Outline

1. Probabilistic Modeling of Data
2. Discriminative and Generative Classifiers
3. Naïve Bayes Models
4. Bayesian Parameter Estimation
5. Multivariate Gaussian Distribution
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 begin putting together a **probabilistic interpretation** of our model and loss, and introduce the concept of **maximum likelihood estimation**.
1 Probabilistic Modeling of Data

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Example: A Biased Coin

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.

We want to create a model to predict the outcome of the next coin flip. That is, we want to answer this question:

What is the probability it will come up heads if we flip again?
The coin is likely biased. Let’s assume that one coin flip outcome $x$ is a Bernoulli random variable for a currently unknown parameter $\theta \in [0, 1]$.

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

or more succinctly

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

Assume that $\{x_1, \ldots, x_N\}$ are independent and identically distributed (i.i.d.). Thus, the joint probability of the outcome $\{x_1, \ldots, x_N\}$ is

$$p(x_1, \ldots, x_N | \theta) = \prod_{i=1}^{N} \theta^{x_i} (1 - \theta)^{1-x_i}$$
The **likelihood function** is the probability of observing the data as a function of the parameters $\theta$:

$$L(\theta) = \prod_{i=1}^{N} \theta^{x_i} (1 - \theta)^{1-x_i} = \theta^{55} (1-\theta)^{45}$$

We usually work with log-likelihoods:

$$\log p(x_1,\ldots,x_N | \theta) = \ell(\theta) = \sum_{i=1}^{N} x_i \log \theta + (1 - x_i) \log (1 - \theta)$$

$$= 55 \log \theta + 45 \log (1-\theta)$$

**55 heads, 45 tails**
Maximum Likelihood Estimation

How can we choose $\theta$? Good values of $\theta$ should assign high probability to the observed data.

The maximum likelihood criterion says that we should pick the parameters that maximize the likelihood. Of data given parameters.

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

We can find the optimal solution by setting derivatives to zero.

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

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

Setting this to zero gives the maximum likelihood estimate:

$$\hat{\theta}_{\text{ML}} = \frac{N_H}{N_H + N_T} = \frac{55}{55 + 45} = 0.55$$
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).
Observe $N$ outcomes of the coin flip \( \{X_1, \ldots, X_N\} \), where $X_i \in \{0, 1\}$. \( X_i = 1 \) means heads (H).

55 heads ($N_H = 55$), 45 tails ($N_T = 45$).

\( \Theta \) is the probability of the coin landing on heads.

\[
Pr(X_i | \Theta) = \Theta^{X_i} (1-\Theta)^{1-X_i} = \begin{cases} 
\Theta, & \text{if } X_i = 1 \\
1-\Theta, & \text{if } X_i = 0.
\end{cases}
\]

\[
Pr(X_1, \ldots, X_N | \Theta) = \prod_{i=1}^{N} \Theta^{X_i} (1-\Theta)^{1-X_i} = \Theta^{55} (1-\Theta)^{45}
\]

\[
L(\Theta) = Pr(X_1, X_2, \ldots, X_N | \Theta) = \prod_{i=1}^{N} \Theta^{X_i} (1-\Theta)^{1-X_i} = \Theta^{55} (1-\Theta)^{45}
\]
\[
\ell(\theta) = \log P_r (X_1, X_2, \ldots, X_N | \theta) = \log \prod_{i=1}^{N} \theta^{X_i} (1-\theta)^{1-X_i}
\]
\[
= \sum_{i=1}^{N} \log (\theta^{X_i} (1-\theta)^{1-X_i})
\]
\[
= \sum_{i=1}^{N} \left( \log \theta^{X_i} + \log (1-\theta)^{1-X_i} \right)
\]
\[
= \sum_{i=1}^{N} \left( X_i \log \theta + (1- X_i) \log (1-\theta) \right)
\]
\[
= N_H \log \theta + N_T \log (1-\theta).
\]
\[
= 55 \log \theta + 45 \log (1-\theta)
\]
$\hat{\theta}_{\text{maximum likelihood}} = \arg \max_{\theta \in [0, 1]} l(\theta)$

