10-701: Introduction to Machine Learning Lecture 7 - Naïve Bayes

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9/20/23

Front Matter

- Announcements:
  - HW1 released 9/6, due 9/20 (today!) at 11:59 PM
  - HW2 released 9/20 (today!), due 10/4 at 11:59 PM
- Recommended Readings:
  - Murphy, Section 3.5

Bayesian Linear Regression

- If we assume a linear model with additive Gaussian noise

$$y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \dots$$

and a **general** (zero-mean) Gaussian prior on the weights …

$$\boldsymbol{\omega} \sim N(\mathbf{0}, \Sigma)$$

then the distribution over $\boldsymbol{y}$ is

$$\boldsymbol{y} \sim N(X\mathbf{0} + \mathbf{0} = \mathbf{0}, X\Sigma X^T + \sigma^2 I)$$

Bayesian Linear Regression

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$$y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \ldots$$

and a **general** (zero-mean) Gaussian prior on the weights …

$$\boldsymbol{\omega} \sim N(\mathbf{0}, \Sigma)$$

then the *joint* distribution over $\boldsymbol{y}$ and $\boldsymbol{\omega}$ is

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{\omega} \end{bmatrix} \sim N\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} X\Sigma X^T + \sigma^2 I & \Sigma X^T \\ X\Sigma & \Sigma \end{bmatrix} \right)$$

Bayesian Linear Regression

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and a **general** (zero-mean) Gaussian prior on the weights …

$$\boldsymbol{\omega} \sim N(\mathbf{0}, \Sigma)$$

then the *conditional* distribution of $\boldsymbol{\omega}$ given $\boldsymbol{y}$ is

$$\boldsymbol{\omega} \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{POST}, \Sigma_{POST})$$

where

$$\boldsymbol{\mu}_{POST} = \Sigma X^T (X \Sigma X^T + \sigma^2 I)^{-1} \boldsymbol{y},$$
$$\Sigma_{POST} = \Sigma - \Sigma X^T (X \Sigma X^T + \sigma^2 I)^{-1} X \Sigma$$

Bayesian Linear Regression

- If we assume a linear model with additive Gaussian noise

$$y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \ldots$$

and a **general** (zero-mean) Gaussian prior on the weights …

$$\boldsymbol{\omega} \sim N(\mathbf{0}, \Sigma)$$

then the *conditional* distribution of $h(\boldsymbol{x}') = \boldsymbol{x}'^T \boldsymbol{\omega}$ given $\boldsymbol{y}$ is

$$h(\boldsymbol{x}') \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

$$\boldsymbol{\mu}_{PRED} = \boldsymbol{x}'^T \Sigma X^T (X \Sigma X^T + \sigma^2 I)^{-1} \boldsymbol{y},$$

$$\Sigma_{PRED} = \boldsymbol{x}'^T \Sigma \boldsymbol{x}' - \boldsymbol{x}'^T \Sigma X^T (X \Sigma X^T + \sigma^2 I)^{-1} X \Sigma \boldsymbol{x}'$$

Kernelized Bayesian Linear Regression = Gaussian Process (GP)

- If we assume a linear model with additive Gaussian noise

$$y = \boldsymbol{\omega}^T \boldsymbol{x} + \epsilon \text{ where } \epsilon \sim N(0, \sigma^2) \rightarrow y \sim N(\boldsymbol{\omega}^T \boldsymbol{x}, \sigma^2) \ldots$$

and a **general** (zero-mean) Gaussian prior on the weights …

$$\boldsymbol{\omega} \sim N(\boldsymbol{0}, \Sigma)$$

then the *conditional* distribution of $h(\boldsymbol{x}') = \boldsymbol{x}'^T \boldsymbol{\omega}$ given $\boldsymbol{y}$ is

$$h(\boldsymbol{x}') \mid \boldsymbol{y} \sim N(\boldsymbol{\mu}_{PRED}, \Sigma_{PRED})$$

where

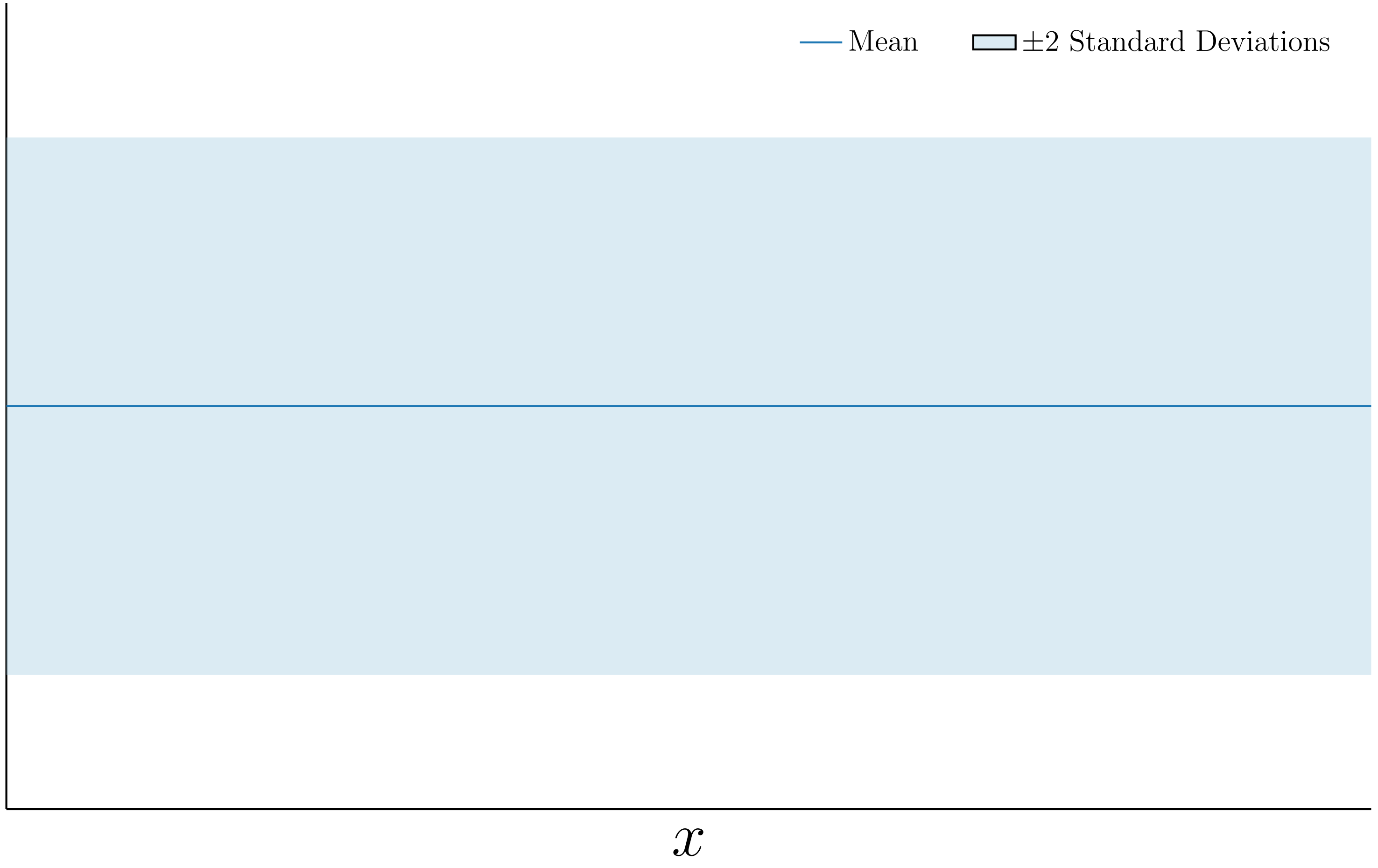
$$K(\boldsymbol{a}, \boldsymbol{b}) = \Phi(\boldsymbol{a})^T \Sigma \Phi(\boldsymbol{b})$$

$$\boldsymbol{\mu}_{PRED} = K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I)^{-1} \boldsymbol{y},$$

$$\Sigma_{PRED} = K(\boldsymbol{x}', \boldsymbol{x}') - K(\boldsymbol{x}', X)(K(X, X) + \sigma^2 I)^{-1} K(X, \boldsymbol{x}')$$

