INT305 Machine Learning
Lecture 9
Probabilistic Models

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Today

- So far in the course we have adopted a modular perspective, in which the model, loss function, optimizer, and regularizer are specified separately.
- Today we will begin putting together a probabilistic interpretation of the choice of model and loss, and introduce the concept of maximum likelihood estimation.
- Let's start with a simple biased coin example.
  - You flip a coin $N = 100$ times and get outcomes $\{x_1, \ldots, x_N\}$ where $x_i \in \{0, 1\}$ and $x_i = 1$ is interpreted as heads H.
  - Suppose you had $N_H = 55$ heads and $N_T = 45$ tails.
  - What is the probability it will come up heads if we flip again? Let's design a model for this scenario, fit the model. We can use the fit model to predict the next outcome.

Model?

- The coin is possibly loaded. So, we can assume that one coin flip outcome x is a Bernoulli random variable for *some currently unknown parameter* $\theta \in [0, 1]$.

$$p(x = 1|\theta) = \theta \quad \text{and} \quad p(x = 0|\theta) = 1 - \theta$$
$$\text{or more succinctly} \quad p(x|\theta) = \theta^x (1 - \theta)^{1-x}$$

- It's sensible to *assume* that $\{x_1, \ldots, x_N\}$ are independent and identically distributed (i.i.d.) Bernoullis.
- Thus the joint probability of the outcome $\{x_1, \ldots, x_N\}$ is

$$p(x_1, ..., x_N|\theta) = \prod_{i=1}^{N} \theta^{x_i} (1 - \theta)^{1-x_i}$$

Loss?

- We call the probability mass (or density for continuous) of the observed data the likelihood function (as a function of the parameters θ):

$$L(\theta) = \prod_{i=1}^{N} \theta^{x_i} (1-\theta)^{1-x_i}$$

- We usually work with log-likelihoods:

$$\ell(\theta) = \sum_{i=1}^{N} x_i \log \theta + (1-x_i) \log(1-\theta)$$

- How can we choose θ? Good values of θ should assign high probability to the observed data. This motivates the maximum likelihood criterion, that we should pick the parameters that maximize the likelihood:

$$\hat{\theta}_{\mathrm{ML}} = \max_{\theta \in [0,1]} \ell(\theta)$$

Maximum Likelihood Estimation for the Coin Example

- Remember how we found the optimal solution to linear regression by setting derivatives to zero? We can do that again for the coin example.

$$
\begin{aligned}
\frac{\mathrm{d}\ell}{\mathrm{d}\theta} &= \frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sum_{i=1}^{N} x_i \log\theta + (1-x_i)\log(1-\theta)\right) \\
&= \frac{\mathrm{d}}{\mathrm{d}\theta}\left(N_H \log\theta + N_T \log(1-\theta)\right) \\
&= \frac{N_H}{\theta} - \frac{N_T}{1-\theta}
\end{aligned}
$$

where $N_H = \sum_i x_i$ and $N_T = N - \sum_i x_i$.

- Setting this to zero gives the maximum likelihood estimate:

$$
\hat{\theta}_{\mathrm{ML}} = \frac{N_H}{N_H + N_T}.
$$

Maximum Likelihood Estimation

- Notice, in the coin example we are actually minimizing cross-entropies!

$$
\begin{aligned}
\hat{\theta}_{\mathrm{ML}} &= \max_{\theta \in [0,1]} \ell(\theta) \\
&= \min_{\theta \in [0,1]} -\ell(\theta) \\
&= \min_{\theta \in [0,1]} \sum_{i=1}^{N} -x_i \log \theta - (1 - x_i) \log(1 - \theta)
\end{aligned}
$$

- This is an example of maximum likelihood estimation.
  - define a model that assigns a probability (or has a probability density at) to a dataset
  - maximize the likelihood (or minimize the neg. log-likelihood).
- Many examples we've considered fall in this framework! Let's consider classification again.

Discriminative VS Generative?

Two approaches to classification:

- Discriminative approach: estimate parameters of decision boundary/class separator directly from labeled examples.
  - Model $p(t|\mathbf{x})$ directly (logistic regression models)
  - Learn mappings from inputs to classes (linear/logistic regression, decision trees etc)
  - Tries to solve: How do I separate the classes?
- Generative approach: model the distribution of inputs characteristic of the class (Bayes classifier).
  - Model $p(\mathbf{x}|t)$
  - Apply Bayes Rule to derive $p(t|\mathbf{x})$.
  - Tries to solve: What does each class "look" like?
- Key difference: is there a distributional assumption over inputs?