$$\frac{d l(\theta)}{d \theta} = \frac{d}{d \theta} \sum_{i=1}^{N} \left( x_i \log \theta + (1-x_i) \log (1-\theta) \right)$$

$$= \sum_{i=1}^{N} \left( \frac{x_i}{\theta} - \frac{1-x_i}{1-\theta} \right)$$

$$= \frac{N_H}{\theta} - \frac{N_T}{1-\theta} = \frac{55}{\theta} - \frac{45}{1-\theta}$$

$$\frac{d l(\theta)}{d \theta} = \frac{N_H}{\theta} - \frac{N_T}{1-\theta} = 0 \Rightarrow \frac{N_H - N_H \theta - N_T \theta}{\theta(1-\theta)} = 0$$

$N_H = \theta (N_H + N_T) \Rightarrow \theta = \frac{N_H}{N_H + N_T} = \frac{55}{55 + 45} = 0.55$
Summary of Maximum Likelihood:
~ model parameters \( \theta \), some data \( D \).

~ calculate the log-likelihood of data given model parameters.
\[
\log p(D|\theta)
\]

~ choose model parameters that maximizes the log-likelihood.
\[
\hat{\theta}_{ML} = \arg \max_{\theta} \log p(D|\theta)
\]

For coin flip example.
\[
\hat{\theta}_{ML} \text{ (prob of heads)} = \frac{\text{# of heads}}{\text{# of coin flips}}
\]
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Spam Classification

For a large company that runs an email service, one of the important predictive problems is the automated detection of spam email.

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Dear Karim,

I think we should postpone the board meeting to be held after Thanksgiving.

Regards,
Anna

---

Dear Toby,

I have an incredible opportunity for mining 2 Bitcoin a day. Please Contact me at the earliest at +1 123 321 1555. You won’t want to miss out on this opportunity.

Regards,
Ark
Discriminative classifiers try to learn mappings directly from the space of inputs $\mathcal{X}$ to class labels $\{0, 1, 2, \ldots , K\}$.

**Features**
- Postpone, board, meeting, Thanksgiving
- Mining, Bitcoin, contact, opportunity

**Class probability**
- $p(y|x)$

**Not spam**

**Spam**
**Generative Classifiers**

Generative classifiers try to build a model of “what data for a class looks like”, i.e. model $p(x, y)$. If we know $p(y)$ we can easily compute $p(x|y)$.

Classification via Bayes rule (thus also called Bayes classifiers)

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

- **Probability of feature given label**
  - $p(x|y)$
- **Class label**
  - $y$

**Not spam**
- postpone, board, meeting, Thanksgiving

**Spam**
- mining, Bitcoin, contact, opportunity
Generative vs Discriminative

- **Discriminative approach**: estimate parameters of decision boundary/class separator directly from labeled examples.
  - Model $p(t|x)$ 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 $p(x|t)$
  - Apply Bayes Rule to derive $p(t|x)$.
  - Tries to solve: What does each class ”look” like?

- Key difference: is there a distributional assumption over inputs?
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Example: Spam Detection

- Classify email into spam ($c = 1$) or non-spam ($c = 0$).
- Binary features $\mathbf{x} = [x_1, \ldots, x_D], x_i \in \{0, 1\}$ saying whether each of $D$ words appears in the e-mail.

Example email: “You are one of the very few who have been selected as a winner for the free $1000$ Gift Card.”

Feature vector for this email:

- “card”: 1
- “winners”: 1
- “winter”: 0
- “you”: 1
Bayesian Classifier

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

\[
p(c|\mathbf{x}) = \frac{p(\mathbf{x}|c)p(c)}{p(\mathbf{x})}
\]

In words,

Posterior for class = \( \frac{\text{Pr. of feature given class} \times \text{Prior for class}}{\text{Pr. of feature}} \)

To compute \( p(c|\mathbf{x}) \) we need: \( p(\mathbf{x}|c) \) and \( p(c) \).
1. explain each term
2. \( p(x|c) \rightarrow p(c|x) \)
3. prior \( \rightarrow \) posterior

\[
\Pr(c|x) = \frac{\Pr(x|c) \Pr(c)}{\Pr(x)}
\]

