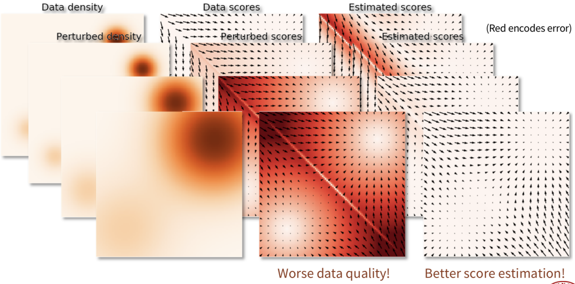
# Multi-scale Noise Perturbation

- Multi-scale noise perturbations.

$$\sigma_1 > \sigma_2 > \cdots > \sigma_{L-1} > \sigma_L$$

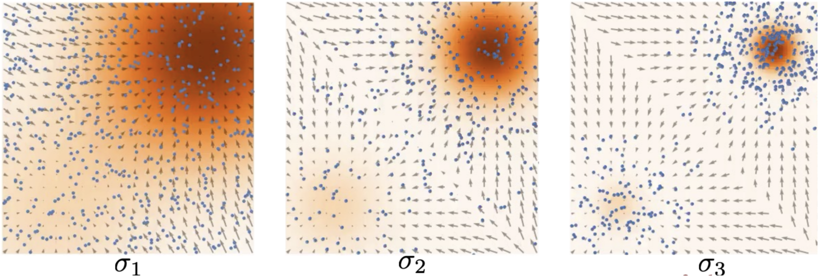


- Trading off data quality and estimator accuracy



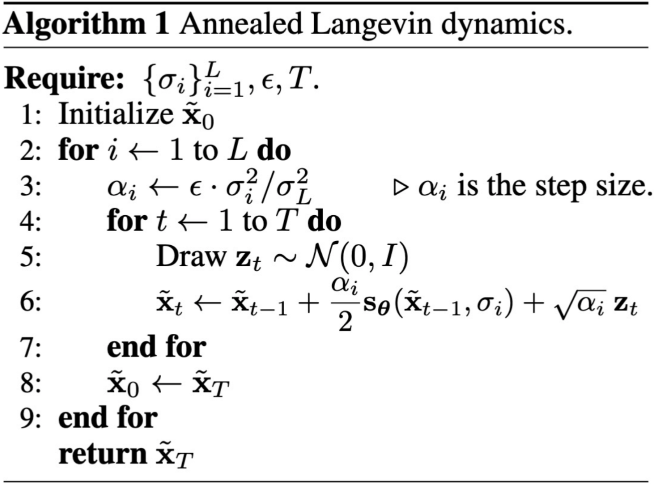
# Annealed Langevin Dynamics

- Sample using $\sigma_1, \ldots, \sigma_L$ sequentially with Langevin dynamics.
- Anneal down the noise level.
- Samples used as initialization for the next level.



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

# Annealed Langevin Dynamics

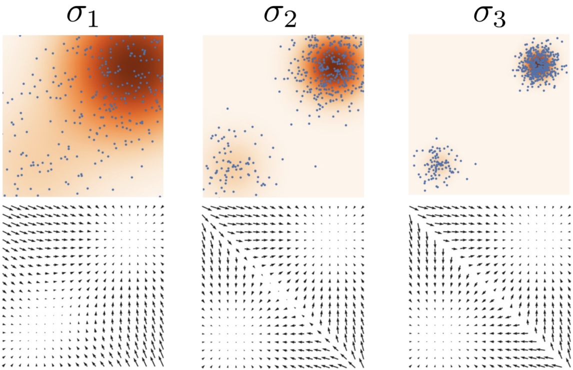


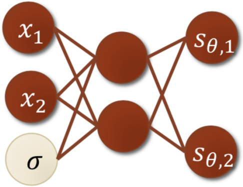
**Algorithm 1** Annealed Langevin dynamics.

```
Require: $\{\sigma_i\}_{i=1}^{L}, \epsilon, T$.
Initialize $\tilde{\mathbf{x}}_0$
for $i \leftarrow 1$ to $L$ do
    $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2/\sigma_L^2$        ▷ $\alpha_i$ is the step size.
    for $t \leftarrow 1$ to $T$ do
        Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
        $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2}\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\,\mathbf{z}_t$
    end for
    $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
end for
return $\tilde{\mathbf{x}}_T$
```

# Noise Conditional Score Networks

- Learning score functions jointly with noise conditional score networks!





Noise Conditional
Score Network
(NCSN)

# Training Noise Conditional Score Networks

- As the goal is to estimate the score of perturbed data distributions, we can use denoising score matching for training.
- Assign different weights to combine denoising score matching losses for different noise levels.

$$
\begin{aligned}
&\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)\mathbb{E}_{\tilde{x}\sim q_{\sigma_i}(\tilde{x})}\|\nabla_{\tilde{x}}\log q_{\sigma_i}(\tilde{x}) - s_\theta(\tilde{x},\sigma_i)\|^2 \\
= &\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)\mathbb{E}_{x\sim p_{\text{data}},\tilde{x}\sim q_{\sigma_i}(\tilde{x}|x)}\|\nabla_{x}\log q_{\sigma_i}(\tilde{x}|x) - s_\theta(\tilde{x},\sigma_i)\|^2 + \text{Const} \\
= &\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)\mathbb{E}_{x\sim p_{\text{data}},z\sim\mathcal{N}(0,I)}\|s_\theta(x+\sigma_i z,\sigma_i) + \frac{z}{\sigma_i}\|^2 + \text{Const.}
\end{aligned}
$$

# Noise Scales and Weighting Functions

- Adjacent noise scales should have sufficient overlap to ease transitioning across noise scales in annealed Langevin dynamics.
- For example, a geometric progression

$$\frac{\sigma_i}{\sigma_{i+1}} = \alpha > 1, \quad i = 1, \ldots, L-1$$

- What about the weighting function $\lambda$?
- Use $\lambda(\sigma) = \sigma^2$ to balance different score matching losses

$$\begin{aligned}
&\frac{1}{L}\sum_{i=1}^{L} \sigma_i^2 \mathbb{E}_{x\sim p_{\text{data}}, z\sim\mathcal{N}(0,I)} \| s_\theta(x+\sigma_i z, \sigma_i) + \frac{z}{\sigma_i} \|^2 \\
=&\frac{1}{L}\sum_{i=1}^{L} \mathbb{E}_{x\sim p_{\text{data}}, z\sim\mathcal{N}(0,I)} \| \sigma_i s_\theta(x+\sigma_i z, \sigma_i) + z \|^2
\end{aligned}$$

# Training Noise Conditional Score Networks

- Sample a mini-batch of datapoints $\{x_1, \ldots, x_n\} \sim p_{\text{data}}$.
- Sample a mini-batch of noise scale indices

$$\{i_1, \ldots, i_n\} \sim \mathcal{U}\{1, 2, \ldots, L\}$$

- Sample a mini-batch of Gaussian noise

$$\{z_1, \ldots, z_n\} \sim \mathcal{N}(0, I)$$

- Estimate the weighted mixture of score matching losses

$$\frac{1}{n}\sum_{k=1}^{n} \|\sigma_{i_k} s_\theta(x_k + \sigma_{i_k} z_k, \sigma_{i_k}) + z_k\|^2$$

- As efficient as training one single non-conditional score-based model.

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