Gaussian Process (GP)

$$f \sim \mathcal{GP}(m(x) = 0, K(x, x') = \exp(-(x - x')^2))$$



$$f \sim \mathcal{GP}(m, K) \rightarrow f(x) \sim \mathcal{N}\big(m(x), K(x, x)\big)$$

Gaussian Process (GP)

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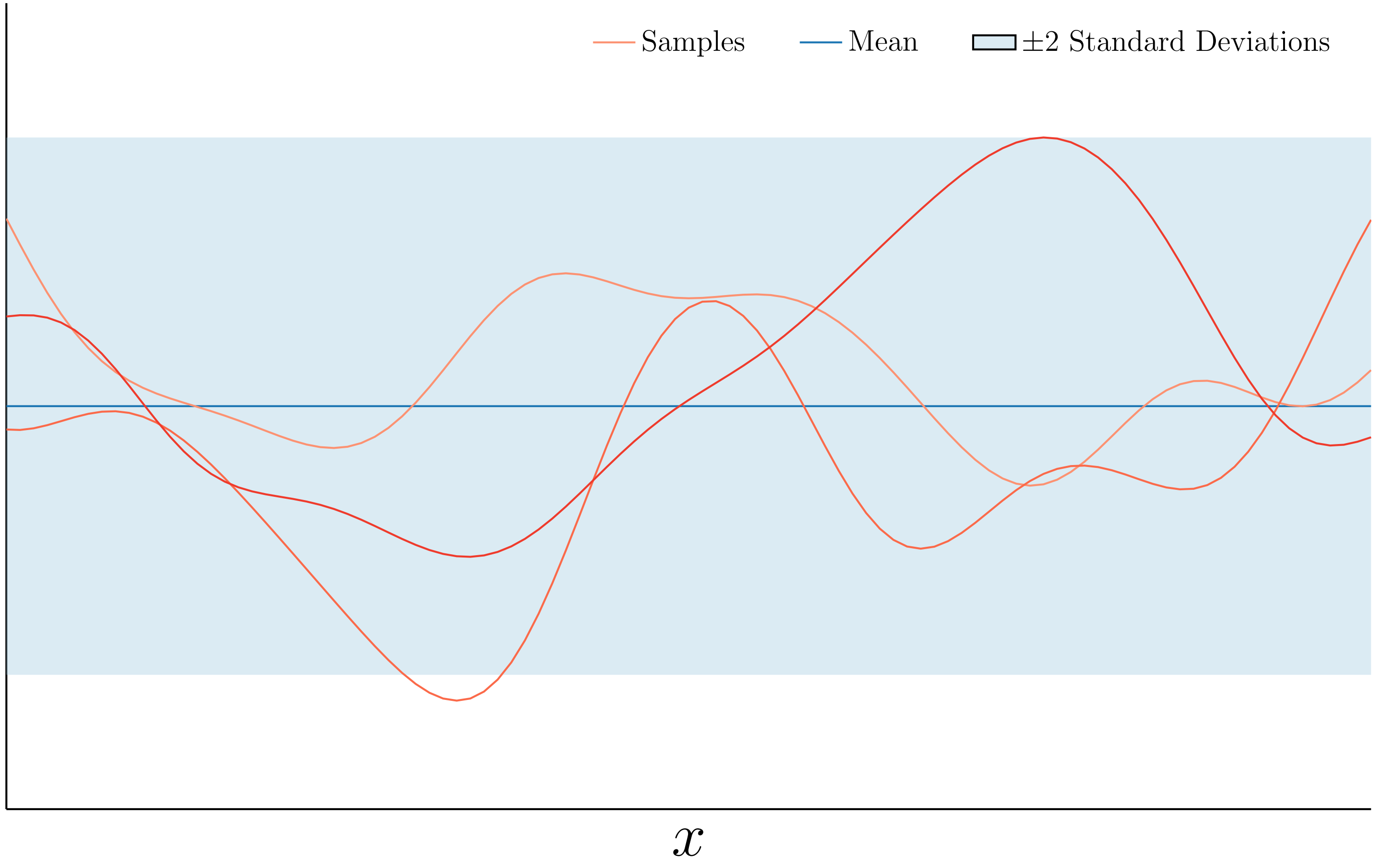

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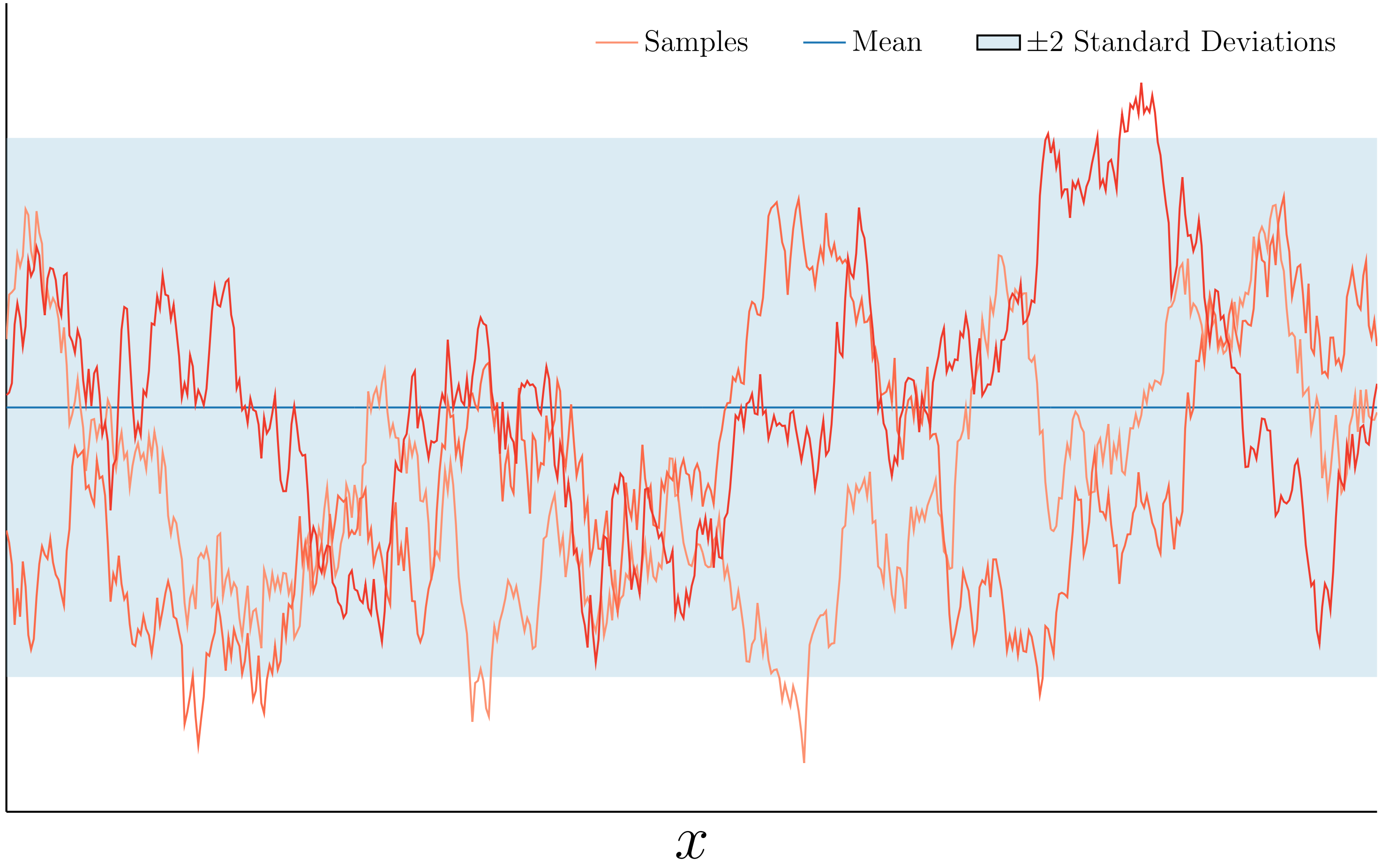
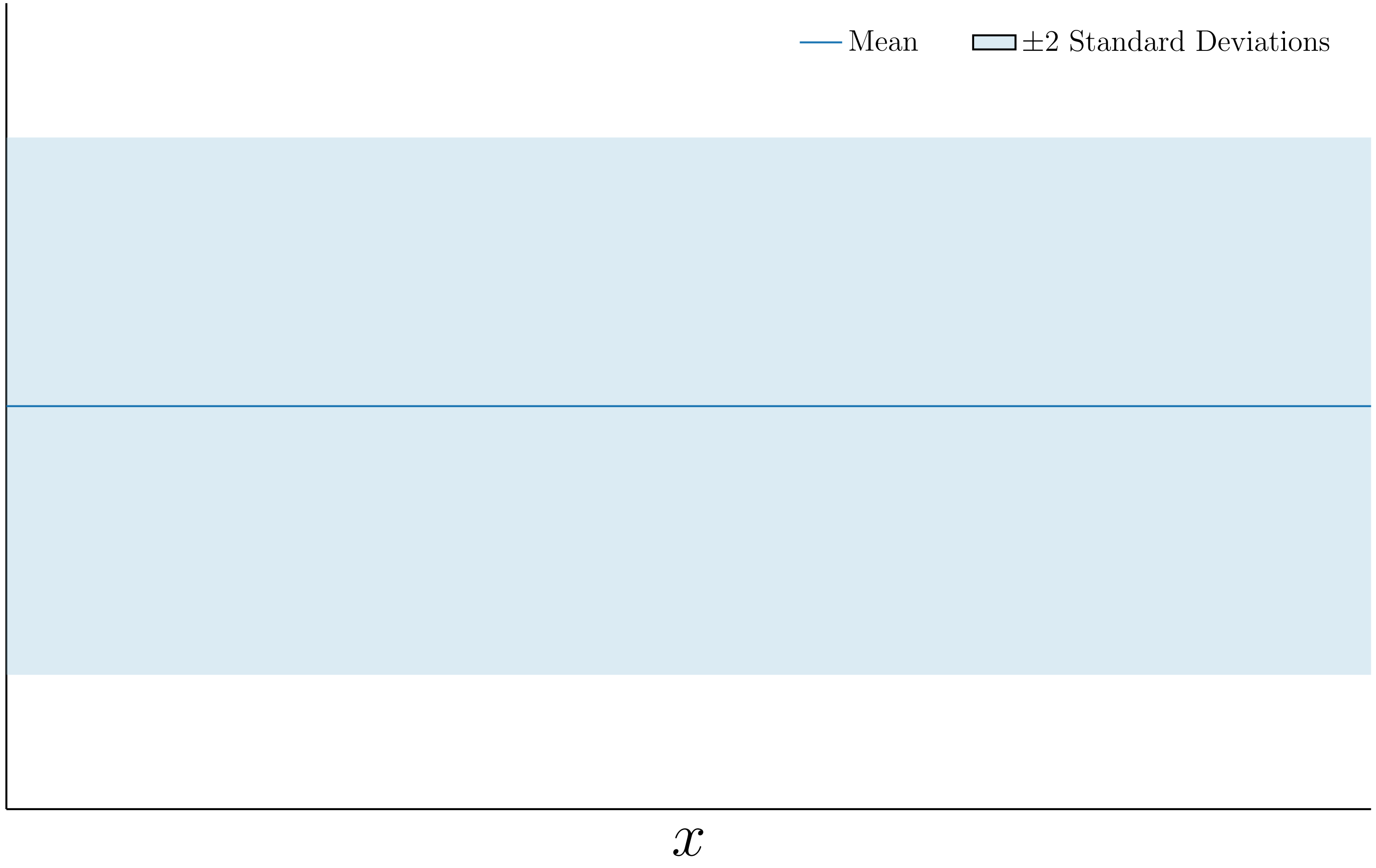