- \( \Pr(x|c) \): word in an email or not
- \( \Pr(c) \): Prior
- \( \Pr(\text{spam}) \)
- \( \Pr(\text{non-spam}) \)
- \( \Pr(x) \): e.g., \( \Pr(\text{"winner"}) \)
- \( \Pr(x) \): e.g., \( \Pr(\text{"you"}) \)
Do not need \( p(x) \) explicitly. It's a normalization constant.

\[
P(c=1|x) = \frac{\frac{p(x|c=1) p(c=1)}{p(x)}}{p(x)}
\]

\[
= \frac{p(x|c=1) p(c=1)}{p(x|c=1) p(c=1) + p(x|c=0) p(c=0)}
\]

1. Calculate \( p(x|c=1) p(c=1) \) and \( p(x|c=0) p(c=0) \).

2. Then normalize. (divide each by the sum of the two.)
Motivation for Compact Representation

- Two classes: \( c \in \{0, 1\} \).
- Binary features \( \mathbf{x} = [x_1, \ldots, x_D], x_i \in \{0, 1\} \).
- Define a joint distribution \( p(c, x_1, \ldots, x_D) \). How many probabilities do we need to specify this joint dist.? \( 2^{D+1} - 1 \)
- Let’s impose structure on the distribution so that the representation is compact and allows for efficient learning and inference.
Naïve Bayes Independence Assumption

Naïve assumption:
the features $x_i$ are conditionally independent given the class $c$.

- Allows us to decompose the joint distribution:

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

Compact representation of the joint distribution

- Prior probability of class:
  $p(c = 1) = \pi$ (e.g. prob of spam)

- Conditional probability of feature given class:
  $p(x_j = 1|c) = \theta_{jc}$ (e.g. prob of word appearing in spam)
Bayesian Network for a Naive Bayes Model

Which probabilities do we need to specify this dist.? 
How many probabilities do we need to specify this dist.? 

\[ 1 + 2D \]
Decomposing the Log-Likelihood

Decompose the log-likelihood into independent terms. Optimize each term independently.

\[
\ell(\theta) = \sum_{i=1}^{N} \log p(c^{(i)}, x^{(i)}) = \sum_{i=1}^{N} \log \left\{ p(x^{(i)}|c^{(i)})p(c^{(i)}) \right\}
\]

\[
= \sum_{i=1}^{N} \log \left\{ p(c^{(i)}) \prod_{j=1}^{D} p(x_j^{(i)} | c^{(i)}) \right\}
\]

\[
= \sum_{i=1}^{N} \left[ \log p(c^{(i)}) + \sum_{j=1}^{D} \log p(x_j^{(i)} | c^{(i)}) \right]
\]

\[
= \sum_{i=1}^{N} \log p(c^{(i)}) + \sum_{j=1}^{D} \sum_{i=1}^{N} \log p(x_j^{(i)} | c^{(i)})
\]

Log-likelihood of labels

Log-likelihood for feature \(x_j\)
Learning the Prior over Class

- To learn the prior, we maximize $\sum_{i=1}^{N} \log p(c^{(i)})$.
- Define $\pi = p(c^{(i)} = 1)$
- \text{Pr. } i\text{-th email: } p(c^{(i)}) = \pi^{c^{(i)}} (1 - \pi)^{1-c^{(i)}}$.
- Log-likelihood of the dataset:
  $$\sum_{i=1}^{N} \log p(c^{(i)}) = \sum_{i=1}^{N} c^{(i)} \log \pi + \sum_{i=1}^{N} (1 - c^{(i)}) \log (1 - \pi)$$
- Maximum likelihood estimate of the prior $\pi$ is the fraction of spams in dataset.
  $$\hat{\pi} = \frac{\sum_{i} \mathbb{1}[c^{(i)} = 1]}{N} = \frac{\# \text{ spams in dataset}}{\text{total } \# \text{ samples}}$$
\( c^{(i)} \in \{0, 1\} \) is the class label for \( i \)th example.

