

# Introduction to Machine Learning

## Generative Models

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## Generative Models for Discrete Data

- Bayesian Concept Learning

- Likelihood

- Adding a Prior

- Posterior

- Posterior Predictive Distribution

## Steps for Learning a Generative Model

- Incorporating Prior

- Beta Distribution

- Conjugate Priors

- Estimating Posterior

- Using Predictive Distribution

- Need for Prior

- Need for Bayesian Averaging

## Learning Gaussian Models

- Estimating Parameters

- Estimating Posterior

- ▶ Let us go back to our tumor example
- ▶  $\mathbf{X}$  represents the data with multiple discrete attributes
  - ▶ Is  $\mathbf{X}$  a discrete or continuous random variable?
- ▶  $Y$  represent the class (benign or malignant)

## Most probable class

$$P(Y = c | \mathbf{X} = \mathbf{x}, \theta) \propto P(\mathbf{X} = \mathbf{x} | Y = c, \theta) P(Y = c, \theta)$$

- ▶  $P(\mathbf{X} = \mathbf{x} | Y = c, \theta) = p(\mathbf{x} | y = c, \theta)$
- ▶  $p(\mathbf{x} | y = c, \theta)$  - **class conditional density**
- ▶ How is the data distributed for each class?

# Bayesian Concept Learning

- ▶ Concept assigns binary labels to examples
- ▶ Features are modeled as a random variable  $X$
- ▶ Class is modeled as a random variable  $Y$
- ▶ We want to find out:  $P(Y = c|X = x)$

# Concept Learning in Number Line

- ▶ I give you a set of numbers (training set  $D$ ) belonging to a concept
- ▶ Choose the most likely hypothesis (concept)
- ▶ Assume that numbers are between 1 and 100
- ▶ Hypothesis Space ( $\mathcal{H}$ ):
  - ▶ All powers of 2
  - ▶ All powers of 4
  - ▶ All even numbers
  - ▶ All prime numbers
  - ▶ Numbers close to a fixed number (say 12)
  - ▶ ⋮

## Socrative Game

- ▶ Goto: <http://b.socrative.com>
- ▶ Enter class ID - UBML18

## Hypothesis Space ( $\mathcal{H}$ )

1. Even numbers
2. Odd numbers
3. Squares
4. Powers of 2
5. Powers of 4
6. Powers of 16
7. Multiples of 5
8. Multiples of 10
9. Numbers within  $20 \pm 5$
10. All numbers between 1 and 100

$$\blacktriangleright D = \{ \}$$

## Hypothesis Space ( $\mathcal{H}$ )

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$$\blacktriangleright D = \{16\}$$

## Hypothesis Space ( $\mathcal{H}$ )

1. Even numbers
2. Odd numbers
3. Squares
4. Powers of 2
5. Powers of 4
6. Powers of 16
7. Multiples of 5
8. Multiples of 10
9. Numbers within  $20 \pm 5$
10. All numbers between 1 and 100

$$\blacktriangleright D = \{60\}$$



## Hypothesis Space ( $\mathcal{H}$ )

1. Even numbers
2. Odd numbers
3. Squares
4. Powers of 2
5. Powers of 4
6. Powers of 16
7. Multiples of 5
8. Multiples of 10
9. Numbers within  $20 \pm 5$
10. All numbers between 1 and 100

$$\blacktriangleright D = \{16, 19, 15, 20, 18\}$$

## Hypothesis Space ( $\mathcal{H}$ )

1. Even numbers
2. Odd numbers
3. Squares
4. Powers of 2
5. Powers of 4
6. Powers of 16
7. Multiples of 5
8. Multiples of 10
9. Numbers within  $20 \pm 5$
10. All numbers between 1 and 100

$$\blacktriangleright D = \{16, 4, 64, 32\}$$

# Computing Likelihood

- ▶ Why choose *powers of 2* concept over *even numbers* concept for  $D = \{16, 4, 64, 32\}$ ?
- ▶ Avoid **suspicious coincidences**
- ▶ Choose concept with higher *likelihood*
- ▶ What is the likelihood of above  $D$  to be generated using the *powers of 2* concept?
- ▶ Likelihood for *even numbers* concept?

