Maximum Likelihood Learning

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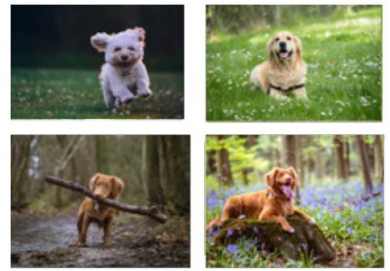
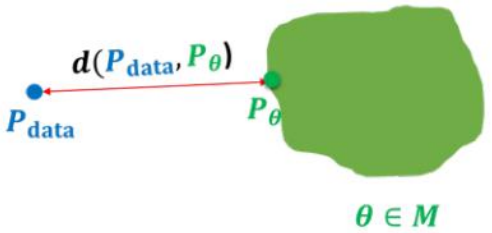
(Slides from: Stefano Ermon)

Learning a Generative Model

- We are given a training set of examples, e.g., images of dogs
- We want to learn a probability distribution $p(x)$ over images 'x' such that we can do:
  - **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) – possible with at least some of the generative models.
- First question: how to represent $p(x)$ – today we'll talk about AR models
- **Second question: how to learn it!** ⟸



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



Model family

Setting

- Let's 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., $(X_{bank} = 1, X_{dollar} = 0, \dots, Y = 1)$ 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

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. Images represented with a vector X of 784 binary variables (black vs. white pixel). 2^{784} possible images/states. Even 10million examples is extremely sparse coverage.
- We want to select P_θ to construct the "best" approximation to the underlying distribution P_{data}
- What is "best"?

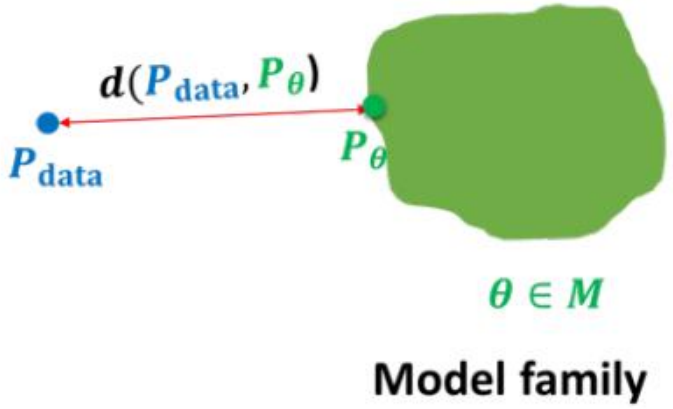
What is “best”?

- This depends on what we want to do
  - Density estimation: we are interested in the full distribution (so later we can compute whatever conditional probabilities we want)
  - 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 (e.g. causal models)
    - 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})
- How do we evaluate "closeness"?

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



KL-divergence (review)

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

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

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

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

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

KL-divergence (review)

- 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.
  - Use a short sequence of bits to encode HHHH (common) and a long sequence for TTTT (rare).
  - Like Morse code: E = •, A = •–, Q = – – •–
- 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:

$$\mathbf{D}(P_{\text{data}}||P_\theta) = \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log\left(\frac{P_{\text{data}}(\mathbf{x})}{P_\theta(\mathbf{x})}\right)\right] = \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \frac{P_{\text{data}}(\mathbf{x})}{P_\theta(\mathbf{x})}$$

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

Expected log-likelihood

- We can simplify this somewhat:

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

No θ

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

- Then, minimizing KL divergence is equivalent to maximizing the expected log-likelihood

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

  - Asks that P_θ assign high probability to instances sampled from P_{data}, so as to reflect the true distribution
  - Because of log, samples x where $P_\theta(x) \approx 0$ weigh heavily in objective
- Although we can now compare models, since we are ignoring $H(P_{data}) = -E_{x\sim P_{data}}[\log P_{data}(x)]$, we don't know how close we are to the optimum.
- This still involves expectation over P_{data}, we do not know P_{data}!

Maximum likelihood

- Approximate the expected log-likelihood

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

using the empirical log-likelihood:

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

- Maximum likelihood learning is then:

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

- Equivalently, maximize likelihood of the data

$$P_\theta(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}) = \prod_{\mathbf{x}\in\mathcal{D}} P_\theta(\mathbf{x})$$

Monte Carlo Estimation (Recap)

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 $x^1, \ldots, x^T$ 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 $x^1, \ldots, x^T$ 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.

