Energy-Based Models

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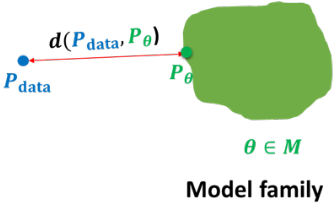
Lecture 12

Recap. of last lecture



- Energy-based models: $p_\theta(\mathbf{x}) = \frac{\exp\{f_\theta(\mathbf{x})\}}{Z(\theta)}$.
  - $Z(\theta)$ is intractable, so no access to likelihood.
  - Comparing the probability of two points is easy: $p_\theta(\mathbf{x}')/p_\theta(\mathbf{x}) = \exp(f_\theta(\mathbf{x}') - f_\theta(\mathbf{x}))$.
- Maximum likelihood training: $\max_\theta\{f_\theta(\mathbf{x}_{train}) - \log Z(\theta)\}$.
  - Contrastive divergence:

$$\nabla_\theta f_\theta(\mathbf{x}_{train}) - \nabla_\theta \log Z(\theta) \approx \nabla_\theta f_\theta(\mathbf{x}_{train}) - \nabla_\theta f_\theta(\mathbf{x}_{sample}),$$

where $\mathbf{x}_{sample} \sim p_\theta(\mathbf{x})$.

Sampling from EBMs: MH-MCMC

Metropolis-Hastings Markov chain Monte Carlo (MCMC).

1. $\mathbf{x}^0 \sim \pi(\mathbf{x})$
2. Repeat for $t = 0, 1, 2, \cdots, T-1$:
   - $\mathbf{x}' = \mathbf{x}^t + \text{noise}$
   - $\mathbf{x}^{t+1} = \mathbf{x}'$ if $f_\theta(\mathbf{x}') \geq f_\theta(\mathbf{x}^t)$
   - If $f_\theta(\mathbf{x}') < f_\theta(\mathbf{x}^t)$, set $\mathbf{x}^{t+1} = \mathbf{x}'$ with probability $\exp\{f_\theta(\mathbf{x}') - f_\theta(\mathbf{x}^t)\}$, otherwise set $\mathbf{x}^{t+1} = \mathbf{x}^t$.

Properties:

- In theory, $\mathbf{x}^T$ converges to $p_\theta(\mathbf{x})$ when $T \to \infty$. Why?
  - Satisfies *detailed balance condition*: $p_\theta(\mathbf{x}) T_{\mathbf{x} \to \mathbf{x}'} = p_\theta(\mathbf{x}') T_{\mathbf{x}' \to \mathbf{x}}$ where $T_{\mathbf{x} \to \mathbf{x}'}$ is the probability of transitioning from $\mathbf{x}$ to $\mathbf{x}'$
  - If $\mathbf{x}^t$ is distributed as p_θ, then $\mathbf{x}^{t+1}$ is distributed as p_θ.
- In practice, need a large number of iterations and convergence slows down exponentially in dimensionality.

Sampling from EBMs: unadjusted Langevin MCMC

Unadjusted Langevin MCMC:

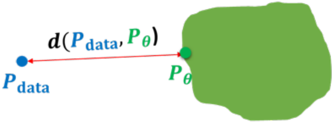
1. $\mathbf{x}^0 \sim \pi(\mathbf{x})$
2. Repeat for $t = 0, 1, 2, \cdots, T-1$:
   - $\mathbf{z}^t \sim \mathcal{N}(0, I)$
   - $\mathbf{x}^{t+1} = \mathbf{x}^t + \epsilon \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})|_{\mathbf{x}=\mathbf{x}^t} + \sqrt{2\epsilon}\mathbf{z}^t$

Properties:

- $\mathbf{x}^T$ converges to a sample from $p_\theta(\mathbf{x})$ when $T \to \infty$ and $\epsilon \to 0$.
- $\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} f_\theta(\mathbf{x})$ for continuous energy-based models.
- Convergence slows down as dimensionality grows.

Sampling converges slowly in high dimensional spaces and is thus very expensive, yet we need sampling for **each training iteration** in contrastive divergence.

