Deep Generative Models (Fall 2024)

CS HUFS

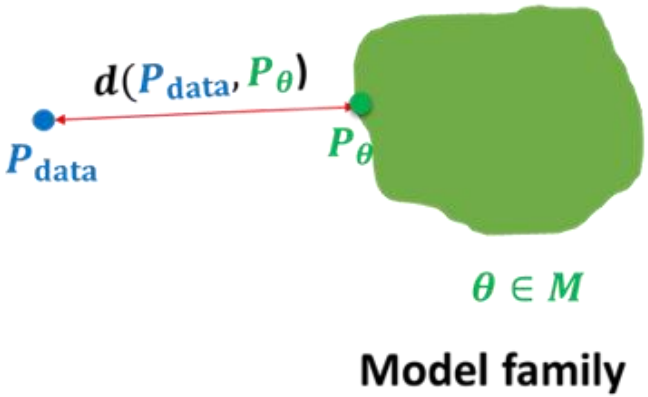
Training Generative Models

- Learning as density estimation
- KL divergence
- Maximum likelihood
- Monte Carlo estimation
- MLE learning: gradience descent
- Overfitting
- Bias-Variance trade off
- Conditional generative models

Learning a generative model

- We are given a training set of examples, e.g., images of dogs

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



- We want to learn a probability distribution $p(x)$ over images x such that
  - **Generation:** If we sample $x_{new} \sim p(x)$, x_{new} should look like a dog (*sampling*)
  - **Density estimation:** $p(x)$ should be high if x looks like a dog, and low otherwise (*anomaly detection*)
  - **Unsupervised representation learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc. (*features*)
- First question: how to represent $p_\theta(x)$. Second question: **how to learn it.**

Setting

- Lets assume that the domain is governed by some underlying distribution P_{data}
- We are given a dataset D of m samples from P_{data}
  - Each sample is an assignment of values to (a subset of) the variables, e.g., $(X_{\text{bank}} = 1, X_{\text{dollar}} = 0, \ldots, Y = 1)$ or pixel intensities.
- The standard assumption is that the data instances are **independent and identically distributed (IID)**
- We are also given a family of models M, and our task is to learn some "good" distribution in this set:
  - For example, M could be all Bayes nets with a given graph structure, for all possible choices of the CPD tables
  - For example, a FVSBN for all possible choices of the logistic regression parameters , θ = concatenation of all logistic regression coefficients

* CPD: Conditional Probability Distribution

Goal of learning

- The goal of learning is to return a model P_θ that precisely captures the distribution P_{data} from which our data was sampled
- This is in general not achievable because of
  - limited data only provides a rough approximation of the true underlying distribution
  - computational reasons
- Example. Suppose we represent each image with a vector X of 784 binary variables (black vs. white pixel). How many possible states (= possible images) in the model? $2^{784} \approx 10^{236}$. Even 10^7 training examples provide *extremely* sparse coverage!
- We want to select P_θ to construct the ″best″ approximation to the underlying distribution P_{data}
- What is ″best″?

What is "best"?