- ▶ Why choose one hypothesis over other?
- ▶ Avoid **suspicious coincidences**
- ▶ Choose concept with higher *likelihood*

$$p(D|h) = \prod_{x \in D} p(x|h)$$

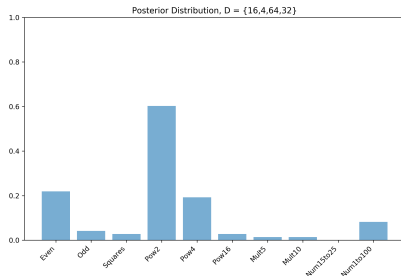
- ▶ *Log Likelihood*

$$\log p(D|h) = \sum_{x \in D} \log p(x|h)$$

# Bayesian Concept Learning

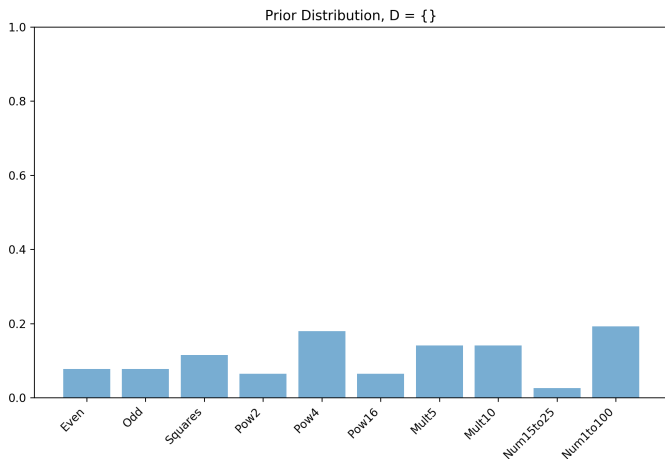
1. Even numbers
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$$D = \{16, 4, 64, 32\}$$



# Adding a Prior

- ▶ Inside information about the hypotheses
- ▶ Some hypotheses are *more likely* a priori
  - ▶ May not be the right hypothesis (**prior can be wrong**)



# Posterior

- ▶ Revised estimates for  $h$  after observing evidence ( $D$ ) and the prior
- ▶  $Posterior \propto Likelihood \times Prior$

$$p(h|D) = \frac{p(D|h)p(h)}{\sum_{h' \in \mathcal{H}} p(D|h')p(h')}$$

	$h$	Prior	Likelihood	Posterior
1	Even	0.3	$0.16 \times 10^{-6}$	$0.621 \times 10^{-3}$
2	Odd	0.075	0	0
3	Squares	0.075	0	0
4	Powers of 2	0.1	$0.77 \times 10^{-3}$	0.997
5	Powers of 4	0.075	0	0
6	Powers of 16	0.075	0	0
7	Multiples of 5	0.075	0	0
8	Multiples of 10	0.075	0	0
9	Numbers within $20 \pm 5$	0.075	0	0
10	All Numbers	0.075	$0.01 \times 10^{-6}$	$0.009 \times 10^{-3}$

# Finding the Best Hypothesis

## Maximum A Priori Estimate

$$\hat{h}_{\text{prior}} = \arg \max_h p(h)$$

## Maximum Likelihood Estimate (MLE)

$$\begin{aligned}\hat{h}_{\text{MLE}} &= \arg \max_h p(D|h) = \arg \max_h \log p(D|h) \\ &= \arg \max_h \sum_{x \in D} \log p(x|H)\end{aligned}$$

## Maximum a Posteriori (MAP) Estimate

$$\hat{h}_{\text{MAP}} = \arg \max_h p(D|h)p(h) = \arg \max_h (\log p(D|h) + \log p(h))$$