A Generative Model: Bayes Classifier

- Aim to classify text into spam/not-spam (yes c=1; no c=0)
- Example: "You are one of the very few who have been selected as a winners for the free $1000 Gift Card."
- Use bag-of-words features, get binary vector $\mathbf{x}$ for each email
- Vocabulary:
  - "a": 1
  - ...
  - "car": 0
  - "card": 1
  - ...
  - "win": 0
  - "winner": 1
  - "winter": 0
  - ...
  - "you": 1

Bayes Classifier

- Given features $\mathbf{x} = [x_1, x_2, \cdots, x_D]^T$ we want to compute class probabilities using Bayes Rule:

$$\underbrace{p(c|\mathbf{x})}_{\text{Pr. class given words}} = \frac{p(\mathbf{x}, c)}{p(\mathbf{x})} = \frac{\overbrace{p(\mathbf{x}|c)}^{\text{Pr. words given class}} \quad p(c)}{p(\mathbf{x})}$$

- More formally

$$\text{posterior} = \frac{\text{Class likelihood} \times \text{prior}}{\text{Evidence}}$$

- How can we compute $p(\mathbf{x})$ for the two class case? (Do we need to?)

$$p(\mathbf{x}) = p(\mathbf{x}|c=0)p(c=0) + p(\mathbf{x}|c=1)p(c=1)$$

- To compute $p(c|\mathbf{x})$ we need: $p(\mathbf{x}|c)$ and $p(c)$

Naive Bayes

- Assume we have two classes: spam and non-spam. We have a dictionary of D words, and binary features $\mathbf{x} = [x_1, \ldots, x_D]$ saying whether each word appears in the e-mail.

- If we define a joint distribution $p(c, x_1, \ldots, x_D)$, this gives enough information to determine $p(c)$ and $p(\mathbf{x}|c)$.

- Problem: specifying a joint distribution over $D + 1$ binary variables requires $2^{D+1} - 1$ entries. This is computationally prohibitive and would require an absurd amount of data to fit.

- We'd like to impose structure on the distribution such that:
  - it can be compactly represented
  - learning and inference are both tractable

Naive Bayes

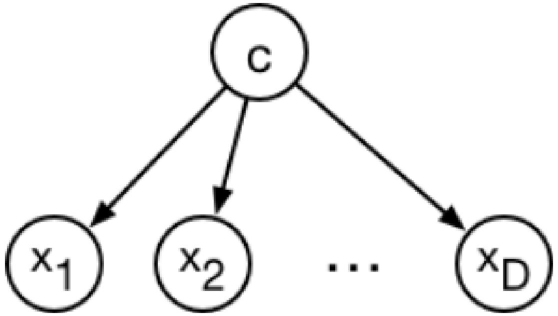
- Naïve assumption: Naïve Bayes assumes that the word features x_i are conditionally independent given the class c.
  - This means x_i and x_j are independent under the conditional distribution $p(\mathbf{x}|c)$.
  - Note: this doesn't mean they're independent.
  - Mathematically,

$$p(c, x_1, \ldots, x_D) = p(c)p(x_1|c) \cdots p(x_D|c).$$

- Compact representation of the joint distribution
  - Prior probability of class: $p(c = 1) = \pi$ (e.g. spam email)
  - Conditional probability of word feature given class: $p(x_j = 1|c) = \theta_{jc}$ (e.g. word "price" appearing in spam)
  - $2D + 1$ parameters total (before $2^{D+1} - 1$)

Bayes Nets

- We can represent this model using an directed graphical model, or Bayesian network:



- This graph structure means the joint distribution factorizes as a product of conditional distributions for each variable given its parent(s).

- Intuitively, you can think of the edges as reflecting a causal structure. But mathematically, this doesn't hold without additional assumptions.