$$f \sim \mathcal{GP}(m, K) \rightarrow f(x) \sim \mathcal{N}\big(m(x), K(x, x)\big)$$

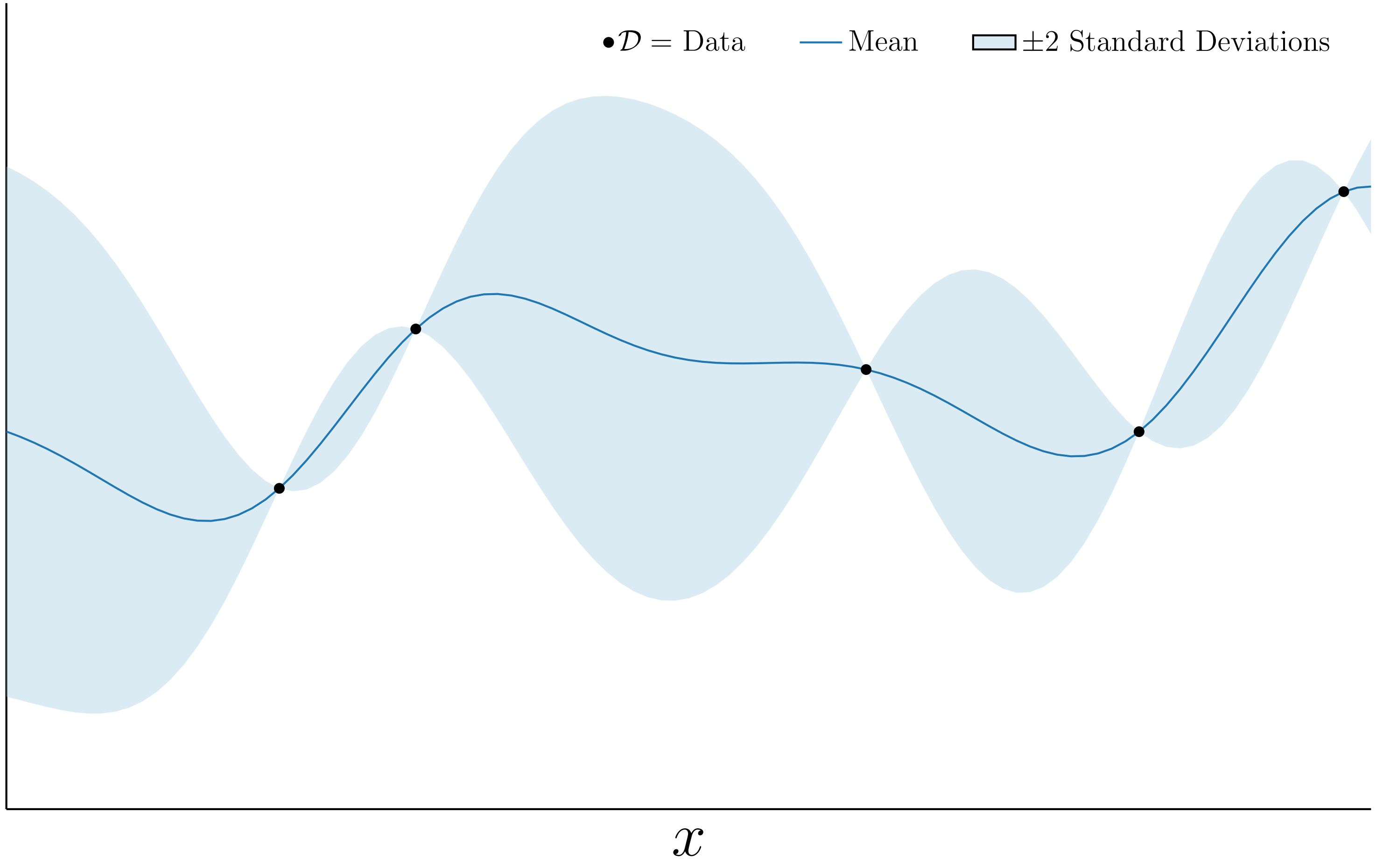
GP Prior

$$f \sim \mathcal{GP}(m(x) = 0, K(x, x') = \exp(-(x - x')^2))$$



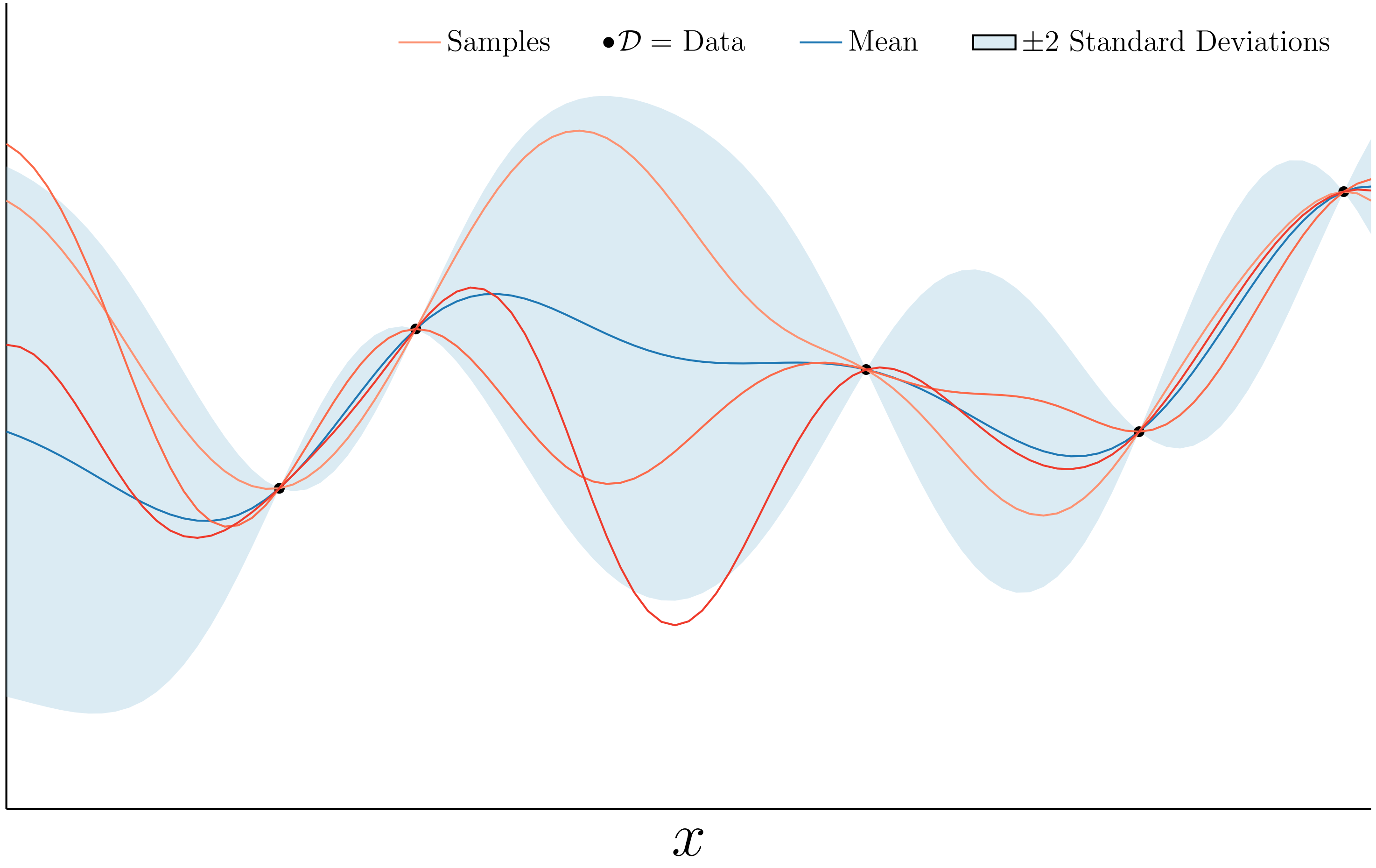
GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(m_{\mathcal{D}}, K_{\mathcal{D}})$$



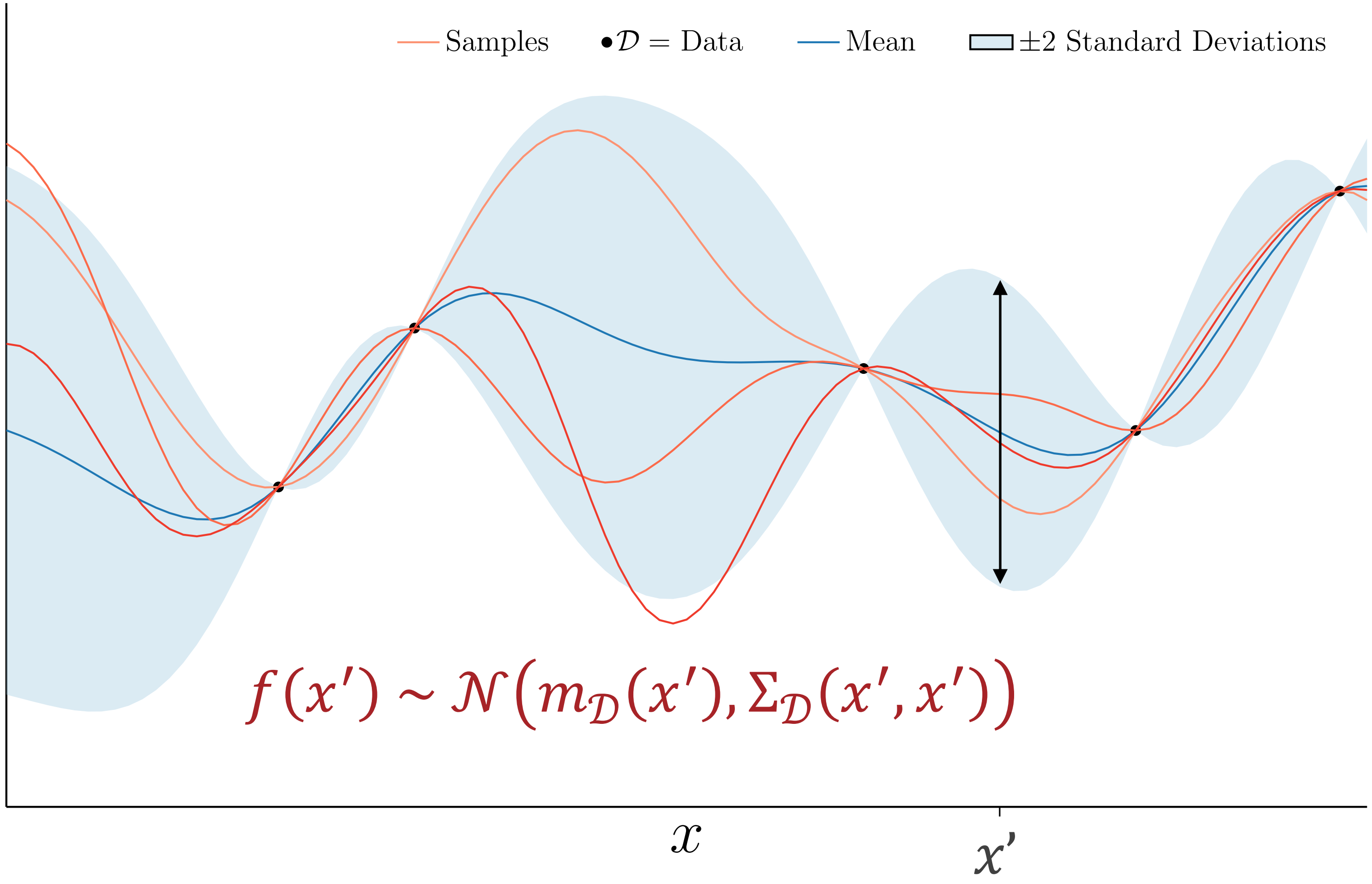
GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(m_{\mathcal{D}}, K_{\mathcal{D}})$$



GP Posterior

$$f \mid \mathcal{D} \sim \mathcal{GP}(m_{\mathcal{D}}, K_{\mathcal{D}})$$



$$f(x') \sim \mathcal{N}\left(m_{\mathcal{D}}(x'), \Sigma_{\mathcal{D}}(x', x')\right)$$

Text Data

- https://www.nytimes.com/2023/09/19/us/politics/senate-dress-code-fetterman-schumer.html
- https://americanwirenews.com/slobs-of-the-world-unite-schumer-changes-senate-dress-code-to-accommodate-fetterman/
- https://triblive.com/news/pennsylvania/u-s-senate-loosens-dress-code-scoring-win-for-casually-dressed-fetterman/
- https://www.theonion.com/fetterman-struggling-to-adapt-to-size-of-capitol-buildi-1849773669

