CSDS 440: Machine Learning

Soumya Ray (he/him, sray@case.edu)
Olin 516

Office hours T, Th 11:15-11:45 or by appointment

Why does Naïve Bayes work well?

- Very simplistic independence assumptions
 - Everyone knows that these assumptions are nearly always wrong
 - But, paradoxically, often works well in practice

Why?

- Works well for classification, but not so great at density estimation
- Most probabilities end up near 0/1 (ask for paper)

Logistic Regression

- Simplest Discriminative model
- Models log odds as a linear function

$$\log \frac{p(Y=1|\mathbf{x})}{p(Y=-1|\mathbf{x})} = \mathbf{w} \cdot \mathbf{x} + b$$

$$p(Y=1|\mathbf{x}) = \left[1 - p(Y=1|\mathbf{x})\right] e^{(\mathbf{w} \cdot \mathbf{x} + b)}$$

$$p(Y=1|\mathbf{x})(1 + e^{(\mathbf{w} \cdot \mathbf{x} + b)}) = e^{(\mathbf{w} \cdot \mathbf{x} + b)}$$

$$p(Y=1|\mathbf{x}) = \frac{e^{(\mathbf{w} \cdot \mathbf{x} + b)}}{1 + e^{(\mathbf{w} \cdot \mathbf{x} + b)}} = \frac{1}{1 + e^{-(\mathbf{w} \cdot \mathbf{x} + b)}}$$

Classification with LR

• LR directly specifies $p(Y=1|\mathbf{x})$, compute and check if greater than 1/2

Estimating parameters

 Use MLE, optimize conditional log likelihood of the data

$$\mathbf{w}, b = \arg\max\prod_{i} p(Y_i = y_i \mid \mathbf{x}_i)$$

$$= \arg\max\sum_{i \in pos} \log p(Y_i = 1 \mid \mathbf{x}_i) + \sum_{i \in neg} \log p(Y_i = -1 \mid \mathbf{x}_i)$$

$$= \arg\max\sum_{i \in pos} \log \left(\frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}}\right) + \sum_{i \in neg} \log \left(1 - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}}\right)$$

Overfitting control

Can include a term for overfitting control:

$$\mathbf{w}, b = \arg\max \sum_{i \in pos} \log \left(\frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}} \right) + \sum_{i \in neg} \log \left(1 - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}} \right)$$

$$\mathbf{w}, b = \arg\min \frac{1}{2} \|\mathbf{w}\|^2 + C \begin{bmatrix} \sum_{i \in pos} -\log\left(\frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}}\right) \\ +\sum_{i \in neg} -\log\left(1 - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x} + b}}\right) \end{bmatrix}$$

Negative Conditional Log Likelihood

Estimating parameters

Can use gradient descent, Newton methods etc

 Very robust method, works extremely well in many practical situations, very easy to code

Logistic Regression Geometry

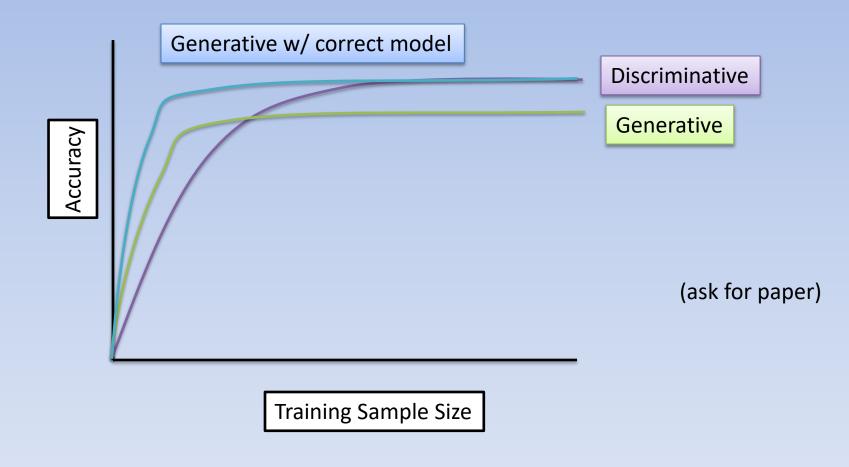
Classify as positive iff:

$$\frac{p(Y=1|\mathbf{x})}{p(Y=-1|\mathbf{x})} > 1$$
or if $\log \frac{p(Y=1|\mathbf{x})}{p(Y=-1|\mathbf{x})} > 0$
But $\log \frac{p(Y=1|\mathbf{x})}{p(Y=-1|\mathbf{x})} = \mathbf{w} \cdot \mathbf{x} + b$
So classify as positive iff $\mathbf{w} \cdot \mathbf{x} + b > 0$