# MAP and MLE

- ▶  $\hat{h}_{prior}$  - Most likely hypothesis based on prior
- ▶  $\hat{h}_{MLE}$  - Most likely hypothesis based on evidence
- ▶  $\hat{h}_{MAP}$  - Most likely hypothesis based on posterior

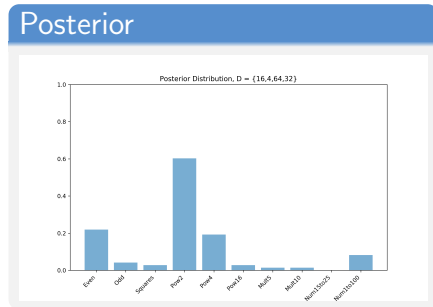
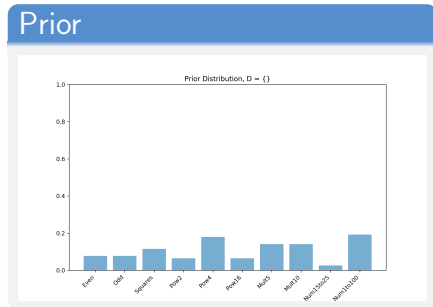
$$\hat{h}_{prior} = \arg \max_h \log p(h)$$

$$\hat{h}_{MLE} = \arg \max_h \log p(D|h)$$

$$\hat{h}_{MAP} = \arg \max_h (\log p(D|h) + \log p(h))$$

- ▶ As data increases, MAP estimate converges towards MLE
  - ▶ Why?
- ▶ MAP/MLE are **consistent estimators**
  - ▶ If concept is in  $\mathcal{H}$ , MAP/ML estimates will converge
- ▶ If  $c \notin \mathcal{H}$ , MAP/ML estimates converge to  $h$  which is closest possible to the truth

# From Prior to Posterior via Likelihood



- ▶ Objective: To *revise* the prior distribution over the hypotheses after observing data (evidence).

# Posterior Predictive Distribution

- ▶ New input,  $x^*$
- ▶ What is the probability that  $x^*$  is also generated by the same concept as  $D$ ?
  - ▶  $P(Y = c|X = x^*, D)$ ?
- ▶ **Option 0:** Treat  $h^{prior}$  as the true concept

$$P(Y = c|X = x^*, D) = P(X = x^*|c = h^{prior})$$

- ▶ **Option 1:** Treat  $h^{MLE}$  as the true concept

$$P(Y = c|X = x^*, D) = P(X = x^*|c = h^{MLE})$$

- ▶ **Option 2:** Treat  $h^{MAP}$  as the true concept

$$P(Y = c|X = x^*, D) = P(X = x^*|c = h^{MAP})$$

- ▶ **Option 3:** *Bayesian Averaging*

$$P(Y = c|X = x^*, D) = \sum_h P(X = x^*|c = h)p(h|D)$$

# Steps for Learning a Generative Model

- ▶ Example:  $D$  is a sequence of  $N$  binary values (0s and 1s) (coin tosses)
- ▶ What is the best distribution that could describe  $D$ ?
- ▶ What is the probability of observing a *head* in future?

## Step 1: Choose the form of the model

- ▶ Hypothesis Space - All possible distributions
  - ▶ Too complicated!!
- ▶ Revised hypothesis space - All Bernoulli distributions ( $X \sim \text{Ber}(\theta), 0 \leq \theta \leq 1$ )
  - ▶  $\theta$  is the hypothesis
  - ▶ Still infinite ( $\theta$  can take infinite possible values)

- ▶ Likelihood of  $D$

$$p(D|\theta) = \theta^{N_1}(1 - \theta)^{N_0}$$

## Maximum Likelihood Estimate

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} p(D|\theta) = \arg \max_{\theta} \theta^{N_1}(1 - \theta)^{N_0} \\ &= \frac{N_1}{N_0 + N_1}\end{aligned}$$