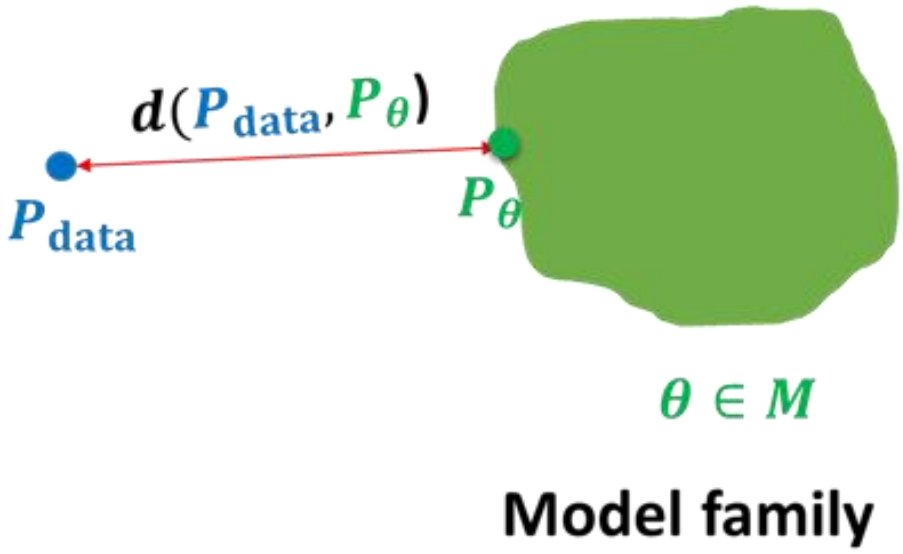
This depends on what we want to do

1. Density estimation: we are interested in the full distribution (so later we can compute whatever conditional probabilities we want)
2. Specific prediction tasks: we are using the distribution to make a prediction
   - Is this email spam or not?
   - **Structured prediction:** Predict next frame in a video or caption given an image
3. Structure or knowledge discovery: we are interested in the model itself
   - How do some genes interact with each other?
   - What causes cancer?

Learning as density estimation

- We want to learn the full distribution so that later we can answer *any* probabilistic inference query
- In this setting we can view the learning problem as **density estimation**
- We want to construct P_θ as "close" as possible to P_{data} (recall we assume we are given a dataset D of samples from P_{data})

$$x_i \sim P_{\text{data}}$$
$$i = 1, 2, \ldots, n$$



- How do we evaluate "closeness"?

KL-divergence

- How should we measure distance between distributions?
- The **Kullback-Leibler divergence** (KL-divergence) between two distributions p and q is defined as

$$D(p\|q) = \sum_{\boldsymbol{x}} p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}$$

- $D(p\|q) \geq 0$ for all p, q, with equality if and only if $p = q$. Proof:

$$E_{\boldsymbol{x}\sim p}\left[-\log \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}\right] \geq -\log\left(E_{\boldsymbol{x}\sim p}\left[\frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}\right]\right) = -\log\left(\sum_{\boldsymbol{x}} p(\boldsymbol{x}) \frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}\right) = 0$$

- Notice that KL-divergence is **asymmetric**, i.e., $D(p\|q) \neq D(q\|p)$
- Measures the expected number of extra bits required to describe *samples from* $p(\mathbf{x})$ using a compression code based on q instead of p

Detour on KL-divergence

- To compress, it is useful to know the probability distribution the data is sampled from
- For example, let $X_1, \cdots, X_{100}$ be samples of an unbiased coin. Roughly 50 heads and 50 tails. Optimal compression scheme is to record heads as 0 and tails as 1. In expectation, use 1 bit per sample, and cannot do better
- Suppose the coin is biased, and $P[H] \gg P[T]$. Then it's more efficient to uses fewer bits on average to represent heads and more bits to represent tails, e.g.
  - Batch multiple samples together
  - Use a short sequence of bits to encode $HHHH$ (common) and a long sequence for $TTTT$ (rare).
  - Like Morse code: $E = \bullet$, $A = \bullet -$, $Q = - - \bullet -$
- KL-divergence: if your data comes from p, but you use a scheme optimized for q, the divergence $D_{KL}(p||q)$ is the number of *extra* bits you'll need on average

Learning as density estimation

- We want to learn the full distribution so that later we can answer *any* probabilistic inference query
- In this setting we can view the learning problem as **density estimation**
- We want to construct P_θ as "close" as possible to P_{data} (recall we assume we are given a dataset D of samples from P_{data})
- How do we evaluate "closeness"?
- **KL-divergence** is one possibility:

$$\mathbf{D}(P_{\text{data}} || P_\theta) = E_{x \sim p}\left[\log \frac{P_{data}(x)}{P_\theta(x)}\right] = \sum_x P_{data}(x) \log \frac{P_{data}(x)}{P_\theta(x)}$$

- $\mathbf{D}(P_{\text{data}} || P_\theta) = 0$ iff the two distributions are the same.
- It measures the "compression loss" (in bits) of using P_θ instead of P_{data}.