Text Data


The TOOTH Book
POCKET ROCKS
HOP ON POP
By Dr. Seuss
The SIMPLEST SEUSS for YOUNGEST USE
THE CAT IN THE HAT
By Dr. Seuss
Go, Dog. Go!
by P.D.Eastman
Lois Ehlert
BLUE FISH
My Mother?
by P.D. Eastman
Chicka Chicka Boom Boom
by Bill Martin Jr and John Archambault
illustrated by Lois Ehlert
幼儿启蒙大全
YOU ER QI MENG DA QUAN
Big Dog... Little Dog
by P.D. Eastman
FRIENDS COLLECTION
Pooh & Eeyore

Bag-of-Words Model

x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	y (Dr. Seuss)

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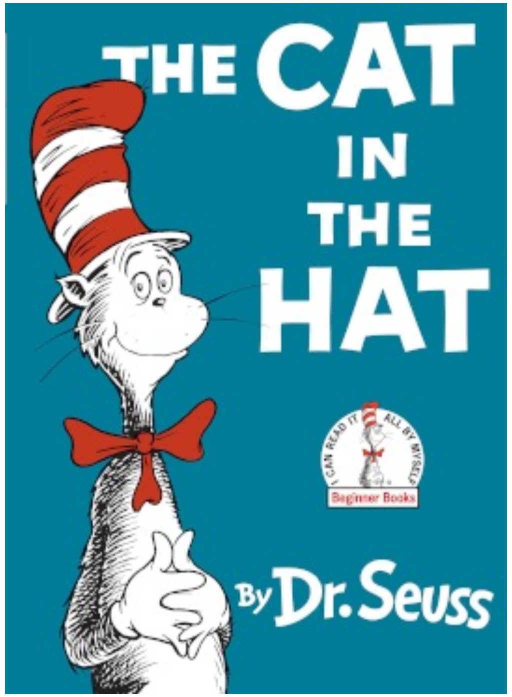
x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	y (Dr. Seuss)
1	1	0	0	0	0	1

The Cat in the Hat
(by Dr. Seuss)



Source: https://en.wikipedia.org/wiki/The_Cat_in_the_Hat#/media/File:The_Cat_in_the_Hat.png

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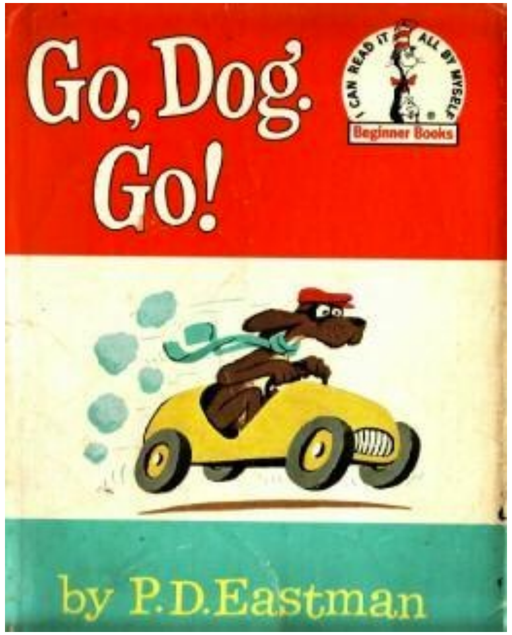
1	1	0	0	0	0	1
0	0	1	0	0	0	0

Go, Dog. Go!
(by P. D. Eastman)



Source: https://en.wikipedia.org/wiki/Go,_Dog._Go!#/media/File:Go_Dog_Go.jpg

Bag-of-Words Model

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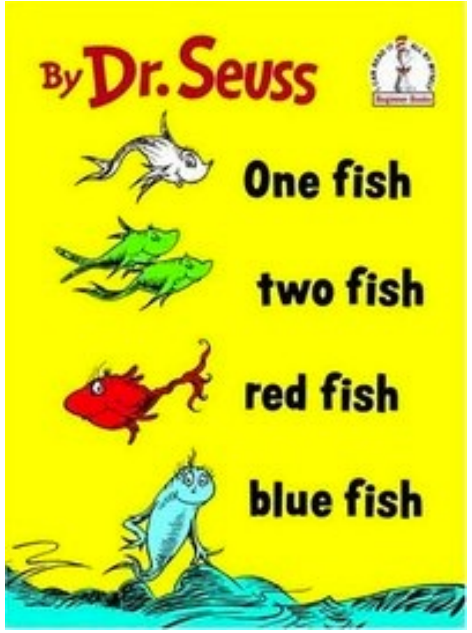
1	1	0	0	0	0	1
0	0	1	0	0	0	0
0	0	0	1	0	0	1

One Fish, Two Fish,
Red Fish, Blue Fish
(by Dr. Seuss)

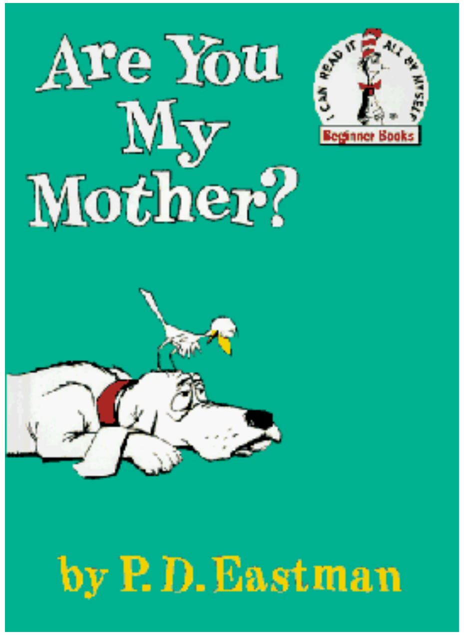


Source: https://en.wikipedia.org/wiki/One_Fish,_Two_Fish,_Red_Fish,_Blue_Fish#/media/File:One_Fish_Two_Fish_Red_Fish_Blue_Fish_(cover_art).jpg

Bag-of-Words Model

x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	y (Dr. Seuss)
1	1	0	0	0	0	1
0	0	1	0	0	0	0
0	0	0	1	0	0	1
0	0	0	0	1	0	0

Are You My Mother?
(by P. D. Eastman)



Source: https://en.wikipedia.org/wiki/Are_You_My_Mother%3F#/media/File:Areyoumymother.gif

Building a Probabilistic Classifier

- Define a decision rule
  - Given a test data point $\boldsymbol{x}'$, predict its label $\hat{y}$ using the posterior distribution $P(Y = y|X = \boldsymbol{x}')$
  - Common choice: $\hat{y} = \underset{y}{\operatorname{argmax}}\, P(Y = y|X = \boldsymbol{x}')$
- Model the posterior distribution
  - Option 1 - Model $P(Y|X)$ directly as some function of X (later)
  - Option 2 - Use Bayes' rule (today!):

$$P(Y|X) = \frac{P(X|Y)\,P(Y)}{P(X)} \propto P(X|Y)\,P(Y)$$

How hard is modelling $P(X|Y)$?