\[
P(c^{(i)} | \pi) = \pi^{c^{(i)}} (1 - \pi)^{1 - c^{(i)}}
\]

\[
P(c^{(1)}, c^{(2)}, \ldots, c^{(N)} | \pi) = \prod_{i=1}^{N} \pi^{c^{(i)}} (1 - \pi)^{1 - c^{(i)}}
\]

\[
\log P(c^{(1)}, \ldots, c^{(N)} | \pi) = \log \prod_{i=1}^{N} \pi^{c^{(i)}} (1 - \pi)^{1 - c^{(i)}}
\]

\[
= \sum_{i=1}^{N} \log \left( \pi^{c^{(i)}} (1 - \pi)^{1 - c^{(i)}} \right)
\]

\[
= \sum_{i=1}^{N} \left( c^{(i)} \log \pi + (1 - c^{(i)}) \log (1 - \pi) \right)
\]

\[
\frac{\partial}{\partial \pi} \log P(c^{(1)}, \ldots, c^{(N)} | \pi) = \sum_{i=1}^{N} \left( c^{(i)} \frac{1}{\pi} - (1 - c^{(i)}) \frac{1}{1 - \pi} \right)
\]
Let \( \sum_{i=1}^{N} \mathbb{I}[c^{(i)}=1] = S \)

\[
\frac{\partial}{\partial \pi} \log p(c^{(1)}, \ldots, c^{(N)} | \pi) = \sum_{i=1}^{N} \left( \frac{1}{\pi} - (1 - c^{(i)}) \frac{1}{1-\pi} \right)
\]

\[
= \frac{S}{\pi} - \frac{N-S}{1-\pi} = 0
\]

\[
\frac{S}{\pi} = \frac{N-S}{1-\pi} \quad \Rightarrow \quad S(1-\pi) = (N-S)\pi
\]

\[
\Rightarrow \quad S = S\pi + (N-S)\pi
\]

\[
\Rightarrow \quad S = N\pi
\]

\[
\Rightarrow \quad \pi = \frac{S}{N} = \frac{\sum_{i=1}^{N} \mathbb{I}[c^{(i)}=1]}{N}
\]
Learning Pr. Feature Given Class

- To learn $p(x_j^{(i)} = 1 \mid c)$, we maximize $\sum_{i=1}^{N} \log p(x_j^{(i)} \mid c^{(i)})$.
- Define $\theta_{jc} = p(x_j^{(i)} = 1 \mid c)$.

Pr. of $i$-th email: $p(x_j^{(i)} \mid c) = \theta_{jc} x_j^{(i)} (1 - \theta_{jc})^{1-x_j^{(i)}}$.

Log-likelihood of the dataset:

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

- Maximum likelihood estimate of $\theta_{jc}$

is the fraction of word $j$ occurrences in each class in the dataset.

$$\hat{\theta}_{jc} = \frac{\sum_i \mathbb{I}[x_j^{(i)} = 1 \& c^{(i)} = c]}{\sum_i \mathbb{I}[c^{(i)} = c]} \quad \text{for } c = 1 \quad \# \text{word } j \text{ appears in class } c \quad \# \text{ class } c \text{ in dataset}$$
\( \chi_j^{(i)} \in \{0, 1\} \) denotes whether \( j \)th word in dictionary occurs in \( i \)th email.

\[
P(\chi_j^{(i)} | c^{(i)}) = \chi_j^{(i)} \left( 1 - p(\chi_j^{(i)} | c^{(i)}) \right)^{1 - \chi_j^{(i)}}
\]

\[
\log p(\chi_j^{(i)} | c^{(i)}) = \chi_j^{(i)} \log p(\chi_j^{(i)} = 1 | c^{(i)})
+ (1 - \chi_j^{(i)}) \log \left( 1 - p(\chi_j^{(i)} = 1 | c^{(i)}) \right)
\]

\[
\sum_{i=1}^{N} \log p(\chi_j^{(i)} | c^{(i)}) = \sum_{i=1}^{N} \left[ \chi_j^{(i)} \log p(\chi_j^{(i)} = 1 | c^{(i)})
+ (1 - \chi_j^{(i)}) \log \left( 1 - p(\chi_j^{(i)} = 1 | c^{(i)}) \right) \right]
\]

