

Unsupervised Learning: Probability

Thanks to Hal Daume for some content

Review: Supervised Learning

- Supervised methods
 - Focus on constructing objective functions
 - Different classifiers (approaches) all trying to solve the same problem
 - Some exceptions (e.g. boosting)

Unsupervised Learning

- Focus on a single objective function (likelihood)
- Cover different frameworks and methods
 - Clustering: outline goals of unsupervised learning and basic approaches
 - EM algorithm: how we learn without labeled data
 - Graphical models: how we construct models
 - Structured prediction: construct models with different output types
 - Manifold learning/dimensionality reduction

Today: Probability

- Probability has shown up in supervised learning
 - Maximize data likelihood
 - Logistic regression
 - Least squares regression
- The language of how we express models
- Today: review core concepts

Probability is Hard

- Probability is not intuitive
- People routinely make wrong decisions
- Examples
 - The lottery
 - Streaks in sports
 - 50/50 chances
 - <http://www.cc.com/video-clips/hzqmb9/the-daily-show-with-jon-stewart-large-hadron-collider>
 - 2:05-3:36

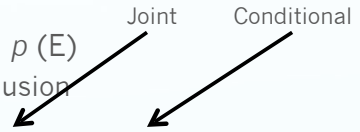
Probability 101

- Probability theory assigns a numerical probability to events
- Probability of an event = *fraction of times* that event would occur if we ran an experiment many times
 - This is the *frequentist* definition of probability
- Events are drawn (they happen) from a sample space Ω (omega)
- A probability model is a function that maps any subset of Ω to a real value between 0 and 1
- Formally, $p : P(\Omega) \rightarrow [0, 1]$

3 Axioms of Probability

- $p(E) \geq 0$ for all $E \subseteq \Omega$
 - Cannot have a negative event
- $p(\Omega) = 1$
 - An event must occur
- If $E_1, E_2, E_3, \dots \subseteq \Omega$, are pairwise disjoint, then:
 $p(E_1 \cup E_2 \cup E_3 \cup \dots) = p(E_1) + p(E_2) + p(E_3) + \dots$
 - Events are additive

Rules of Probability

- $p(A \cup B) = p(A) + p(B) - p(A \cap B)$
 - Decomposition of “or”
 - $p(\Omega \setminus E) = 1 - p(E)$
 - Inclusion/exclusion
 - $p(A \cap B) = p(A, B) = p(A|B) p(B)$
 - Decomposition of “and”, called the product rule
 - $p(\emptyset) = 0$
 - Null event
- 

Why We Need These Rules

- Many machine learning models are probabilistic
 - Assume data fits some probability distribution
 - Example: logistic regression
 - The label is given by a conditional probability based on the data $p(y|x)$
 - Alternatively: define a joint probability of label and data $p(y, x)$

$$p(y, x) = p(y|x)p(x) = p(x|y)p(y)$$

- We can model these separately
- What is $p(y = 0|x)$

$$p(y = 0|x) = 1 - p(y = 1|x)$$

Expectations

- We assign values to these probabilities given data
- Using our learned probabilities, we want to make predictions about what we **expect** will happen
 - The “average” result of an event
- If A is a random variable, the expectation is

$$E_p[A] = \begin{cases} \sum_{a \in A} p(A = a)a & \text{discrete} \\ \int_A da p(A = a)a & \text{continuous} \end{cases}$$

Bayes Rule

- Sometimes we cannot measure $p(y|x)$ directly
 - Ex. y is a disease and x is a symptom
- But we can measure $p(x|y)$

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

Medical Test

- You take a test for a disease. The results are positive.
- The probability that the test shows positive given a negative sample is 10,000 to 1
- Do you have the disease?

Applications of Bayes Rule

- $p(\text{test}=\text{positive} | \text{disease}=\text{negative}) = 0.0001$
- $p(\text{test}=\text{negative} | \text{disease}=\text{negative}) = 0.9999$
- $p(\text{test}=\text{positive} | \text{disease}=\text{positive}) = 0.9999$
- $p(\text{disease}=\text{negative}) = 0.999999$
- $p(\text{disease}=\text{negative} | \text{test}=\text{positive}) = \frac{p(\text{test}=\text{positive} | \text{disease}=\text{negative})}{p(\text{test}=\text{positive})} = 9 \times 10^{-5} * K$
- $p(\text{disease}=\text{positive} | \text{test}=\text{positive}) = \frac{p(\text{test}=\text{positive} | \text{disease}=\text{positive})}{p(\text{test}=\text{positive})} = 9 \times 10^{-7} * K$
- $(9 \times 10^{-5} + 9 \times 10^{-7}) * K = 1$
- $p(\text{disease}=\text{positive} | \text{test}=\text{positive}) \approx 0.01$ (1%)

Chain Rule

- We want to know the probability of many things happening
- $p(x_1, x_2, x_3, \dots, x_n)$
 - Often difficult to manage a large joint probability
- Break apart using the chain rule

$$p(x_1, x_2, x_3, \dots, x_N) = \prod_{n=1}^N p(x_n | x_1, x_2, \dots, x_{n-1})$$

Why the Chain Rule?