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How hard is modelling $P(X|Y)$?

x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	$P(X\|Y=1)$	$P(X\|Y=0)$
0	0	0	0	0	0	θ_1	θ_{64}
1	0	0	0	0	0	θ_2	θ_{65}
1	1	0	0	0	0	θ_3	θ_{66}
1	0	1	0	0	0	θ_4	θ_{67}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
1	1	1	1	1	1	$1-\sum_{i=1}^{63}\theta_i$	$1-\sum_{i=64}^{126}\theta_i$

Naïve Bayes Assumption

- ***Assume*** features are conditionally independent given the label:

$$P(X|Y) = \prod_{d=1}^{D} P(X_d|Y)$$

- Pros:
  - Significantly reduces computational complexity
  - Also reduces model complexity, combats overfitting
- Cons:
  - Is a strong, often illogical assumption
    - We'll see a relaxed version of this next week when we discuss Bayesian networks

General Recipe for Machine Learning

- Define a model and model parameters

- Write down an objective function

- Optimize the objective w.r.t. the model parameters

Recipe for Naïve Bayes

- Define a model and model parameters
  - Make the Naïve Bayes assumption
  - Assume independent, identically distributed (iid) data
  - Parameters: $\pi = P(Y = 1)$, $\theta_{d,y} = P(X_d = 1 | Y = y)$
- Write down an objective function
  - Maximize the log-likelihood
- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take partial derivatives, set to 0 and solve

Setting the Parameters via MLE

$$\ell_{\mathcal{D}}(\pi, \boldsymbol{\theta}) = \log P\left(\mathcal{D} = \left\{\boldsymbol{x}^{(1)}, y^{(1)}, \dots, \boldsymbol{x}^{(N)}, y^{(N)}\right\} \middle| \pi, \boldsymbol{\theta}\right)$$

$$= \log \prod_{n=1}^{N} P\left(\boldsymbol{x}^{(n)}, y^{(n)} \middle| \pi, \boldsymbol{\theta}\right) = \log \prod_{n=1}^{N} P\left(\boldsymbol{x}^{(n)} \middle| y^{(n)}, \boldsymbol{\theta}\right) P\left(y^{(n)} \middle| \pi\right)$$

$$= \log \prod_{n=1}^{N} \left(\prod_{d=1}^{D} P\left(x_d^{(n)} \middle| y^{(n)}, \theta_{d,1}, \theta_{d,0}\right) \right) P\left(y^{(n)} \middle| \pi\right)$$

$$= \sum_{n=1}^{N} \left(\sum_{d=1}^{D} \log P\left(x_d^{(n)} \middle| y^{(n)}, \theta_{d,1}, \theta_{d,0}\right) \right) + \log P\left(y^{(n)} \middle| \pi\right)$$

$$= \sum_{n:y^{(n)}=1} \left(\sum_{d=1}^{D} \log P\left(x_d^{(n)} \middle| \theta_{d,1}\right) \right)$$

$$+ \sum_{n:y^{(n)}=0} \left(\sum_{d=1}^{D} \log P\left(x_d^{(n)} \middle| \theta_{d,0}\right) \right) + \sum_{n=1}^{N} \log P\left(y^{(n)} \middle| \pi\right)$$

Setting the Parameters via MLE

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}/_{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Binary features
  - $X_d | Y = y \sim \text{Bernoulli}(\theta_{d,y})$
  - $\hat{\theta}_{d,y} = {}^{N_{Y=y,\, X_d=1}}/_{N_{Y=y}}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=1}$ = # of data points with label y and feature $X_d = 1$

Bernoulli Naïve Bayes

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}/_{N}$
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- Binary features
  - $X_d | Y = y \sim \text{Bernoulli}(\theta_{d,y})$
  - $\hat{\theta}_{d,y} = {}^{N_{Y=y,\, X_d=1}}/_{N_{Y=y}}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=1}$ = # of data points with label y and feature $X_d = 1$

Multiclass Bernoulli Naïve Bayes

- Discrete label (Y can take on one of M possible values)
  - $Y \sim \text{Categorical}(\pi_1, \dots, \pi_M)$
  - $\hat{\pi}_m = {}^{N_{Y=m}}/_{N}$
    - N = # of data points
    - $N_{Y=m}$ = # of data points with label m
- Binary features
  - $X_d | Y = m \sim \text{Bernoulli}\left(\theta_{d,m}\right)$
  - $\hat{\theta}_{d,m} = {}^{N_{Y=m,\, X_d=1}}/_{N_{Y=m}}$
    - $N_{Y=m}$ = # of data points with label m
    - $N_{Y=m,\, X_d=1}$ = # of data points with label m and feature $X_d = 1$

Multinomial Naïve Bayes

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}/_{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Discrete features (X_d can take on one of K possible values)
  - $X_d | Y = y \sim \text{Categorical}\left(\theta_{d,1,y}, \dots, \theta_{d,K,y}\right)$
  - $\hat{\theta}_{d,k,y} = {}^{N_{Y=y,\, X_d=k}}/_{N_{Y=y}}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=k}$ = # of data points with label y and feature $X_d = k$

Gaussian Naïve Bayes

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}\!/_{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Real-valued features
  - $X_d | Y = y \sim \text{Gaussian}\left(\mu_{d,y}, \sigma_{d,y}^2\right)$
  - $\hat{\mu}_{d,y} = \frac{1}{N_{Y=y}} \sum_{n: y^{(n)}=y} x_d^{(n)}$
  - $\hat{\sigma}_{d,y}^2 = \frac{1}{N_{Y=y}} \sum_{n: y^{(n)}=y} \left(x_d^{(n)} - \hat{\mu}_{d,y}\right)^2$
    - $N_{Y=y}$ = # of data points with label y

Recall: Fisher Iris Dataset

- Fisher (1936) used 150 measurements of flowers from 3 different species: Iris setosa (0), Iris virginica (1), Iris versicolor (2) collected by Anderson (1936)

Species	Sepal Length	Sepal Width
0	4.3	3.0
0	4.9	3.6
0	5.3	3.7
1	4.9	2.4
1	5.7	2.8
1	6.3	3.3
1	6.7	3.0

Visualizing Gaussian Naïve Bayes (2 classes)