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



$\theta \in M$

Model family

Goal: Training without sampling

- Score Matching
- Noise Contrastive Estimation
- Adversarial training

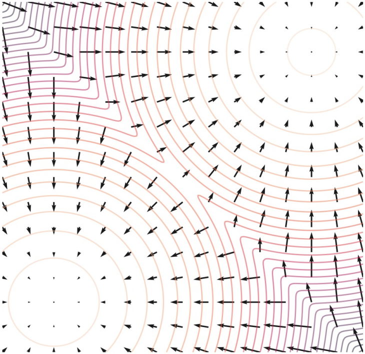
Score function

Energy-based model: $p_\theta(\mathbf{x}) = \frac{\exp\{f_\theta(\mathbf{x})\}}{Z(\theta)}$, $\log p_\theta(\mathbf{x}) = f_\theta(\mathbf{x}) - \log Z(\theta)$

(Stein) Score function:

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

- Gaussian distribution
  $p_\theta(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
  $\longrightarrow s_\theta(x) = -\frac{x-\mu}{\sigma^2}$
- Gamma distribution
  $p_\theta(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}$
  $\longrightarrow s_\theta(x) = \frac{\alpha-1}{x} - \beta$



$p_\theta(\mathbf{x})$ vs. $s_\theta(\mathbf{x})$

Score matching

Observation

$s_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})$ is independent of the partition function $Z(\theta)$.

Fisher divergence between $p(\mathbf{x})$ and $q(\mathbf{x})$:

$$D_F(p, q) := \frac{1}{2} E_{\mathbf{x}\sim p}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - \nabla_{\mathbf{x}} \log q(\mathbf{x})\|_2^2]$$

Score matching: minimizing the Fisher divergence between $p_{\text{data}}(\mathbf{x})$ and the EBM $p_\theta(\mathbf{x}) \propto \exp\{f_\theta(\mathbf{x})\}$

$$\frac{1}{2} E_{\mathbf{x}\sim p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - s_\theta(\mathbf{x})\|_2^2]$$
$$= \frac{1}{2} E_{\mathbf{x}\sim p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \nabla_{\mathbf{x}} f_\theta(\mathbf{x})\|_2^2]$$

Score matching

$$\frac{1}{2}E_{\mathbf{x}\sim p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})\|_2^2]$$

How to deal with $\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$ given only samples? Integration by parts!

$$\frac{1}{2}E_{x\sim p_{\text{data}}}[(\nabla_x \log p_{\text{data}}(x) - \nabla_x \log p_\theta(x))^2] \quad \text{(Univariate case)}$$

$$= \frac{1}{2}\int p_{\text{data}}(x)[(\nabla_x \log p_{\text{data}}(x) - \nabla_x \log p_\theta(x))^2]\mathrm{d}x$$

$$= \frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_{\text{data}}(x))^2\mathrm{d}x + \frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_\theta(x))^2\mathrm{d}x$$

$$- \int p_{\text{data}}(x)\nabla_x \log p_{\text{data}}(x)\nabla_x \log p_\theta(x)\mathrm{d}x$$

Recall Integration by parts: $\int f'g = fg - \int g'f$.

$$- \int p_{\text{data}}(x)\nabla_x \log p_{\text{data}}(x)\nabla_x \log p_\theta(x)\mathrm{d}x$$

$$= -\int p_{\text{data}}(x)\frac{1}{p_{\text{data}}(x)}\nabla_x p_{\text{data}}(x)\nabla_x \log p_\theta(x)\mathrm{d}x$$

$$= \underbrace{-p_{\text{data}}(x)\nabla_x \log p_\theta(x)\Big|_{x=-\infty}^{\infty}}_{=0} + \int p_{\text{data}}(x)\nabla_x^2 \log p_\theta(x)\mathrm{d}x$$

$$= \int p_{\text{data}}(x)\nabla_x^2 \log p_\theta(x)\mathrm{d}x$$

Note: we need to assume p_{data} decays sufficiently rapidly, $p_{\text{data}}(x) \to 0$ when $x \to \pm\infty$.