- Assume you have many events you want to predict
 - e.x., probability of an image- prediction for each pixel
- $P(\text{image}) = P(\text{pixel}_1, \text{pixel}_2, \text{pixel}_3, \dots)$
 - This is a very large probability
 - Hard to make good estimates
 - Most of the time it will be 0
- Break down using the chain rule
 - $P(\text{image}) = P(\text{pixel}_n | \text{pixel}_1, \text{pixel}_2, \dots) * P(\text{pixel}_{n-1} | \text{pixel}_1, \text{pixel}_2, \dots)$

This would be useful if we could remove terms on the RHS of the probability...

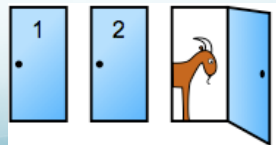
Marginalization

- We want to compute $p(x)$
- But we only know $p(x|y)$
- Solution: sum over all possible y

$$p(X = x) = \sum_y p(X = x | Y = y) p(Y = y)$$

Monty Hall: A Game Show

- Three doors: behind 1 door is a car, the other two have goats
 - You want the car
- You pick a door
- The host opens a different door and reveals a goat
 - He knows where the car is
- Should you switch doors?



Simulation

Probability Distributions

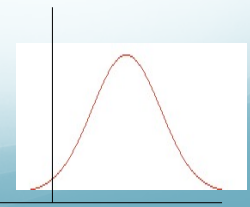
- Function that maps input to an output such that
 - Output must be between 0 and 1
 - Total area under the function must be 1

Gaussian Distribution

- Gaussian distribution (aka. normal distribution)

$$N(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

- μ - mean
- σ - standard deviation, σ^2 variance
- Continuous distribution (assigns probabilities to real valued numbers)
- Many special properties that will be useful to us



Bernoulli Distribution

- Simple distribution that records probability of two discrete events

- Coin flip

$$\text{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x}$$

- Parameter μ controls the distribution
 - It is the mean

Likelihood

- Given:
 - A sample of data
 - A probability distribution (a model) for the data
- We want to know how likely that data is given our model
 - $P(D|\text{model})$
- Why do we want to do this?
 - When we learn, we want the model that best explains the data
 - Select a model that makes the data most probable

Likelihood

- Suppose we had a single coin flip (event)
- We can write the probability of this event

$$p(x|\mu) = \mu^x(1-\mu)^{1-x}$$

- What about the probability of n events?
- We need to assume independence
 - Each coin flip is independent
 - IID: independent and identically distributed
 - Each data point is obtained independently from the same distribution

Likelihood

- Writing out the entire likelihood

$$p(D|\mu) = \prod_{n=1}^N p(x_n|\mu) = \prod_{n=1}^N \mu^{x_n}(1-\mu)^{1-x_n}$$

- Remember our useful log trick

$$\log p(D|\mu) = \sum_{n=1}^N \log p(x_n|\mu) = \sum_{n=1}^N x_n \log \mu + (1-x_n) \log(1-\mu)$$

Logistic Regression: Conditional Log Likelihood

$$p(Y|X, w) = \prod_{i=1}^n p(y_i | x_i, w)$$

$$\ell(Y, X, w) = \log p(Y|X, w) = \sum_{i=1}^n \log p(y_i | x_i, w)$$

$$p(y=1|x, w) = \frac{1}{1 + e^{-w^T \cdot x}} \quad p(y=0|x, w) = \frac{e^{-w^T \cdot x}}{1 + e^{-w^T \cdot x}}$$

Finding the Best Model

- How should we find the best model?
- First approach: maximum likelihood
 - Find the model parameters that maximize the likelihood of the data
- Function maximization
 - Take the derivative, set equal to 0

$$\mu = \frac{1}{N} \sum_{n=1}^N x_n$$

Maximum Likelihood

- Maximum likelihood estimation (MLE) is a common approach to estimating model parameters
- Straightforward: compute derivative, find parameters most likely to give observed data
- Problem: over fits data
 - Suppose we saw three coin flips, each one heads
 - MLE estimate $\mu=1$
 - We saw similar behavior in linear regression
 - MLE for gaussians over-fits by under-estimating true variance

Bayesian Probabilities

- So far probabilities are frequencies of random events
- Bayesian view
 - Probabilities are quantifications of uncertainty
 - Not all events are repeatable
 - Ex. What grade will you get in this class
 - Over the semester our guess will get better
- Prior probability $p(a)$
- Likelihood of data given observations $p(D|a)$

Bayesian Estimation

- We have some idea of the value of μ
 - Most coins $\mu=0.5$
- This is a prior
 - A belief as to the value of μ that isn't based on the data
 - Our prior: $p(\mu=0.5)$ is high
- We can use this prior to "smooth" our estimation

MAP

- Maximum posterior estimation (MAP)
 - Maximize the posterior distribution
- Posterior \propto likelihood * prior
 - Likelihood: $P(D|\mu)$
 - Prior: $P(\mu)$
 - Posterior: $P(\mu|D)$
- Find the most probable value of μ given the data (and the prior)