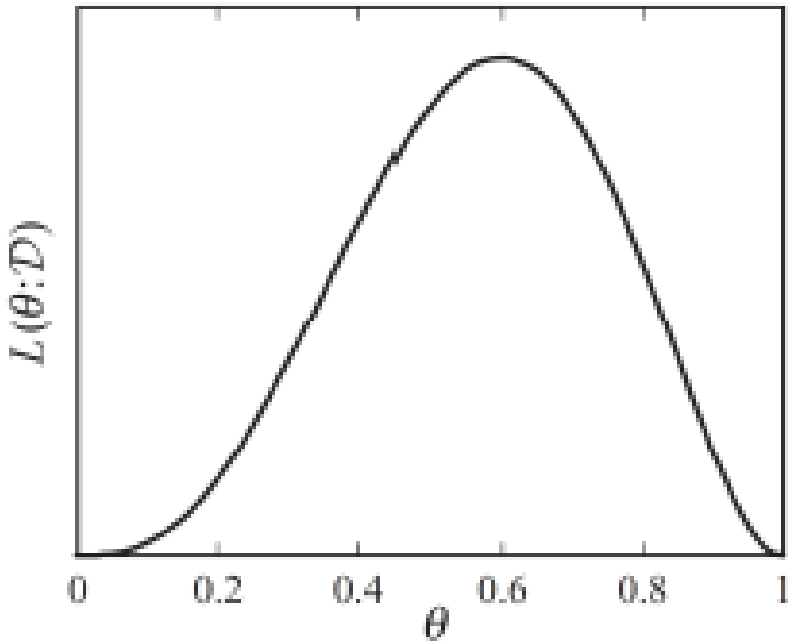
Example

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 $P_{data}(x)$ where x ∈ {H,T}
- Class of models M: all probability distributions over x ∈ {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 $D = \{H, H, T, H, T\}$
  - 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? θ = 0.6, optimization problem can be solved in closed-form

MLE principle for Autoregressive Models

Given an autoregressive model with n variables and factorization

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

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

- Decomposition of Likelihood function

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

- 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

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

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

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

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

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

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 $\nabla_\theta(\theta)$ (by back prop)
3. $\theta^{k+1} = \theta^t + \alpha_t \nabla_\theta(\theta)$

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 $p_{neural}(x_i | x_{<i}; \theta_i)$ 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 $\nabla_\theta(\theta)$ (by back prop)
3. $\theta^{k+1} = \theta^t + \alpha_t \nabla_\theta(\theta)$

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

What if $m = |D|$ is huge?

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

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 (memorize 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

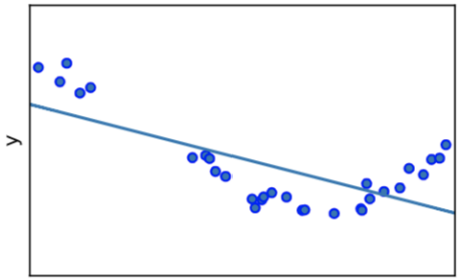
- If the hypothesis space is very limited, it might not be able to represent P_{data}, even with unlimited data
  - This type of limitation is called bias, as the learning is limited on how close it can approximate the target distribution

- If we select a highly expressive hypothesis class, we might represent better 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 call the variance.

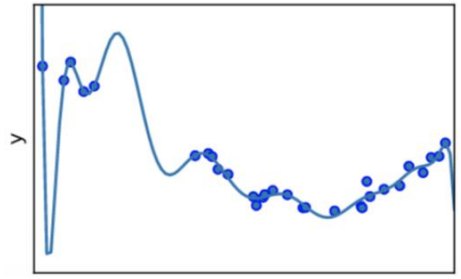
Bias-Variance trade off

There is an inherent bias-variance trade off when selecting the hypothesis class. Error in learning due to both things: bias and variance.

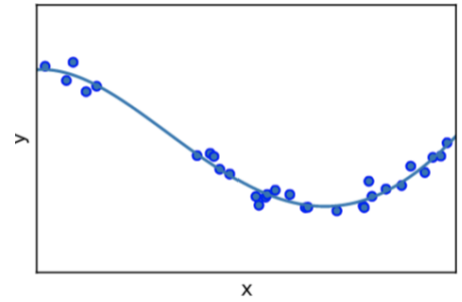
- Hypothesis space: linear relationship
  - Does it fit well? Underfits



- Hypothesis space: high degree polynomial
  - Overfits



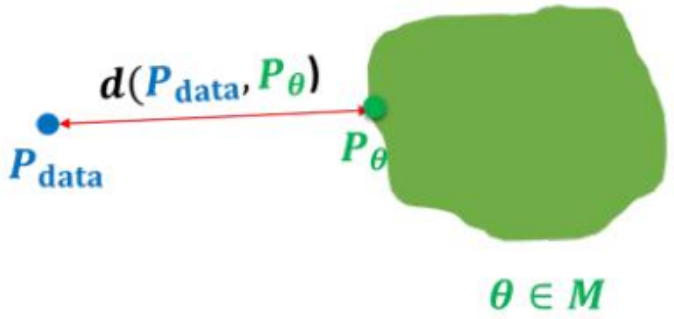
- Hypothesis space: low degree polynomial
  - Right tradeof



How to avoid overfitting?

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

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



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

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

- Evaluate **generalization performance** on a held-out validation set

Conditional generative models

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

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

- Since the loss function only depends on $P_\theta(\mathrm{y} \mid \mathrm{x})$, 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 $p_\theta(\mathrm{x})$
  - Ideally, evaluate in parallel each conditional $\log p_{neural}(x_i^{(j)} | x_{<i}^{(j)}; \theta_i)$. 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)