Score matching

Univariate score matching

$$\frac{1}{2}E_{x\sim p_{\text{data}}}[(\nabla_x \log p_{\text{data}}(x) - \nabla_x \log p_\theta(x))^2]$$
$$= \frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_{\text{data}}(x))^2 \mathrm{d}x + \frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_\theta(x))^2 \mathrm{d}x$$
$$- \int p_{\text{data}}(x)\nabla_x \log p_{\text{data}}(x)\nabla_x \log p_\theta(x)\mathrm{d}x$$
$$= \underbrace{\frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_{\text{data}}(x))^2 \mathrm{d}x}_{\text{const. wrt } \theta} + \frac{1}{2}\int p_{\text{data}}(x)(\nabla_x \log p_\theta(x))^2 \mathrm{d}x$$
$$+ \int p_{\text{data}}(x)\nabla_x^2 \log p_\theta(x)\mathrm{d}x$$
$$= E_{x\sim p_{\text{data}}}[\tfrac{1}{2}(\nabla_x \log p_\theta(x))^2 + \nabla_x^2 \log p_\theta(x)] + \text{const.}$$

Multivariate score matching (integration by parts, i.e. Gauss theorem)

$$\frac{1}{2}E_{\mathbf{x}\sim p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})\|_2^2]$$
$$= E_{\mathbf{x}\sim p_{\text{data}}}\left[\frac{1}{2}\|\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})\|_2^2 + \operatorname{tr}\Big(\underbrace{\nabla_{\mathbf{x}}^2 \log p_\theta(\mathbf{x})}_{\text{Hessian of } \log p_\theta(\mathbf{x})}\Big)\right] + \text{const.}$$

Score matching

1. Sample a mini-batch of datapoints $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\} \sim p_{\text{data}}(\mathbf{x})$.
2. Estimate the score matching loss with the empirical mean

$$\frac{1}{n}\sum_{i=1}^{n}\left[\frac{1}{2}\|\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}_i)\|_2^2 + \text{tr}(\nabla_{\mathbf{x}}^2 \log p_\theta(\mathbf{x}_i))\right]$$
$$=\frac{1}{n}\sum_{i=1}^{n}\left[\frac{1}{2}\|\nabla_{\mathbf{x}} f_\theta(\mathbf{x}_i)\|_2^2 + \text{trace}(\nabla_{\mathbf{x}}^2 f_\theta(\mathbf{x}_i))\right]$$

3. Stochastic gradient descent.
4. No need to sample from the EBM!

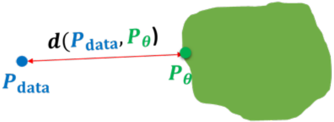
Caveat

Computing the trace of Hessian $\text{tr}(\nabla_{\mathbf{x}}^2 \log p_\theta(\mathbf{x}))$ is in general very expensive for large models.

Denoising score matching (Vincent 2010) and sliced score matching (Song et al. 2019). More on this in the next lecture!

Recap.

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



$\theta \in M$

Model family

Distances used for training energy-based models.

- KL divergence = maximum likelihood.

$$\nabla_\theta f_\theta(\mathbf{x}_{data}) - f_\theta(\mathbf{x}_{sample}) \quad \text{(contrastive divergence)}$$

- Fisher divergence = score matching.

$$\frac{1}{2} E_{\mathbf{x} \sim p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \nabla_{\mathbf{x}} f_\theta(\mathbf{x})\|_2^2]$$

Noise contrastive estimation

Learning an energy-based model by contrasting it with a noise distribution.

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

$$\max_\theta E_{\mathbf{x} \sim p_{\text{data}}}[\log D_\theta(\mathbf{x})] + E_{\mathbf{x} \sim p_n}[\log(1 - D_\theta(\mathbf{x}))]$$

- What is the Optimal discriminator $D_{\theta^*}(\mathbf{x})$?

