# Deep Generative Models <br> Lecture 4: Maximum Likelihood Learning 

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- Goal: learn a probability distribution $p(x)$ over images $x$
- Generation: If we sample $x_{\text {new }} \sim p(x), x_{\text {new }}$ 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 $p_{\theta}(x)$.


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- First question: how to represent $p_{\theta}(x)$. Second question: how to learn it.


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- For example, a FVSBN for all possible choices of the logistic regression parameters. $\mathcal{M}=\left\{P_{\theta}, \theta \in \Theta\right\}, \theta=$ concatenation of all logistic regression coefficients


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3. Structure or knowledge discovery: we are interested in the model itself

- How do some genes interact with each other?
- What causes cancer?


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- 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 code based on $q$ instead of $p$


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- Batch multiple samples together
- Use a short sequence of bits to encode HHHH (common) and a long sequence for TTTT (rare).
- Like Morse code: $E=\bullet, A=\bullet-, Q=--\bullet-$


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- 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 $D_{K L}(p \| q)$ 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 $P_{\theta}$ as "close" as possible to $P_{\text {data }}$ (recall we assume we are given a dataset $\mathcal{D}$ of samples from $P_{\text {data }}$ )
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- Because of log, samples $\mathbf{x}$ where $P_{\theta}(\mathbf{x}) \approx 0$ weigh heavily in objective


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- The first term does not depend on $P_{\theta}$.
- Then, minimizing KL divergence is equivalent to maximizing the expected log-likelihood
- Asks that $P_{\theta}$ assign high probability to instances sampled from $P_{\text {data }}$, so as to reflect the true distribution
- Because of log, samples $\mathbf{x}$ where $P_{\theta}(\mathbf{x}) \approx 0$ weigh heavily in objective
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## Expected log-likelihood

- We can simplify this somewhat:

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- Problem: In general we do not know $P_{\text {data }}$.


## Maximum likelihood

- Approximate the expected log-likelihood

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\mathbf{E}_{\mathbf{x} \sim P_{\text {data }}}\left[\log P_{\theta}(\mathbf{x})\right]
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with the empirical log-likelihood:

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\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})
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- Equivalently, maximize likelihood of the data

$$
P_{\theta}\left(\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}\right)=\prod_{\mathbf{x} \in \mathcal{D}} P_{\theta}(\mathbf{x})
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## Main idea in Monte Carlo Estimation

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

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- Variance:

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V_{P}[\hat{g}]=V_{P}\left[\frac{1}{T} \sum_{t=1}^{T} g\left(x^{t}\right)\right]=\frac{V_{P}[g(x)]}{T}
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Thus, variance of the estimator can be reduced by increasing the number of samples.

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Single variable example: A biased coin

- Two outcomes: heads $(H)$ and tails $(T)$


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- Class of models $\mathcal{M}$ : all probability distributions over $x \in\{H, T\}$.
- Example learning task: How should we choose $P_{\theta}(x)$ from $\mathcal{M}$ if 60 out of 100 tosses are heads in $\mathcal{D}$ ?


## MLE scoring for the coin example

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

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- Optimize for $\theta$ which makes $\mathcal{D}$ most likely. What is the solution in this case?


## MLE scoring for the coin example: Analytical derivation

Distribution: $P_{\theta}(x=H)=\theta$ and $P_{\theta}(x=T)=1-\theta$

- More generally, log-likelihood function

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L(\theta)=\theta^{\# \text { heads }} \cdot(1-\theta)^{\# \text { tails }}
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## Extending the MLE principle to autoregressive models

Given an autoregressive model with $n$ variables and factorization

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P_{\theta}(\mathbf{x})=\prod_{i=1}^{n} p_{\text {neural }}\left(x_{i} \mid \mathbf{x}_{<i} ; \theta_{i}\right)
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$\theta=\left(\theta_{1}, \cdots, \theta_{n}\right)$ are the parameters of all the conditionals.

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- We no longer have a closed form solution


## MLE Learning: Gradient Descent

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2. Compute $\nabla_{\theta} \ell(\theta)$ (by back propagation)
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Non-convex optimization problem, but often works well in practice

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Each conditional $p_{\text {neural }}\left(x_{i} \mid \mathbf{x}_{<i} ; \theta_{i}\right)$ can be optimized separately if there is no parameter sharing.

## MLE Learning: Stochastic Gradient Descent

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Each conditional $p_{\text {neural }}\left(x_{i} \mid \mathbf{x}_{<i} ; \theta_{i}\right)$ can be optimized separately if there is no parameter sharing. In practice, parameters $\theta_{i}$ are shared (e.g., NADE, PixeIRNN, PixeICNN, etc.)

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- Thus, we typically restrict the hypothesis space of distributions that we search over


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- Evaluate generalization performance on a held-out validation set


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Input: image

## Recap

- For autoregressive models, it is easy to compute $p_{\theta}(x)$
- Ideally, evaluate in parallel each conditional $\log p_{\text {neural }}\left(x_{i}^{(j)} \mid \mathbf{x}_{<i}^{(j)} ; \theta_{i}\right)$.


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- 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)