- ▶ Likelihood of  $D$

$$p(D|\theta) = \theta^{N_1}(1 - \theta)^{N_0}$$

## Maximum Likelihood Estimate

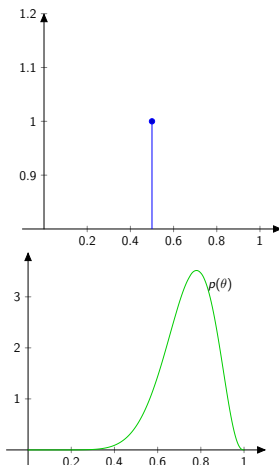
$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} p(D|\theta) = \arg \max_{\theta} \theta^{N_1}(1 - \theta)^{N_0} \\ &= \frac{N_1}{N_0 + N_1}\end{aligned}$$

- ▶ **We can stop here (MLE approach)**
- ▶ Probability of getting a head next:

$$p(x^* = 1|D) = \hat{\theta}_{MLE}$$

# Incorporating Prior

- ▶ Prior *encodes* our prior belief on  $\theta$
- ▶ How to set a Bayesian prior?
  1. A point estimate:  $\theta_{prior} = 0.5$
  2. A probability distribution over  $\theta$  (**a random variable**)
    - ▶ Which one?
    - ▶ For a bernoulli distribution  $0 \leq \theta \leq 1$
    - ▶ *Beta* Distribution





# Beta Distribution as Prior

- ▶ Continuous random variables defined between 0 and 1

$$\text{Beta}(\theta|a, b) \triangleq p(\theta|a, b) = \frac{1}{B(a, b)} \theta^{a-1} (1 - \theta)^{b-1}$$

- ▶  $a$  and  $b$  are the (hyper-)parameters for the distribution
- ▶  $B(a, b)$  is the **beta function**

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a + b)}$$

$$\Gamma(x) = \int_0^{\infty} u^{x-1} e^{-u} du$$

If  $x$  is integer

$$\Gamma(x) = (x - 1)!$$

- ▶ “Control” the shape of the pdf
- ▶ **We can stop here as well (prior approach)**

$$p(x^* = 1) = \theta_{\text{prior}}$$

- ▶ Another reason to choose Beta distribution

$$p(D|\theta) = \theta^{N_1} (1 - \theta)^{N_0}$$

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

- ▶ Posterior  $\propto$  Likelihood  $\times$  Prior

$$p(\theta|D) \propto \theta^{N_1} (1 - \theta)^{N_0} \theta^{a-1} (1 - \theta)^{b-1}$$

$$\propto \theta^{N_1+a-1} (1 - \theta)^{N_0+b-1}$$

- ▶ **Posterior has same form as the prior**
- ▶ Beta distribution is a conjugate prior for Bernoulli/Binomial distribution

- ▶ Posterior

$$\begin{aligned} p(\theta|D) &\propto \theta^{N_1+a-1}(1-\theta)^{N_0+b-1} \\ &= \text{Beta}(\theta|N_1+a, N_0+b) \end{aligned}$$

- ▶ We start with a belief that

$$\mathbb{E}[\theta] = \frac{a}{a+b}$$

- ▶ After observing  $N$  trials in which we observe  $N_1$  heads and  $N_0$  trails, we update our belief as:

$$\mathbb{E}[\theta|D] = \frac{a + N_1}{a + b + N}$$

- ▶ We know that posterior over  $\theta$  is a beta distribution
- ▶ MAP estimate

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} p(\theta | a + N_1, b + N_0) \\ &= \frac{a + N_1 - 1}{a + b + N - 2}\end{aligned}$$

- ▶ What happens if  $a = b = 1$ ?
- ▶ **We can stop here as well (MAP approach)**
- ▶ Probability of getting a head next:

$$p(x^* = 1 | D) = \hat{\theta}_{MAP}$$

# True Bayesian Approach

- ▶ All values of  $\theta$  are possible
- ▶ Prediction on an unknown input ( $x^*$ ) is given by *Bayesian Averaging*

$$\begin{aligned} p(x^* = 1|D) &= \int_0^1 p(x = 1|\theta)p(\theta|D)d\theta \\ &= \int_0^1 \theta \text{Beta}(\theta|a + N_1, b + N_0) \\ &= \mathbb{E}[\theta|D] \\ &= \frac{a + N_1}{a + b + N} \end{aligned}$$