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

Noise contrastive estimation

What if the discriminator is parameterized by

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

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

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

- By training the discriminator, we are implicitly learning $p_{\theta^*}(\mathbf{x}) \approx p_{\text{data}}(\mathbf{x})$. Particularly suitable for cases where $p_\theta(\mathbf{x})$ is defined up to a normalization constant (EBMs)
- Equivalently,

$$p_{\theta^*}(\mathbf{x}) = \frac{p_n(\mathbf{x}) D_{\theta^*}(\mathbf{x})}{1 - D_{\theta^*}(\mathbf{x})} = p_{\text{data}}(\mathbf{x})$$

  Classifier is used to correct density estimates from p_n. Can be used to improve a base generative model (*Boosted Generative Models*, Grover et al., 2018)

Noise contrastive estimation for training EBMs

Energy-based model:

$$p_\theta(\mathbf{x}) = \frac{e^{f_\theta(\mathbf{x})}}{Z(\theta)}$$

The constraint $Z(\theta) = \int e^{f_\theta(\mathbf{x})} \mathrm{d}\mathbf{x}$ is hard to satisfy.
Solution: Modeling $Z(\theta)$ with an additional trainable parameter Z that is not explicitly constrained to satisfy $Z = \int e^{f_\theta(\mathbf{x})} \mathrm{d}\mathbf{x}$.

$$p_{\theta, Z}(\mathbf{x}) = \frac{e^{f_\theta(\mathbf{x})}}{Z}$$

With noise contrastive estimation, the optimal parameters θ^*, Z^* are

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

The optimal parameter Z^* is the correct partition function, because

$$\int \frac{e^{f_{\theta^*}(\mathbf{x})}}{Z^*} \mathrm{d}\mathbf{x} = \int p_{\text{data}}(\mathbf{x}) \mathrm{d}\mathbf{x} = 1 \implies Z^* = \int e^{f_{\theta^*}(\mathbf{x})} \mathrm{d}\mathbf{x}$$

Noise contrastive estimation for training EBMs

The discriminator $D_{\theta,Z}(\mathbf{x})$ for probabilistic model $p_{\theta,Z}(\mathbf{x})$ is

$$D_{\theta,Z}(\mathbf{x}) = \frac{\frac{e^{f_\theta(\mathbf{x})}}{Z}}{\frac{e^{f_\theta(\mathbf{x})}}{Z} + p_n(\mathbf{x})} = \frac{e^{f_\theta(\mathbf{x})}}{e^{f_\theta(\mathbf{x})} + p_n(\mathbf{x})Z}$$

Noise contrastive estimation training

$$\max_{\theta,Z} E_{\mathbf{x}\sim p_{\text{data}}}[\log D_{\theta,Z}(\mathbf{x})] + E_{\mathbf{x}\sim p_n}[\log(1 - D_{\theta,Z}(\mathbf{x}))]$$

Equivalently,

$$\begin{aligned}\max_{\theta,Z} E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x}) - \log(e^{f_\theta(\mathbf{x})} + Zp_n(\mathbf{x}))] \\ + E_{\mathbf{x}\sim p_n}[\log(Zp_n(\mathbf{x})) - \log(e^{f_\theta(\mathbf{x})} + Zp_n(\mathbf{x}))]\end{aligned}$$

Log-sum-exp trick for numerical stability:

$$\begin{aligned}\log(e^{f_\theta(\mathbf{x})} + Zp_n(\mathbf{x})) &= \log(e^{f_\theta(\mathbf{x})} + e^{\log Z + \log p_n(\mathbf{x})}) \\ &= \text{logsumexp}(f_\theta(\mathbf{x}), \log Z + \log p_n(\mathbf{x}))\end{aligned}$$

Noise contrastive estimation for training EBMs

1. Sample a mini-batch of datapoints $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n \sim p_{\text{data}}(\mathbf{x})$.
2. Sample a mini-batch of noise samples $\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_n \sim p_n(\mathbf{y})$.
3. Estimate the NCE loss.

$$\frac{1}{n}\sum_{i=1}^{n}[f_\theta(\mathbf{x}_i) - \text{logsumexp}(f_\theta(\mathbf{x}_i), \log Z + \log p_n(\mathbf{x}_i))$$
$$+ \log Z + p_n(\mathbf{y}_i) - \text{logsumexp}(f_\theta(\mathbf{y}_i), \log Z + \log p_n(\mathbf{y}_i))]$$

4. Stochastic gradient ascent with respect to θ and Z.
5. 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 (recall likelihood not tractable in EBM).

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 (Gao et al. 2020)

Observations:

- We need to both evaluate the probability of $p_n(\mathbf{x})$, and sample from it efficiently.
- We hope to make the classification task as hard as possible, i.e., $p_n(\mathbf{x})$ should be close to $p_{\text{data}}(\mathbf{x})$ (but not exactly the same).