Expected log-likelihood

- We can simplify this somewhat:

$$\begin{aligned}\mathbf{D}(P_{\text{data}} \,||P_\theta) &= \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log \frac{P_{data}(x)}{P_\theta(x)}\right] \\ &= \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{data}}(\mathbf{x})\right] - \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right]\end{aligned}$$

- The first term does not depend on P_θ.
- Then, *minimizing* KL divergence is equivalent to *maximizing* the **expected log-likelihood**

$$\arg\min_{P_\theta} \mathbf{D}(P_{\text{data}}||P_\theta) = \arg\min_{P_\theta} -\mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right] = \arg\max_{P_\theta} \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right]$$

  - Asks that P_θ assign high probability to instances sampled from P_{data}, so as to reflect the true distribution
  - Because of log, samples $\mathbf{x}$ where $P_\theta(\mathbf{x}) \approx 0$ weigh heavily in objective
- Although we can now compare models, since we are ignoring $\mathbf{H}(P_{\text{data}}) = -\mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{data}}(\mathbf{x})\right]$, we don't know how close we are to the optimum
- Problem: In general, we do not know P_{data}.

Maximum likelihood

- Approximate the expected log-likelihood

$$\mathbf{E}_{\mathbf{x} \sim P_{\text{data}}} [\log P_\theta(\mathbf{x})]$$

with the *empirical log-likelihood*:

$$\mathbf{E}_D [\log P_\theta(\mathbf{x})] = \frac{1}{|D|} \sum_{\mathbf{x} \in D} \log P_\theta(\mathbf{x})$$

- **Maximum likelihood learning** is then:

$$\max_{P_\theta} \frac{1}{|D|} \sum_{\mathbf{x} \in D} \log P_\theta(\mathbf{x})$$

- Equivalently, maximize likelihood of the data $P_\theta(\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}) = \prod_{\mathbf{x} \in D} P_\theta(\mathbf{x})$

Main idea in Monte Carlo Estimation

1. **Express the quantity of interest as the expected value of a random variable.**

$$E_{x\sim P}[g(x)] = \sum_x g(x)P(x)$$

2. Generate T samples $\mathbf{x}^1, \ldots, \mathbf{x}^T$ from the distribution P with respect to which the expectation was taken.
3. Estimate the expected value from the samples using:

$$\hat{g}(\mathbf{x}^1, \cdots, \mathbf{x}^T) \triangleq \frac{1}{T} \sum_{t=1}^{T} g(\mathbf{x}^t)$$

where $\mathbf{x}^1, \ldots, \mathbf{x}^T$ are independent samples from P. Note: $\hat{g}$ is a random variable. Why?

Properties of the Monte Carlo Estimate

- **Unbiased:**

$$E_P[\hat{g}] = E_P[g(x)]$$

- **Convergence:** By law of large numbers

$$\hat{g} = \frac{1}{T}\sum_{t=1}^{T} g(x^t) \rightarrow E_P[g(x)] \text{ for } T \rightarrow \infty$$

- **Variance:**

$$V_P[\hat{g}] = V_P\left[\frac{1}{T}\sum_{t=1}^{T} g(x^t)\right] = \frac{V_P[g(x)]}{T}$$

Thus, variance of the estimator can be reduced by increasing the number of samples.

Example

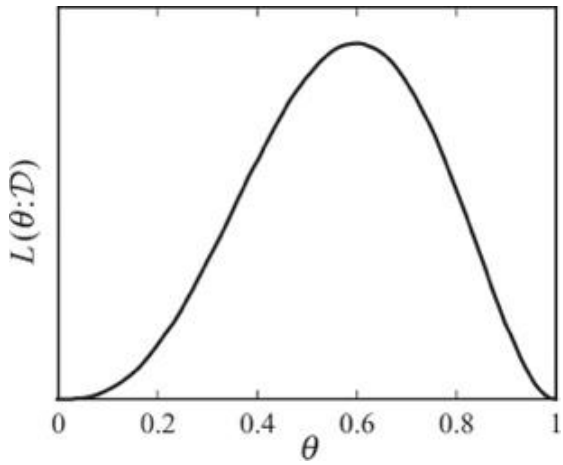
Single variable example: A biased coin

- Two outcomes: *heads* (H) and *tails* (T)
- Data set: Tosses of the biased coin, e.g., $D = \{H, H, T, H, T\}$
- Assumption: the process is controlled by a probability distribution $P_{\text{data}}(x)$ where $x \in \{H, T\}$
- Class of models M: all probability distributions over $x \in \{H, T\}$.
- Example learning task: How should we choose $P_\theta(x)$ from M if 3 out of 5 tosses are heads in D?