Naive Bayes: Learning

- The parameters can be learned efficiently because the log-likelihood decomposes into independent terms for each feature.

$$
\begin{aligned}
\ell(\boldsymbol{\theta}) &= \sum_{i=1}^{N} \log p(c^{(i)}, \mathbf{x}^{(i)}) = \sum_{i=1}^{N} \log \left\{ p(\mathbf{x}^{(i)} | c^{(i)}) p(c^{(i)}) \right\} \\
&= \sum_{i=1}^{N} \log \left\{ p(c^{(i)}) \prod_{j=1}^{D} p(x_j^{(i)} \mid c^{(i)}) \right\} \\
&= \sum_{i=1}^{N} \left[\log p(c^{(i)}) + \sum_{j=1}^{D} \log p(x_j^{(i)} \mid c^{(i)}) \right] \\
&= \underbrace{\sum_{i=1}^{N} \log p(c^{(i)})}_{\substack{\text{Bernoulli log-likelihood} \\ \text{of labels}}} + \sum_{j=1}^{D} \underbrace{\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)})}_{\substack{\text{Bernoulli log-likelihood} \\ \text{for feature } x_j}}
\end{aligned}
$$

- Each of these log-likelihood terms depends on different sets of parameters, so they can be optimized independently.

Naive Bayes: Learning

- We can handle these terms separately. For the prior we maximize: $\sum_{i=1}^{N} \log p(c^{(i)})$
- This is a minor variant of our coin flip example. Let $p(c^{(i)} = 1) = \pi$. Note $p(c^{(i)}) = \pi^{c^{(i)}}(1-\pi)^{1-c^{(i)}}$.
- Log-likelihood:

$$\sum_{i=1}^{N} \log p(c^{(i)}) = \sum_{i=1}^{N} c^{(i)} \log \pi + \sum_{i=1}^{N} (1 - c^{(i)}) \log(1-\pi)$$

- Obtain MLEs by setting derivatives to zero:

$$\hat{\pi} = \frac{\sum_i \mathbb{I}[c^{(i)} = 1]}{N} = \frac{\text{\# spams in dataset}}{\text{total \# samples}}$$

Naive Bayes: Learning

- Each θ_{jc}'s can be treated separately: maximize $\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)})$
- This is (again) a minor variant of our coin flip example.

  Let $\theta_{jc} = p(x_j^{(i)} = 1 \mid c)$. Note $p(x_j^{(i)} \mid c) = \theta_{jc}^{x_j^{(i)}} (1 - \theta_{jc})^{1 - x_j^{(i)}}$.
- Log-likelihood:

$$\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)}) = \sum_{i=1}^{N} c^{(i)} \left\{ x_j^{(i)} \log \theta_{j1} + (1 - x_j^{(i)}) \log(1 - \theta_{j1}) \right\} + \sum_{i=1}^{N} (1 - c^{(i)}) \left\{ x_j^{(i)} \log \theta_{j0} + (1 - x_j^{(i)}) \log(1 - \theta_{j0}) \right\}$$

- Obtain MLEs by setting derivatives to zero:

$$\hat{\theta}_{jc} = \frac{\sum_i \mathbb{I}[x_j^{(i)} = 1 \ \& \ c^{(i)} = c]}{\sum_i \mathbb{I}[c^{(i)} = c]} \stackrel{\text{for } c = 1}{=} \frac{\#\text{word } j \text{ appears in spams}}{\#\text{ spams in dataset}}$$

Naive Bayes: Inference

- We predict the category by performing inference in the model.
- Apply Bayes' Rule:

$$p(c \,|\, \mathbf{x}) = \frac{p(c)p(\mathbf{x} \,|\, c)}{\sum_{c'} p(c')p(\mathbf{x} \,|\, c')} = \frac{p(c) \prod_{j=1}^{D} p(x_j \,|\, c)}{\sum_{c'} p(c') \prod_{j=1}^{D} p(x_j \,|\, c')}$$

- We need not compute the denominator if we're simply trying to determine the most likely c.
- Shorthand notation:

$$p(c \,|\, \mathbf{x}) \propto p(c) \prod_{j=1}^{D} p(x_j \,|\, c)$$

- For input $\mathbf{x}$, predict by comparing the values of $p(c) \prod_{j=1}^{D} p(x_j \,|\, c)$ for different c (e.g. choose the largest).

Naive Bayes

- Naïve Bayes is an amazingly cheap learning algorithm!
- Training time: estimate parameters using maximum likelihood
  - Compute co-occurrence counts of each feature with the labels.
  - Requires only one pass through the data!
- Test time: apply Bayes' Rule
  - Cheap because of the model structure. (For more general models, Bayesian inference can be very expensive and/or complicated.)
- We covered the Bernoulli case for simplicity. But our analysis easily extends to other probability distributions.
- Unfortunately, it's usually less accurate in practice compared to discriminative models due to its "naïve" independence assumption.