Flow contrastive estimation:

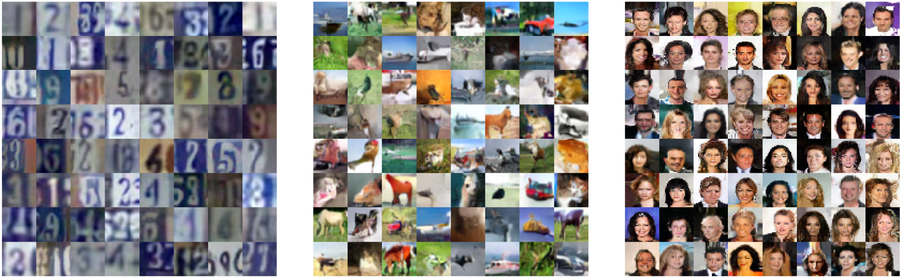
- Parameterize the noise distribution with a normalizing flow model $p_{n,\phi}(\mathbf{x})$.
- Parameterize the discriminator $D_{\theta,Z,\phi}(\mathbf{x})$ as

$$D_{\theta,Z,\phi}(\mathbf{x}) = \frac{\frac{e^{f_\theta(\mathbf{x})}}{Z}}{\frac{e^{f_\theta(\mathbf{x})}}{Z} + p_{n,\phi}(\mathbf{x})} = \frac{e^{f_\theta(\mathbf{x})}}{e^{f_\theta(\mathbf{x})} + p_{n,\phi}(\mathbf{x})Z}$$

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

$$\min_\phi \max_{\theta,Z} E_{\mathbf{x}\sim p_{\text{data}}}[\log D_{\theta,Z,\phi}(\mathbf{x})] + E_{\mathbf{x}\sim p_{n,\phi}}[\log(1 - D_{\theta,Z,\phi}(\mathbf{x}))]$$

Flow contrastive estimation (Gao et al. 2020)



Samples from SVHN, CIFAR-10, and CelebA datasets.

Image source: Gao et al. 2020.

Adversarial training for EBMs

Energy-based model:

$$p_\theta(\mathbf{x}) = \frac{e^{f_\theta(\mathbf{x})}}{Z(\theta)}$$

Upper bounding its log-likelihood with a variational distribution $q_\phi(\mathbf{x})$:

$$\begin{aligned}
E_{\mathbf{x}\sim p_{\text{data}}}[\log p_\theta(\mathbf{x})] &= E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - \log Z(\theta) \\
&= E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - \log \int e^{f_\theta(\mathbf{x})} \mathrm{d}\mathbf{x} \\
&= E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - \log \int q_\phi(\mathbf{x}) \frac{e^{f_\theta(\mathbf{x})}}{q_\phi(\mathbf{x})} \mathrm{d}\mathbf{x} \\
&\leq E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - \int q_\phi(\mathbf{x}) \log \frac{e^{f_\theta(\mathbf{x})}}{q_\phi(\mathbf{x})} \mathrm{d}\mathbf{x} \\
&= E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - E_{\mathbf{x}\sim q_\phi}[f_\theta(\mathbf{x})] - H(q_\phi(\mathbf{x}))
\end{aligned}$$

Adversarial training

$$\max_\theta \min_\phi E_{\mathbf{x}\sim p_{\text{data}}}[f_\theta(\mathbf{x})] - E_{\mathbf{x}\sim q_\phi}[f_\theta(\mathbf{x})] - H(q_\phi(\mathbf{x}))$$

What do we require for the model $q_\phi(\mathbf{x})$?

Conclusion

- Energy-based models are very flexible probabilistic models with intractable partition functions.
- Sampling is hard and typically requires iterative MCMC approaches.
- Computing the likelihood is hard.
- Comparing the likelihood/probability of two different points is tractable.
- Maximum likelihood training by contrastive divergence. Requires sampling for each training iteration.
- Sampling-free training: score matching.
- Sampling-free training: noise contrastive estimation. Additionally provides an estimate of the partition function.
- Sampling-free training: adversarial optimization.
- Reference: *How to Train Your Energy-Based Models* by Yang Song and Durk Kingma.