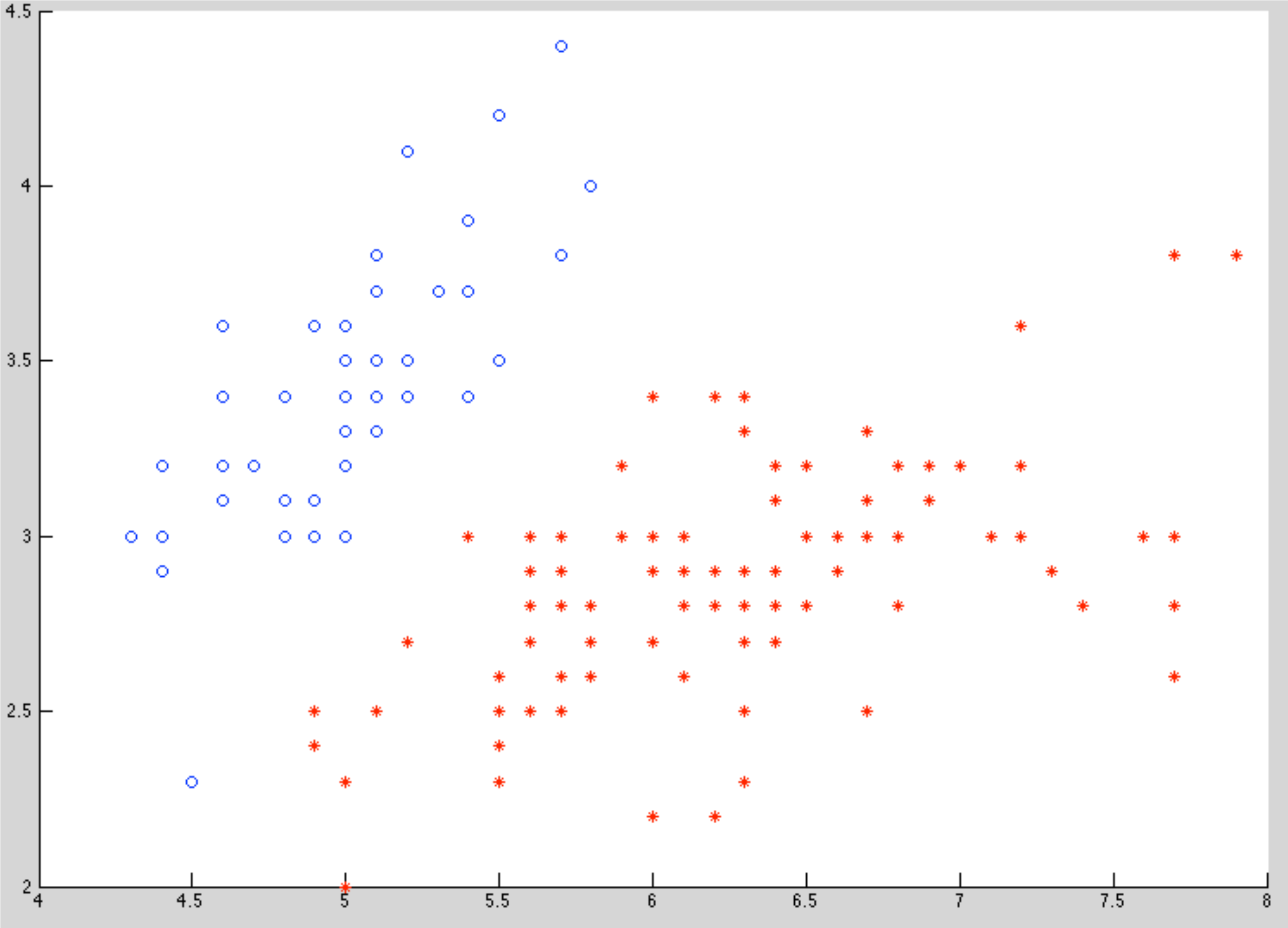

Figure courtesy of William Cohen

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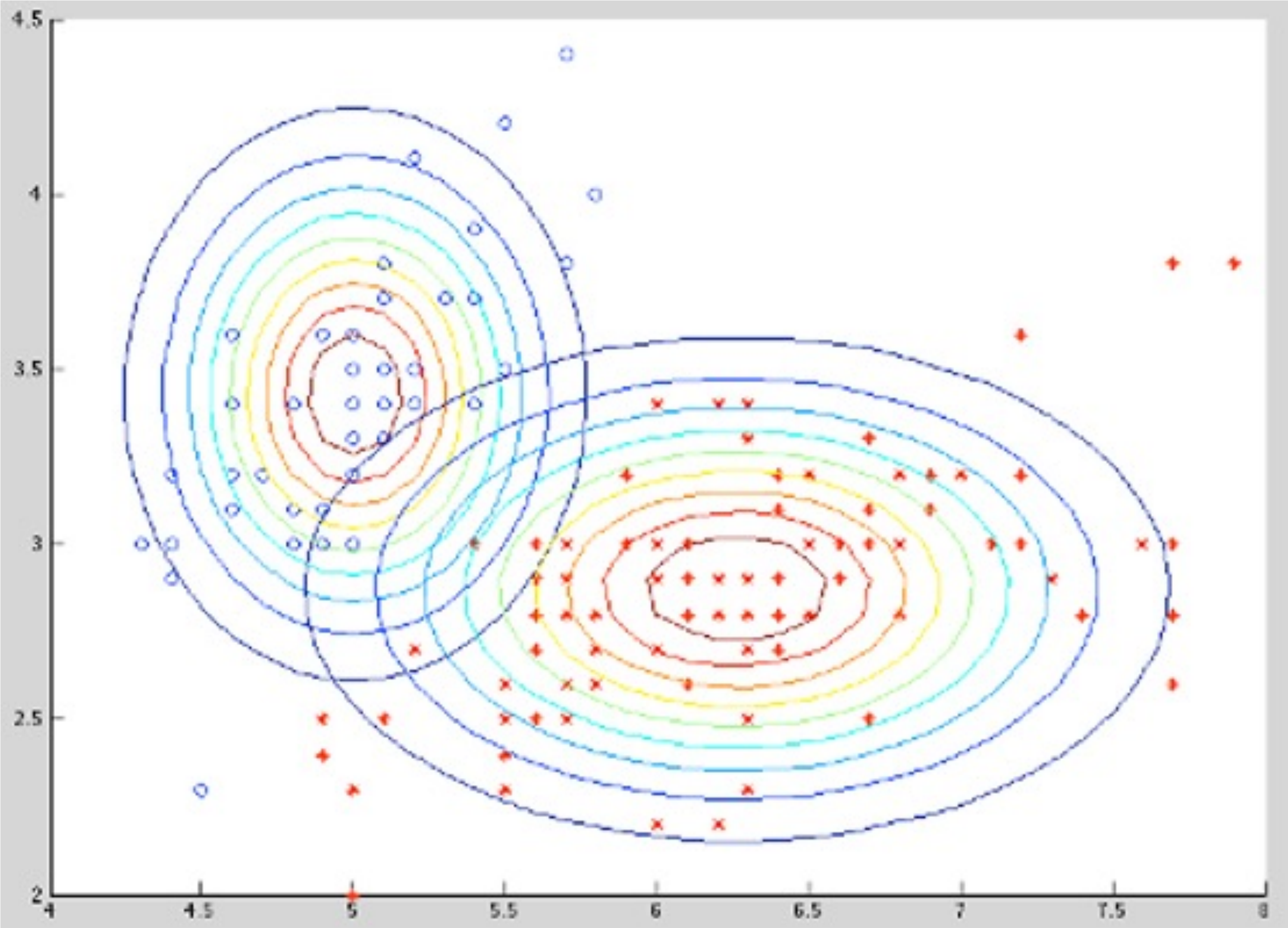

Figure courtesy of William Cohen

Visualizing Gaussian Naïve Bayes (2 classes, equal variances)

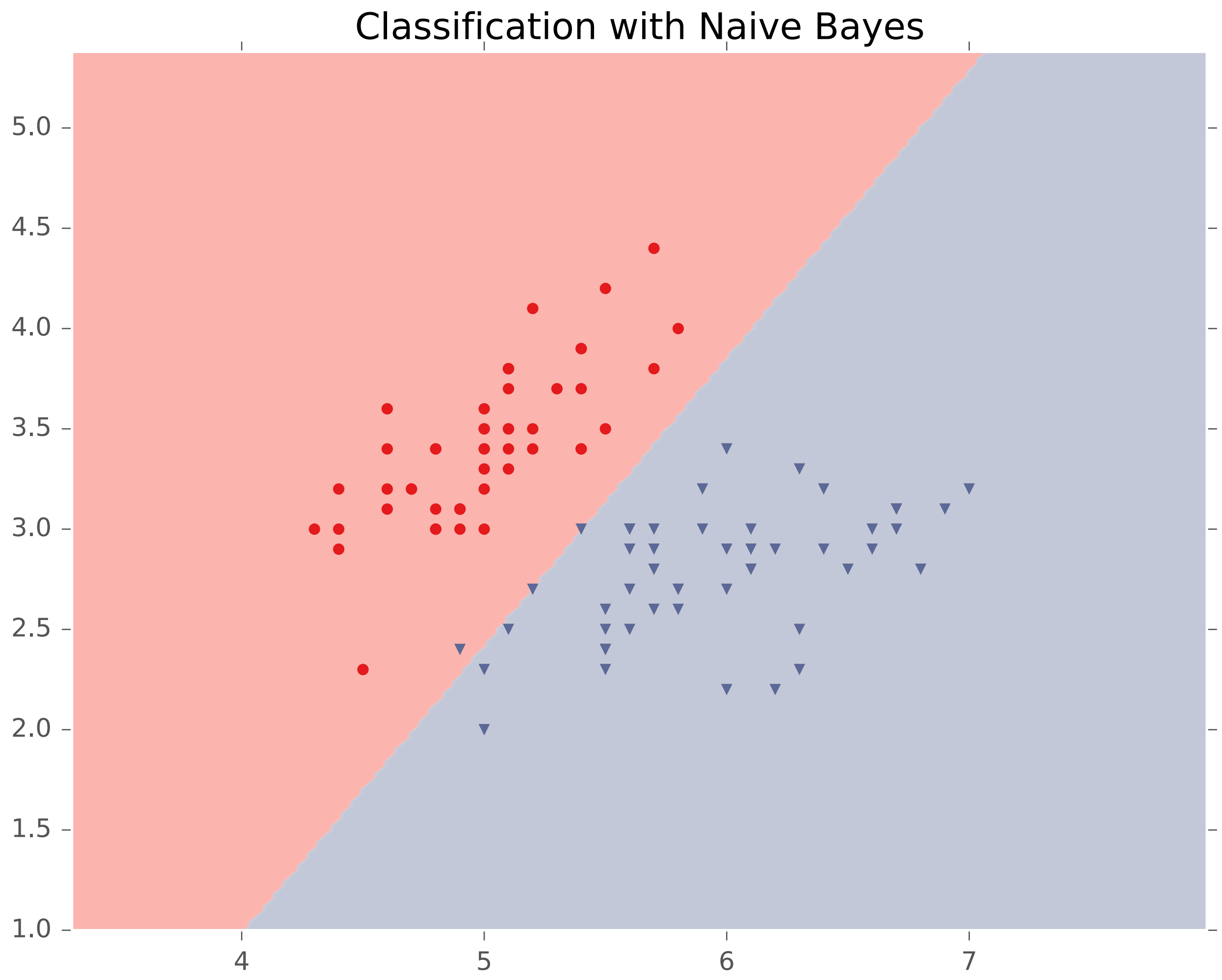

Figure courtesy of Matt Gormley

Visualizing Gaussian Naïve Bayes (2 classes, learned variances)