MLE issue: Data Sparsity

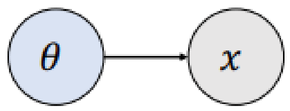
- Maximum likelihood has a pitfall: if you have too little data, it can overfit.
- E.g., what if you flip the coin twice and get H both times?

$$\theta_{\mathrm{ML}} = \frac{N_H}{N_H + N_T} = \frac{2}{2+0} = 1$$

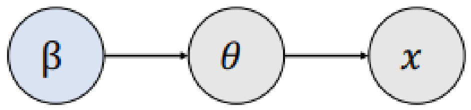
- Because it never observed T, it assigns this outcome probability 0. This problem is known as data sparsity.

Bayesian Parameter Estimation

- In maximum likelihood, the observations are treated as random variables, but the parameters are not.



- The Bayesian approach treats the parameters as random variables as well. β is the set of parameters in the prior distribution of θ.



- To define a Bayesian model, we need to specify two distributions:
  - The prior distribution $p(\boldsymbol{\theta})$, which encodes our beliefs about the parameters *before* we observe the data
  - The likelihood $p(\mathcal{D} \,|\, \boldsymbol{\theta})$, same as in maximum likelihood

Bayesian Parameter Estimation

- When we update our beliefs based on the observations, we compute the posterior distribution using Bayes' Rule:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{p(\boldsymbol{\theta})p(\mathcal{D} \mid \boldsymbol{\theta})}{\int p(\boldsymbol{\theta}')p(\mathcal{D} \mid \boldsymbol{\theta}')\,\mathrm{d}\boldsymbol{\theta}'}.$$

- We rarely ever compute the denominator explicitly. In general, it is computationally intractable.

Bayesian Parameter Estimation

- Let's revisit the coin example. We already know the likelihood:

$$L(\theta) = p(\mathcal{D}|\theta) = \theta^{N_H}(1-\theta)^{N_T}$$

- It remains to specify the prior $p(\theta)$.
  - We can choose an uninformative prior, which assumes as little as possible. A reasonable choice is the uniform prior.
  - But our experience tells us 0.5 is more likely than 0.99. One particularly useful prior that lets us specify this is the beta distribution:

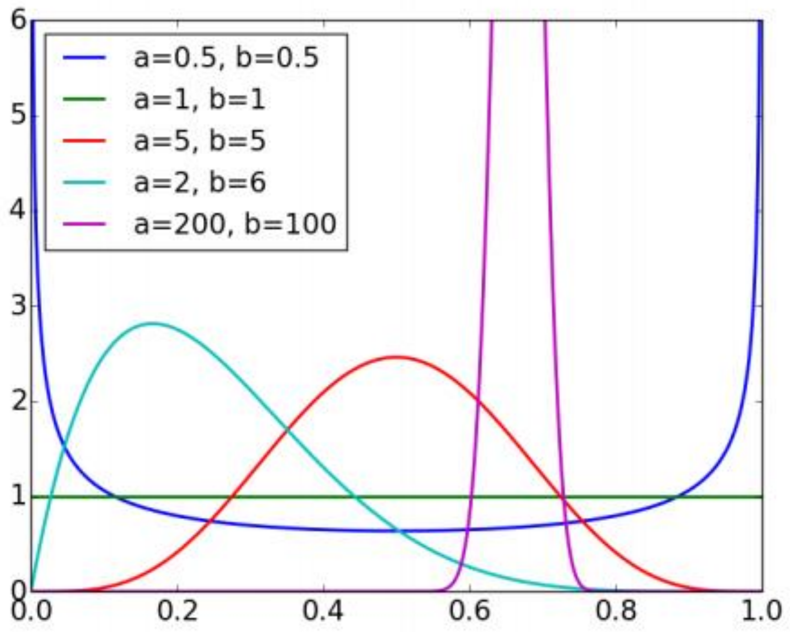
$$p(\theta; a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\,\theta^{a-1}(1-\theta)^{b-1}.$$

  - This notation for proportionality lets us ignore the normalization constant:

$$p(\theta; a, b) \propto \theta^{a-1}(1-\theta)^{b-1}.$$

Bayesian Parameter Estimation

- Beta distribution for various values of a, b:



- Some observations:
  - The expectation $\mathbb{E}[\theta] = a/(a+b)$ (easy to derive).
  - The distribution gets more peaked when a and b are large.
  - The uniform distribution is the special case where $a = b = 1$.
- The beta distribution is used for is as a prior for the Bernoulli distribution.