MLE scoring for the coin example

We represent our model: $P_\theta(x = H) = \theta$ and $P_\theta(x = T) = 1 - \theta$

- Example data: $D = \{H, H, T, H, T\}$
- Likelihood of data = $\prod_i P_\theta(x_i) = \theta \cdot \theta \cdot (1 - \theta) \cdot \theta \cdot (1 - \theta)$



- Optimize for θ which makes D most likely. What is the solution in this case? $\theta = 0.6$, optimization problem can be solved in closed-form

Extending the MLE principle to autoregressive models

Given an autoregressive model with n variables and factorization

$$P_\theta(\mathbf{x}) = \prod_{i=1}^{n} p_{\text{neural}}(x_i \,|\, \mathbf{x}_{<i}; \theta_i)$$

$\theta = (\theta_1, \cdots, \theta_n)$ are the parameters of all the conditionals. Training data $D = \{\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}\}$. Maximum likelihood estimate of the parameters θ?

- Decomposition of Likelihood function

$$L(\theta, D) = \prod_{j=1}^{m} P_\theta(\mathbf{x}^{(j)}) = \prod_{j=1}^{m} \prod_{i=1}^{n} p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

- Goal : maximize $\arg\max_\theta L(\theta, D) = \arg\max_\theta \log L(\theta, D)$
- We no longer have a closed form solution

MLE Learning: Gradient Descent

$$L(\theta, D) = \prod_{j=1}^{m} P_\theta(\mathbf{x}^{(j)}) = \prod_{j=1}^{m} \prod_{i=1}^{n} p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

Goal : maximize $\arg\max_\theta L(\theta, D) = \arg\max_\theta \log L(\theta, D)$

$$\ell(\theta) = \log L(\theta, D) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize $\theta^0 = (\theta_1, \cdots, \theta_n)$ at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

Non-convex optimization problem, but often works well in practice

MLE Learning: Stochastic Gradient Descent

$$\ell(\theta) = \log L(\theta, D) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize θ^0 at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

What is the gradient with respect to θ_i?

$$\nabla_{\theta_i} \ell(\theta) = \sum_{j=1}^{m} \nabla_{\theta_i} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) = \sum_{j=1}^{m} \nabla_{\theta_i} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

Each conditional $p_{\text{neural}}(x_i | \mathbf{x}_{<i}; \theta_i)$ can be optimized separately if there is no parameter sharing. In practice, parameters θ_i are shared (e.g., NADE, PixelRNN, PixelCNN, etc.)

MLE Learning: Stochastic Gradient Descent

$$\ell(\theta) = \log L(\theta, \mathcal{D}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize θ^0 at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

$$\nabla_\theta \ell(\theta) = \sum_{j=1}^{m} \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

What if $m = |\mathcal{D}|$ is huge?

$$\begin{aligned} \nabla_\theta \ell(\theta) &= m \sum_{j=1}^{m} \frac{1}{m} \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) \\ &= m E_{x^{(j)} \sim \mathcal{D}} \left[\sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) \right] \end{aligned}$$

Monte Carlo: Sample $x^{(j)} \sim \mathcal{D}; \nabla_\theta \ell(\theta) \approx m \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$