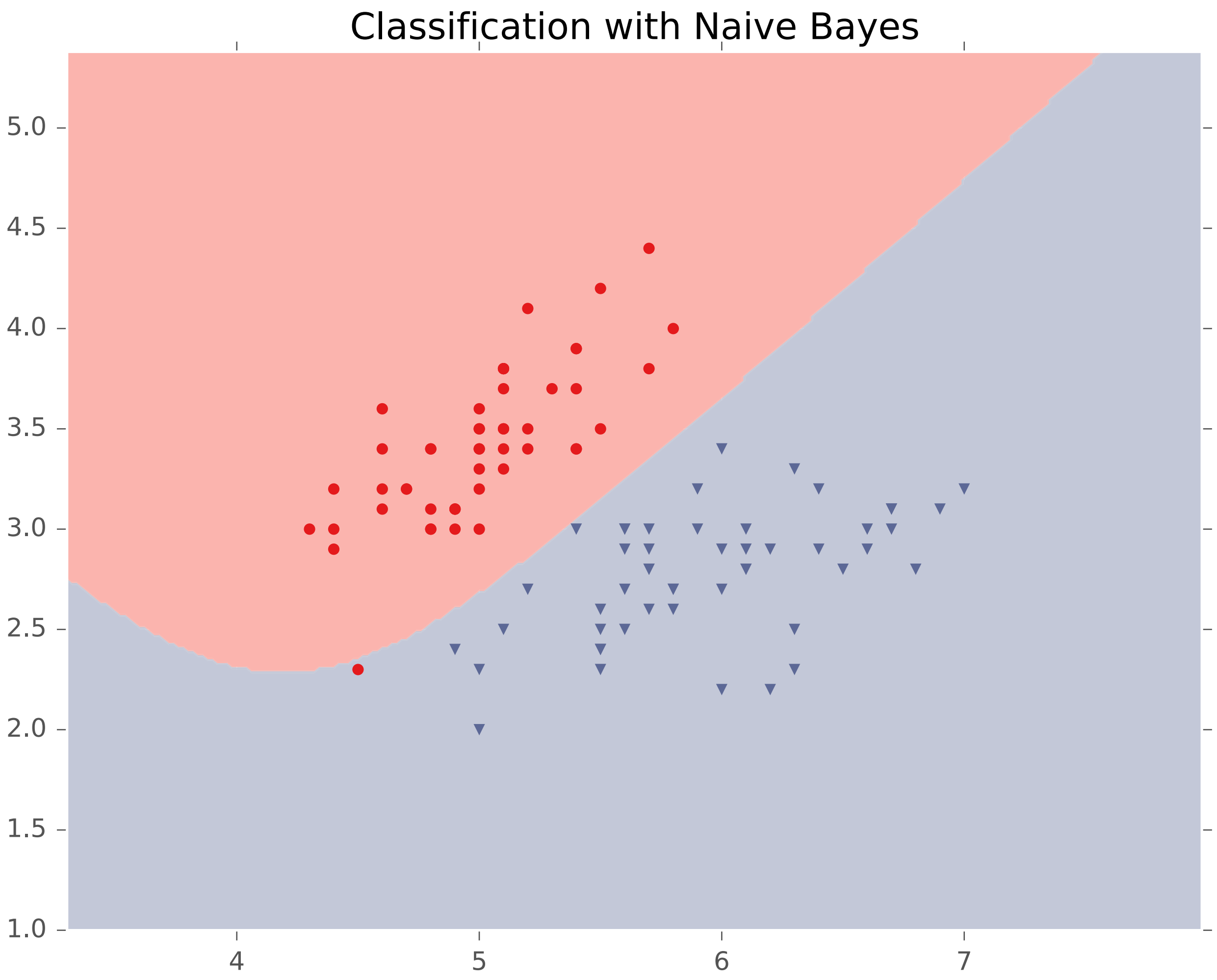

Figure courtesy of Matt Gormley

Bernoulli Naive Bayes: Making Predictions

What if some word-label pair never appears in our training data?

- Given a test data point $\boldsymbol{x}' = [x_1', \ldots, x_D']^T$

$$P(Y = 1|\boldsymbol{x}') \propto P(Y = 1)P(\boldsymbol{x}'|Y = 1)$$

$$= \hat{\pi} \prod_{d=1}^{D} \hat{\theta}_{d,1}^{x_d'} \left(1 - \hat{\theta}_{d,1}\right)^{1-x_d'}$$

$$P(Y = 0|\boldsymbol{x}') \propto (1 - \hat{\pi}) \prod_{d=1}^{D} \hat{\theta}_{d,0}^{x_d'} \left(1 - \hat{\theta}_{d,0}\right)^{1-x_d'}$$

$$\hat{y} = \begin{cases} 1 \text{ if } \hat{\pi} \prod_{d=1}^{D} \hat{\theta}_{d,1}^{x_d'} \left(1 - \hat{\theta}_{d,1}\right)^{1-x_d'} > \\ (1 - \hat{\pi}) \prod_{d=1}^{D} \hat{\theta}_{d,0}^{x_d'} \left(1 - \hat{\theta}_{d,0}\right)^{1-x_d'} \\ 0 \text{ otherwise} \end{cases}$$

What if some Word-Label pair never appears in our training data?

x_1 ("hat")	x_2 ("cat")	x_3 ("dog")	x_4 ("fish")	x_5 ("mom")	x_6 ("dad")	y (Dr. Seuss)
1	1	0	0	0	0	1
0	0	1	0	0	0	0
0	0	0	1	0	0	1
0	0	0	0	1	0	0

The Cat in the Hat gets a Dog (by ???)

- If some $\hat{\theta}_{d,y} = 0$ and that word appears in our test data $\boldsymbol{x}'$, then $P(Y = y|\boldsymbol{x}') = 0$ even if all the other features in $\boldsymbol{x}'$ point to the label being y!
- The model has been overfit to the training data…
- We can address this with a prior over the parameters!

Setting the Parameters via MAP

- Binary label
  - $Y \sim \text{Bernoulli}(\pi)$
  - $\hat{\pi} = {}^{N_{Y=1}}\!/_{N}$
    - N = # of data points
    - $N_{Y=1}$ = # of data points with label 1
- Binary features
  - $X_d|Y = y \sim \text{Bernoulli}(\theta_{d,y})$ and $\theta_{d,y} \sim \text{Beta}(\alpha, \beta)$
  - $\hat{\theta}_{d,y} = {}^{N_{Y=y,\, X_d=1}+(\alpha-1)}\!/_{N_{Y=y}+(\alpha-1)+(\beta-1)}$
    - $N_{Y=y}$ = # of data points with label y
    - $N_{Y=y,\, X_d=1}$ = # of data points with label y and feature $X_d = 1$
    - α and β are "pseudocounts" of imagined data points that help avoid zero-probability predictions.
    - Common choice: $\alpha = \beta = 2$

What can we do when this is a bad/incorrect assumption, e.g., when our features are words in a sentence?

- ***Assume*** features are conditionally independent given the label:

$$P(X|Y) = \prod_{d=1}^{D} P(X_d|Y)$$

- Pros:
  - Significantly reduces computational complexity
  - Also reduces model complexity, combats overfitting
- Cons:
  - Is a strong, often illogical assumption
    - We'll see a relaxed version of this next week when we discuss Bayesian networks

Key Takeaways

- Text data
  - Bag-of-words feature representation
- Naïve Bayes
  - Conditional independence assumption
    - Pros and cons
  - Different Naïve Bayes models based on type of features
  - MLE vs. MAP for Bernoulli Naïve Bayes