\[
= \sum_{i=1}^{N} c^{(i)} \left[ \chi_j^{(i)} \log p(\chi_j^{(i)} = 1 | c^{(i)} = 1)
+ (1 - \chi_j^{(i)}) \log \left( 1 - p(\chi_j^{(i)} = 1 | c^{(i)} = 1) \right) \right]
+ \sum_{i=1}^{N} (1 - c^{(i)}) \left[ \chi_j^{(i)} \log p(\chi_j^{(i)} = 1 | c^{(i)} = 0)
+ (1 - \chi_j^{(i)}) \log \left( 1 - p(\chi_j^{(i)} = 1 | c^{(i)} = 0) \right) \right]
\]
\[
\frac{\partial}{\partial p(x_j^{(i)} = 1 | c^{(i)} = 1)} \sum_{i=1}^{N} \log p(x_j^{(i)} | c^{(i)}) = \sum_{i=1}^{N} \left[ c^{(i)} \left( \frac{x_j^{(i)}}{p(x_j^{(i)} = 1 | c^{(i)} = 1)} - \frac{1 - x_j^{(i)}}{p(x_j^{(i)} = 1 | c^{(i)} = 1)} \right) \right] = 0
\]

Let \( \theta_{j1} = p(x_j^{(i)} = 1 | c^{(i)} = 1) \)

\[
\Rightarrow \sum_{i=1}^{N} c^{(i)} \left( x_j^{(i)} \left( 1 - \theta_{j1} \right) - \left( 1 - x_j^{(i)} \right) \theta_{j1} \right) = 0
\]

\[
\Rightarrow \sum_{i=1}^{N} c^{(i)} \left( x_j^{(i)} - \theta_{j1} \right) = 0
\]

\[
\Rightarrow \frac{\sum_{i=1}^{N} c^{(i)} x_j^{(i)}}{\sum_{i=1}^{N} c^{(i)}} = \theta_{j1} \Rightarrow \theta_{j1} = \frac{\sum_{i=1}^{N} c^{(i)} x_j^{(i)}}{\sum_{i=1}^{N} c^{(i)}}
\]
Predicting the Most Likely Class

- We predict the class by performing inference in the model.
- Apply Bayes’ Rule:

\[
p(c \mid x) = \frac{p(c)p(x \mid c)}{\sum_{c'} p(c')p(x \mid c')} = \frac{p(c) \prod_{j=1}^{D} p(x_j \mid c)}{\sum_{c'} p(c') \prod_{j=1}^{D} p(x_j \mid c')}
\]

- For input \( x \), predict \( c \) with the largest \( p(c) \prod_{j=1}^{D} p(x_j \mid c) \)

  (the most likely class).
Naïve Bayes Properties

- 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.)
- Analysis easily extends to prob. distributions other than Bernoulli.
- Less accurate in practice compared to discriminative models due to its “naïve” independence assumption.
Naive Bayes Summary.

Model Parameters:
\[
\begin{align*}
\sum \Pr(c) &= \pi \\
\Pr(x_j | c) &= \theta_{jc}
\end{align*}
\]

1. Learning the model parameters.
   ~ Learn \( \pi \) by maximum likelihood.
   ~ Learn \( \theta_{jc} \) by maximum likelihood.

2. Making a prediction.
   For input \( x \), predict class \( c \) w/ largest
   \[
   \frac{\prod_{j=1}^{D} \Pr(x_j | c) \Pr(c)}{\sum \Pr(c) \prod_{j=1}^{D} \Pr(x_j | c)}
   \]
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Data Sparsity

Maximum likelihood can overfit if there is too little data.

Example: what if you flip the coin twice and get H both times?

\[ \theta_{\text{ML}} = \frac{N_H}{N_H + N_T} = \frac{2}{2 + 0} = 1 \]

The model assigned probability 0 to T. This problem is known as data sparsity.
We need to specify two distributions:

- **The prior distribution** $p(\theta)$ encodes our beliefs about the parameters before we observe the data.