Bayesian Parameter Estimation

- Computing the posterior distribution:

$$\begin{aligned} p(\boldsymbol{\theta} \,|\, \mathcal{D}) &\propto p(\boldsymbol{\theta}) p(\mathcal{D} \,|\, \boldsymbol{\theta}) \\ &\propto \left[\theta^{a-1}(1-\theta)^{b-1}\right] \left[\theta^{N_H}(1-\theta)^{N_T}\right] \\ &= \theta^{a-1+N_H}(1-\theta)^{b-1+N_T}. \end{aligned}$$

- This is just a beta distribution with parameters $N_H + a$ and $N_T + b$.
- The posterior expectation of θ is:

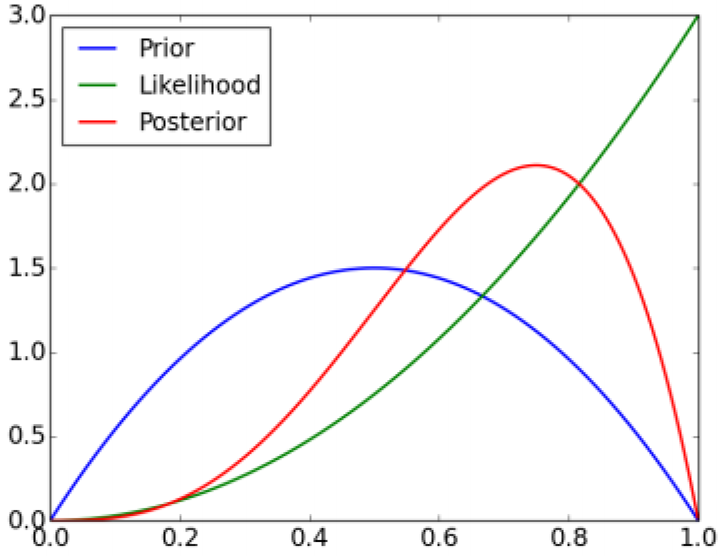
$$\mathbb{E}[\theta \,|\, \mathcal{D}] = \frac{N_H + a}{N_H + N_T + a + b}$$

- The parameters a and b of the prior can be thought of as pseudo-counts.
  - The reason this works is that the prior and likelihood have the same functional form. This phenomenon is known as conjugacy (conjugate priors), and it's very useful.

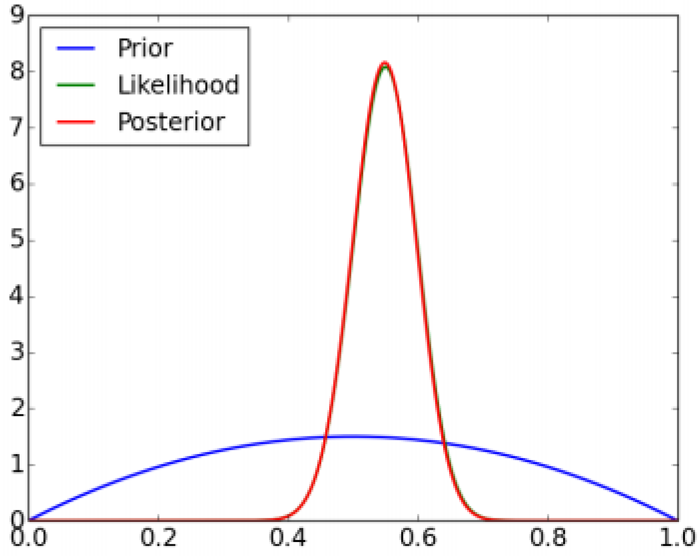
Bayesian Parameter Estimation

Bayesian inference for the coin flip example:

Small data setting
$N_H = 2,\ N_T = 0$



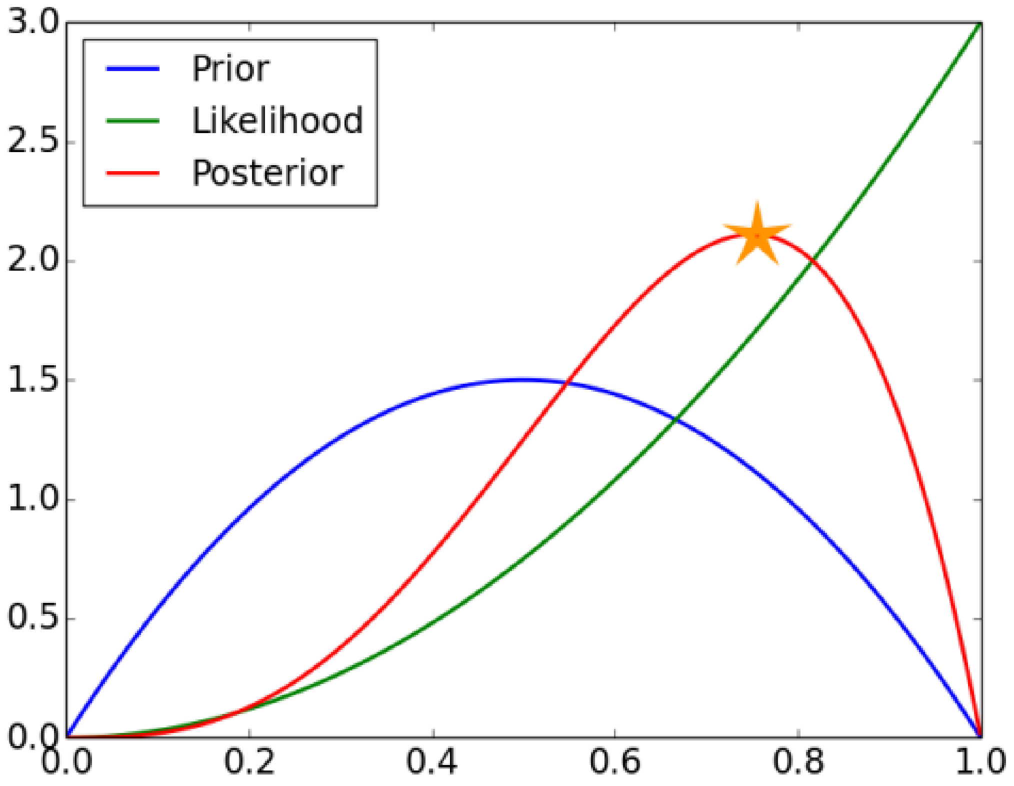
Large data setting
$N_H = 55,\ N_T = 45$



When you have enough observations, the data overwhelm the prior.

Maximum A-Posteriori Estimation

- Maximum a-posteriori (MAP) estimation: find the most likely parameter settings under the posterior



Maximum A-Posteriori Estimation

- This converts the Bayesian parameter estimation problem into a maximization problem

$$\begin{aligned}\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} &= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta} \,|\, \mathcal{D}) \\ &= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta}, \mathcal{D}) \\ &= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta})\, p(\mathcal{D} \,|\, \boldsymbol{\theta}) \\ &= \arg\max_{\boldsymbol{\theta}} \; \log p(\boldsymbol{\theta}) + \log p(\mathcal{D} \,|\, \boldsymbol{\theta})\end{aligned}$$

- We already saw an example of this in the homework.

Maximum A-Posteriori Estimation

- Joint probability in the coin flip example:

$$\begin{aligned}\log p(\theta, \mathcal{D}) &= \log p(\theta) + \log p(\mathcal{D} \mid \theta)\\ &= \text{Const} + (a-1)\log\theta + (b-1)\log(1-\theta) + N_H \log\theta + N_T \log(1-\theta)\\ &= \text{Const} + (N_H + a - 1)\log\theta + (N_T + b - 1)\log(1-\theta)\end{aligned}$$

- Maximize by finding a critical point

$$0 = \frac{\mathrm{d}}{\mathrm{d}\theta}\log p(\theta, \mathcal{D}) = \frac{N_H + a - 1}{\theta} - \frac{N_T + b - 1}{1-\theta}$$

- Solving for θ,

$$\hat{\theta}_{\mathrm{MAP}} = \frac{N_H + a - 1}{N_H + N_T + a + b - 2}$$

Maximum A-Posteriori Estimation

Comparison of estimates in the coin flip example:

	Formula	$N_H = 2, N_T = 0$	$N_H = 55, N_T = 45$
$\hat{\theta}_{\text{ML}}$	$\frac{N_H}{N_H+N_T}$	1	$\frac{55}{100} = 0.55$
$\mathbb{E}[\theta \mid \mathcal{D}]$	$\frac{N_H+a}{N_H+N_T+a+b}$	$\frac{4}{6} \approx 0.67$	$\frac{57}{104} \approx 0.548$
$\hat{\theta}_{\text{MAP}}$	$\frac{N_H+a-1}{N_H+N_T+a+b-2}$	$\frac{3}{4} = 0.75$	$\frac{56}{102} \approx 0.549$

$\hat{\theta}_{\text{MAP}}$ assigns nonzero probabilities as long as $a, b > 1$.