- ▶ This is same as using  $\mathbb{E}[\theta|D]$  as a point estimate for  $\theta$

# The Black Swan Paradox

- ▶ Why use a *prior*?
- ▶ Consider  $D = \text{tails, tails, tails}$
- ▶  $N_1 = 0, N = 3$
- ▶  $\hat{\theta}_{MLE} = 0$
- ▶  $p(x^* = 1|D) = 0!!$ 
  - ▶ Never observe a heads
  - ▶ The *black swan* paradox
- ▶ How does the Bayesian approach help?

$$p(x^* = 1|D) = \frac{a}{a + b + 3}$$



# Why is MAP Estimate Insufficient?

- ▶ MAP is only one part of the posterior
  - ▶  $\theta$  at which the posterior probability is maximum
  - ▶ But is that enough?
  - ▶ What about the posterior variance of  $\theta$ ?

$$\text{var}[\theta|D] = \frac{(a + N_1)(b + N_0)}{(a + b + N)^2(a + b + N + 1)}$$

- ▶ If variance is high then  $\theta_{MAP}$  is not trustworthy
- ▶ Bayesian averaging helps in this case

- ▶ pdf for MVN with  $d$  dimensions:

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \triangleq \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp \left[ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right]$$



## Problem Statement

Given a set of  $N$  **independent and identically distributed** (iid) samples,  $D$ , learn the parameters  $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  of a Gaussian distribution that generated  $D$ .

- ▶ MLE approach - maximize log-likelihood
- ▶ Result

$$\hat{\boldsymbol{\mu}}_{MLE} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i \triangleq \bar{\mathbf{x}}$$

$$\hat{\boldsymbol{\Sigma}}_{MLE} = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

# Estimating Posterior

- ▶ We need posterior for both  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$

$$p(\boldsymbol{\mu})$$

$$p(\boldsymbol{\Sigma})$$

- ▶ What distribution do we need to sample  $\boldsymbol{\mu}$ ?
  - ▶ A Gaussian distribution!

$$p(\boldsymbol{\mu}) = \mathcal{N}(\boldsymbol{\mu} | \mathbf{m}_0, \mathbf{V}_0)$$

- ▶ What distribution do we need to sample  $\boldsymbol{\Sigma}$ ?
  - ▶ An *Inverse-Wishart* distribution.

$$\begin{aligned} p(\boldsymbol{\Sigma}) &= IW(\boldsymbol{\Sigma} | \mathbf{S}, \nu) \\ &= \frac{1}{Z_{IW}} |\boldsymbol{\Sigma}|^{-(\nu+D+1)/2} \exp\left(-\frac{1}{2} \text{tr}(\mathbf{S}^{-1} \boldsymbol{\Sigma}^{-1})\right) \end{aligned}$$

where,

$$Z_{IW} = |\mathbf{S}|^{-\nu/2} 2^{\nu D/2} \Gamma_D(\nu/2)$$

## Posterior for $\mu$ - Also a MVN

$$\begin{aligned}p(\mu|D, \Sigma) &= \mathcal{N}(\mathbf{m}_N, \mathbf{V}_N) \\ \mathbf{V}_N^{-1} &= \mathbf{V}_0^{-1} + N\Sigma^{-1} \\ \mathbf{m}_N &= \mathbf{V}_N(\Sigma^{-1}(N\bar{\mathbf{x}}) + \mathbf{V}_0^{-1}\mathbf{m}_0)\end{aligned}$$

## Posterior for $\Sigma$ - Also an Inverse Wishart

$$\begin{aligned}p(\Sigma|D, \mu) &= IW(\mathbf{S}_N, \nu_N) \\ \nu_N &= \nu_0 + N \\ \mathbf{S}_N^{-1} &= \mathbf{S}_0 + \mathbf{S}_\mu\end{aligned}$$

# References