Building Classifiers

- Let's use probabilities to build a new classifier
- For regression we used likelihood
 - $p(D|w)$ as a Gaussian
- For logistic regression we used conditional likelihood
 - We only had $p(y|x)$
 - Couldn't write out $p(D|w)$
- Let's try and write likelihood for classification
 - $P(D|w)$

Likelihood

- Each example is independent

$$p(Y, X) = \prod_{i=1}^n p(y_i, x_i)$$

- Rewrite probability as conditional

$$p(y_i, x_i) = p(y_i | x_i) p(x_i)$$

- Substitute

$$p(Y, X) = \prod_{i=1}^n p(y_i | x_i) p(x_i)$$

Likelihood

- Consider the first term $p(y_i | x_i)$
- How do we compute it?
- Let's use Bayes rule

$$p(y_i | x_i) = \frac{p(x_i | y_i) p(y_i)}{p(x_i)}$$

Likelihood

- Substitute $p(Y, X) = \prod_{i=1}^n \frac{p(x_i | y_i) p(y_i)}{p(x_i)} p(x_i)$
- Simplify $p(Y, X) = \prod_{i=1}^n p(x_i | y_i) p(y_i)$

Likelihood

- What is $p(y)$?
- The expected number of labels of each type
 - Easy to compute

Conditional

- What is $p(x|y)$?
 - Probability of generating example x given that it has label y
- How hard is this?
 - Remember that x is a vector
 - Equivalent to $p(x_{i1}, x_{i2}, x_{i3}, \dots, x_{iM} | y_i)$
 - Assuming binary features and binary label, how many parameters do we need?
 - $2 * (2^M \cdot 1)$ parameters!
 - $(2^M \cdot 1)$ combinations for x
 - 2 labels

Assumptions

- Not enough data to observe all combinations even a single time
- Need to make simplifying assumptions

Conditional Independence

- **RV (random variable) X is conditionally independent of RV Y given RV Z if the probability of each is independent given Z**
- $p(x,y|z) = p(x|z)p(y|z)$
- Example
 - Probability that I need an umbrella and the ground is wet
 - Not independent! If its wet I probably need an umbrella because it is raining
 - I am told it is raining
 - Given this the probability that I need an umbrella is independent of the ground being wet
 - I gain no new information knowing that the ground is wet

Conditional Independence

- Assume each feature in x is independent given y
 - Once I know y each feature in x is independent
- Why is this helpful?

$$p(\mathbf{x}_i | y_i) = \prod_{j=1}^M p(x_{ij} | y_i)$$

- This is a naïve assumption (it's very unlikely)

Conditional Independence

- How to estimate $p(\mathbf{x}_{ij} | y_i)$?
 - Lots of data- every time feature x_{ij} occurs with y_i
- How many parameters do I need?
 - Before: $2 * (2^M - 1)$
 - Now: $2 * M$
 - One parameter for each of M features
- Should be easier to learn so many fewer parameters

Maximum Likelihood Solution

- Solution is the mean of the probabilities in the data

$$p(y) = \frac{\text{number of times } y \text{ appears}}{\text{number of examples}}$$

$$p(x_j | y) = \frac{\text{number of times } x_j \text{ and } y \text{ appear together}}{\text{number of times } y \text{ appears}}$$

Predictions

- Given an example x , how do we make predictions?

$$\arg \max_{y \in \{0,1\}} p(y | x)$$

- Bayes rule and conditional assumption

$$\arg \max_{y \in \{0,1\}} \frac{\prod_{j=1}^M \{p(x_j | y)\} p(y)}{p(x)}$$

- Observe that $p(x)$ does not depend on y

$$\arg \max_{y \in \{0,1\}} \prod_{j=1}^M \{p(x_j | y)\} p(y)$$

Naïve vs. Reality

- Positive: we now can parameterize our model
- Reality: naïve assumption very unlikely to be true
- Example:
 - Document classification: sports vs. finance
 - Each word in a document is a feature
 - Naïve assumption: once I know the topic is sports, every word is conditionally independent
 - Not true! Would be total nonsense
- Reality: works pretty well in practice
 - Assuming you don't have features that are highly correlated

Problem: Not enough data

- Recall that maximum likelihood is biased
 - Maximum likelihood over-fits the data
- In naïve Bayes this can be extreme
- What is the learned value of $p(x|y)$ when I have never seen x and y together?
 - What happens to $p(x|y)$?

Solution: Bias Model Parameters

- Smoothing
 - Balances fitting the observed data with a prior bias
 - Laplacian smoothing (+1 smoothing)
 - Pretend we saw extra examples with every possible feature and label
 - Effectively add 1 to each count
- Bayesian methods
 - Put priors over model parameters

Naive Bayes

Fitting a function to data

- Fitting: Closed form solution: just count!
- Function: data likelihood (joint X and Y)
- Data: Naive feature conditional independence assumption