Empirical Risk and Overfitting

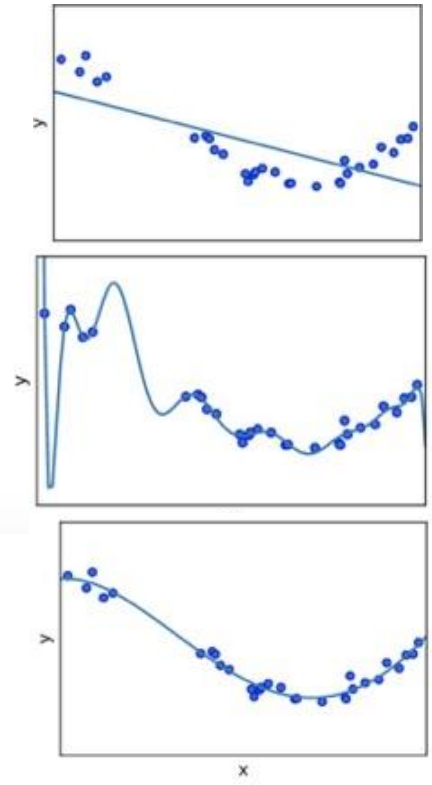
- Empirical risk minimization can easily **overfit** the data
  - Extreme example: The data is the model (remember all training data).
- Generalization: the data is a sample, usually there is vast amount of samples that you have never seen. Your model should generalize well to these "never-seen" samples.
- Thus, we typically restrict the **hypothesis space** of distributions that we search over

Bias-Variance trade off

- If the hypothesis space is very limited, it might not be able to represent P_{data}, even with unlimited data
  - This type of limitation is called **bias**, as the learning is limited on how close it can approximate the target distribution
- If we select a highly expressive hypothesis class, we might better represent the data
  - When we have small amount of data, multiple models can fit well, or even better than the true model. Moreover, small perturbations on D will result in very different estimates
  - This limitation is called the **variance**.

Bias-Variance trade off

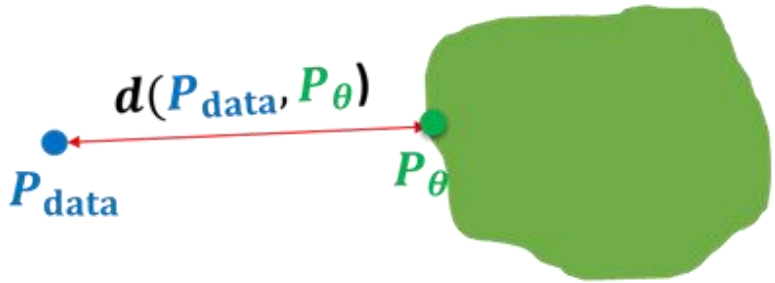
- There is an inherent **bias-variance trade off** when selecting the hypothesis class. Error in learning due to both things: bias and variance.
- Hypothesis space: linear relationship
  - Does it fit well? Underfits
- Hypothesis space: high degree polynomial
  - Overfits
- Hypothesis space: low degree polynomial
  - Right tradeoff



How to avoid overfitting?

- Hard constraints, e.g. by selecting a less expressive model family:
  - Smaller neural networks with less parameters
  - Weight sharing

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



Model family

- Soft preference for "simpler" models: **Occam Razor.**
- Augment the objective function with **regularization**:

"The simplest explanation for a phenomenon is usually the correct one"

$$objective(\mathbf{x}, M) = loss(\mathbf{x}, M) + R(M)$$

- Evaluate generalization performance on a held-out validation set

Conditional generative models

- Suppose we want to generate a set of variables $\mathbf{Y}$ given some others $\mathbf{X}$, e.g., text to speech
- We concentrate on modeling $p(\mathbf{Y}|\mathbf{X})$, and use a **conditional** loss function

$$-\log P_\theta(\mathbf{y}\,|\,\mathbf{x}).$$

- Since the loss function only depends on $P_\theta(\mathbf{y}\,|\,\mathbf{x})$, it suffices to estimate the conditional distribution, not the joint

Input : image

$\mapsto$

Brown horse in grass field

Output: caption

Recap

- For autoregressive models, it is easy to compute $p_\theta(x)$
  - Ideally, evaluate in parallel each conditional $\log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$. Not like RNNs.
- Natural to train them via maximum likelihood
- Higher log-likelihood doesn't necessarily mean better looking samples
- Other ways of measuring similarity are possible (Generative Adversarial Networks, GANs)