- **The likelihood** $p(D|\theta)$ encodes the likelihood of observing the data given the parameters.
When we **update** our beliefs based on the observations, we compute the **posterior distribution** using Bayes’ Rule:

\[
p(\theta | D) = \frac{p(\theta)p(D | \theta)}{\int p(\theta')p(D | \theta') \, d\theta'}.
\]

- Rarely ever compute the denominator explicitly.
- In general, computing the denominator is **intractable**.
Revisiting Coin Flip Example

We already know the likelihood:

\[ L(\theta) = p(D|\theta) = \theta^N_H (1 - \theta)^N_T \]

It remains to specify the prior \( p(\theta) \).

- An uninformative prior, which assumes as little as possible. A reasonable choice is the uniform prior.
- But, experience tells us \( 0.5 \) is more likely than \( 0.99 \). One particularly useful prior is the beta distribution:

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

- We can ignore the normalization constant.

\[
p(\theta; a, b) \propto \theta^{a-1}(1 - \theta)^{b-1}.
\]
The expectation is $\mathbb{E}[\theta] = a/(a + b)$. $a = b$ symmetric about 0.5.

The distribution gets more peaked when $a$ and $b$ are large.

When $a = b = 1$, it becomes the uniform distribution.

Defined on $[0, 1]$. 

![Graph of Beta Distribution](image)
Posterior for the Coin Flip Example

- Computing the posterior distribution: 
  \[ p(\theta | D) = \frac{p(\theta) p(D | \theta)}{p(D)} \]

  \[ p(\theta | D) \propto p(\theta) p(D | \theta) \]
  \[ \propto [\theta^{a-1}(1 - \theta)^{b-1}] [\theta^{N_H}(1 - \theta)^{N_T}] \]
  \[ = \theta^{a-1+N_H}(1 - \theta)^{b-1+N_T}. \]

  A beta distribution with parameters \( N_H + a \) and \( N_T + b \).

- The posterior expectation of \( \theta \) is:
  \[ E[\theta | D] = \frac{N_H + a}{N_H + N_T + a + b} \]
  \[ \text{For prior uniform } \quad E[\theta] = \frac{a}{a+b} \]

- Think of \( a \) and \( b \) as pseudo-counts.
  beta(a, b) = beta(1, 1) + a - 1 heads + b - 1 tails.

- The prior and likelihood have the same functional form (conjugate priors). prior & posterior in the same dist. family.
Bayesian Inference for the Coin Flip Example

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

Small data setting
\[ N_H = 2, \quad N_T = 0 \]

- \( a = 1 + 2 \) heads
- \( b = 1 \) tails

Large data setting
\[ N_H = 55, \quad N_T = 45 \]

- \( a = 1 + 55 \) heads
- \( b = 1 + 45 \) tails.
Maximum A-Posteriori (MAP) Estimation

Finds the most likely parameters under the posterior (i.e. the mode).

\[ p(\theta|D) \]

Graph showing the Prior, Likelihood, and Posterior distributions with the mode indicated by a star.
Converts the Bayesian parameter estimation problem into a maximization problem

\[
\hat{\theta}_{\text{MAP}} = \arg \max_{\theta} p(\theta | D) = \arg \max_{\theta} \log p(\theta) + \log p(D | \theta)
\]

if uniform prior, MAP = ML.

since \( p(\theta) \) is a constant.

Maximum Likelihood.

\[
\hat{\theta}_{\text{ML}} = \arg \max_{\theta} p(D | \theta)
\]
Maximum A-Posteriori Estimation

Joint probability of parameters and data:
\[
\log p(\theta, D) = \log p(\theta) + \log p(D | \theta) = \text{Const} + (N_H + a - 1) \log \theta + (N_T + b - 1) \log(1 - \theta)
\]

Maximize by finding a critical point
\[
\frac{d}{d\theta} \log p(\theta, D) = \frac{N_H + a - 1}{\theta} - \frac{N_T + b - 1}{1 - \theta} = 0
\]

Solving for \(\theta\),
\[
\hat{\theta}_{\text{MAP}} = \frac{N_H + a - 1}{N_H + N_T + a + b - 2}
\]

- \(a - 1 + N_H\) heads
- \(b - 1 + N_T\) tails.
Estimate Comparison for Coin Flip Example