Relationship to Naïve Bayes

- LR does not make the independence assumptions of NB
 - Can be more robust than NB, especially in the presence of irrelevant attributes
 - Also handles continuous attributes nicely
 - But (as with all discriminative models) no easy way to handle data issues such as missing data

Generative and Discriminative Pairs



Pros and Cons of Probabilistic Classification

- + Optimal approach in decision-theoretic terms
- + Can incorporate prior knowledge (possibly later)
- + Produces confidence measures
- + Very well studied
- + Simple models are easy to implement
- + Can nicely capture causal influences (CSDS 442)
- Inference and estimation are in general hard
- Discriminative approaches can be hard to interpret

High dimensional Generative Models

- Suppose we wish to generate an image of a face
- This is hard!
- These are samples from a VERY high dimensional distribution
- And, the "axes" are not independent







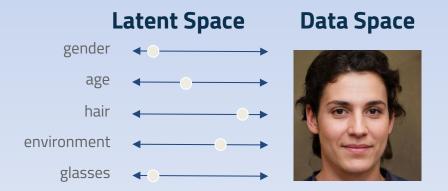






Latent Variable Models

- To make the problem easier, we introduce "latent variables" z
 - These are hidden features which capture (hopefully independent) abstractions that constrain the space of images



Maximizing Likelihood

Observe

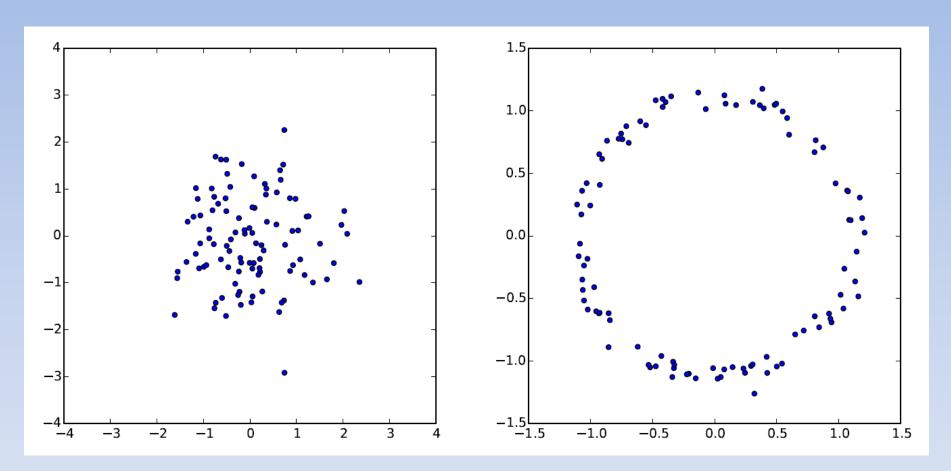
$$p(X) = \int p(X \mid z) p(z) dz$$

- To train a model, want to maximize LHS as before
- 1. What should z be?
- 2. How to compute the p(X) above?

First clever idea

- We have no idea what z could be
- Let us just sample z from $N(\mathbf{0}, \mathbf{I})$ and use a nonlinear function to transform this input into the output we need
 - Does such a function exist?
 - In many cases yes! under "compatibility" conditions for p(X) and sufficiently rich nonlinear transformations

You're Joking, Right?



Left: samples z from 2D N(0,I). Right: f(z)=z/10+z/||z||

And so

• We'll choose a trainable family $f_{\theta}(z)$, typically a neural network

• With this choice, $p(X|z)=N(f_{\theta}(z), \sigma^2I)$

Evaluating Likelihood

$$p(X) = \int p(X \mid z) p(z) dz, z \sim N(0, I)$$

$$\approx \frac{1}{n} \sum_{i} p(X \mid z_{i})$$

• Unfortunately, in high dimensions, most $p(X|z_i)$ will be near zero, so this is going to be VERY inefficient

Second key idea

• What if we had a function $Q(z \mid X)$, that could return a distribution over those z's that are likely to produce X?

• Then maybe we could use $E_{z\sim Q}p(X\mid z)$ to get a good approximation to the likelihood?

Aside: Kullback-Liebler divergence

 One way to measure the "dissimilarity" between two distributions

$$D(X(z) || Y(z)) = E_{z \sim X} \left(\log \left(X(z) \right) - \log \left(Y(z) \right) \right)$$