<table>
<thead>
<tr>
<th>Formula</th>
<th>( N_H = 2, N_T = 0 )</th>
<th>( N_H = 55, N_T = 45 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{\theta}_{\text{ML}} )</td>
<td>( \frac{N_H}{N_H + N_T} )</td>
<td>1 ( \frac{55}{100} = 0.55 )</td>
</tr>
<tr>
<td>( \mathbb{E}[\theta</td>
<td>\mathcal{D}] )</td>
<td>( \frac{N_H + a}{N_H + N_T + a + b} )</td>
</tr>
<tr>
<td>( \hat{\theta}_{\text{MAP}} )</td>
<td>( \frac{N_H + a - 1}{N_H + N_T + a + b - 2} )</td>
<td>( \frac{3}{4} = 0.75 ), ( \frac{56}{102} \approx 0.549 )</td>
</tr>
</tbody>
</table>

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

avoids overfitting.
Bayesian Parameter Estimation

- Maximum Likelihood overfits when there is little data.
- Add a prior (our belief before observing data).

\[
p(\theta | D) \propto p(\theta) p(D | \theta)
\]

posterior \quad prior \quad likelihood.

- Maximum A Posteriori Estimation:

choose model parameters that have the largest posterior probability.

\[
\hat{\theta}_{\text{MAP}} = \arg\max_{\theta} \log p(\theta | D) = \arg\max_{\theta} \log p(\theta) + \log p(D | \theta)
\]

\[
\text{prior} \quad (\text{regularizer}) \quad \text{maximum likelihood}.
\]
Maximum A Posteriori Estimation for Coin Flip.

Prior is the beta distribution.

\[ p(\theta) = \theta^{a-1} (1 - \theta)^{b-1} \]

\[ \log p(\theta) = (a-1) \log \theta + (b-1) \log (1 - \theta) \]

Likelihood:

\[ \log p(D|\theta) = N_H \log \theta + N_T \log (1 - \theta) \]

Posterior:

\[ \log p(\theta|D) \propto \log p(\theta) + \log p(D|\theta) \]

\[ = (N_H + a - 1) \log \theta + (N_T + b - 1) \log (1 - \theta) \]

\[ \hat{\theta}_{\text{MAP}} = \frac{N_H + a - 1}{(N_H + a - 1) + (N_T + b - 1)} \]
1. Probabilistic Modeling of Data
2. Discriminative and Generative Classifiers
3. Naïve Bayes Models
4. Bayesian Parameter Estimation
5. Multivariate Gaussian Distribution
Classification: Diabetes Example

- Observation per patient: White blood cell count & glucose value.

- \( p(\mathbf{x} | t = k) \) for each class is shaped like an ellipse
  \[ \implies \text{we model each class as a multivariate Gaussian} \]
Univariate Gaussian distribution

- Recall the Gaussian, or normal, distribution:

\[ \mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \]

- Parameterized by mean \( \mu \) and variance \( \sigma^2 \).

- The Central Limit Theorem says that sums of lots of independent random variables are approximately Gaussian.

- In machine learning, we use Gaussians a lot because they make the calculations easy.
Multivariate Mean and Covariance

- **Mean**
  \[
  \mu = \mathbb{E}[x] = \begin{pmatrix} 
  \mu_1 \\
  \vdots \\
  \mu_d 
  \end{pmatrix}
  \]

- **Covariance**
  \[
  \Sigma = \text{Cov}(x) = \mathbb{E}[(x - \mu)(x - \mu)^\top] = 
  \begin{pmatrix}
  \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1D} \\
  \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2D} \\
  \vdots & \vdots & \ddots & \vdots \\
  \sigma_{D1} & \sigma_{D2} & \cdots & \sigma_D^2
  \end{pmatrix}
  \]

- The statistics \((\mu, \Sigma)\) uniquely define a **multivariate Gaussian** (or **multivariate Normal**) distribution, denoted \(\mathcal{N}(\mu, \Sigma)\) or \(\mathcal{N}(x; \mu, \Sigma)\)
  - This is not true for distributions in general!