COMS 4771
Introduction to Machine Learning

Nakul Verma

Machine learning: what?

Study of making machines **learn** a concept ***without*** having to explicitly program it.

- Constructing algorithms that can:
  - learn from input data, and be able to make predictions.
  - find interesting patterns in data.

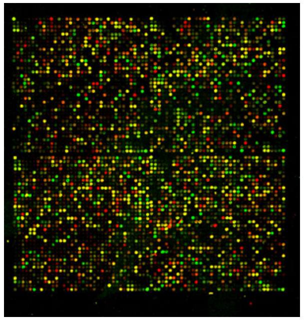
- Analyzing these algorithms to understand the limits of ‘learning’

Machine learning: why?

We are smart programmers, why can’t we just write some code with a set of rules to solve a particular problem?

Write down a set of rules to code to distinguish these two faces:

What if we don’t even know the explicit task we want to solve?



Machine learning: problems in the real world

- Recommendation systems (Netflix, Amazon, Overstock)
- Stock prediction (Goldman Sachs, Morgan Stanley)
- Risk analysis (Credit card, Insurance)
- Face and object recognition (Cameras, Facebook, Microsoft)
- Speech recognition (Siri, Cortana, Alexa, Dragon)
- Search engines and content filtering (Google, Yahoo, Bing)

Machine learning: how?

so…. how do we do it?

This is what we will focus on in this class!

This course

We will learn:

- Study a prediction problem in an **abstract manner** and come up with a solution which is **applicable to many problems** simultaneously.

- Different types of paradigms and algorithms that have been successful in prediction tasks.

- How to systematically **analyze** how good an algorithm is for a prediction task.

Prerequisites

Mathematical prerequisites

- Basics of probability and statistics
- Linear algebra
- Calculus

Computational prerequisites

- Basics of algorithms and datastructure design
- Ability to program in a high-level language.

Administrivia

Website:

`http://www.cs.columbia.edu/~verma/classes/sp18/coms4771/`

The team:

Instructor: Nakul Verma (me)

TAs

Students: you!

Evaluation:

- Homeworks (40%)
- Exam 1 (30%)
- Exam 2 (30%)

Policies

Homeworks:

- No late homework
- **Must** type your homework (no handwritten homework)
- Please include your name and UNI
- Submit a pdf copy of the assignment via gradescope (**98644J**)
- Except for HW0, students are encouraged to do it in groups (at max 3 people)

- We encourage discussing the problems (piazza), but **please don't copy**.

Announcement!

- Visit the course website
- Review the basics (prerequisites)
- HW0 is out!
- Sign up on Piazza & Gradescope
- Students have access to recitation section on Fri 1:10-2:25p Math 207.

Let’s get started!

Machine Learning: the basics…

A closer look at some prediction problems…

- Handwritten character recognition:

{ 0, 1, 2, …, 9 }

- Spam filtering:

murdered during the recent civil war in Libya in March 2011, before his death my late father was a strong supporter and a member of late Moammar Gadhafi Government in Tripoli. Meanwhile before the incident, my late Father came to Cotonou Benin republic with the sum of USD4, 200,000.00 (US$4.2M) which he deposited in a Bank here in Cotonou Benin Republic West Africa for safe keeping.

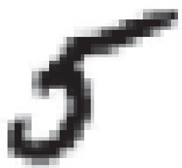
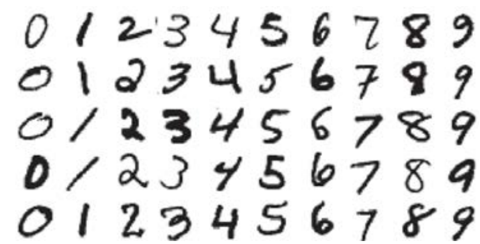
{ spam, not spam }

- Object recognition:

{ building, tree, car, road, sky,... }

Machine Learning: the basics…

Commonalities in a prediction problem:

Input:  $= \vec{x} = \begin{pmatrix} x^{(1)} \\ \vdots \\ x^{(d)} \end{pmatrix} \in \mathcal{X}$ 

To learn: f

Output: **5** $= y \in \mathcal{Y}$ **{ 0, 1, 2, …, 9 }**

Machine Learning: the basics...

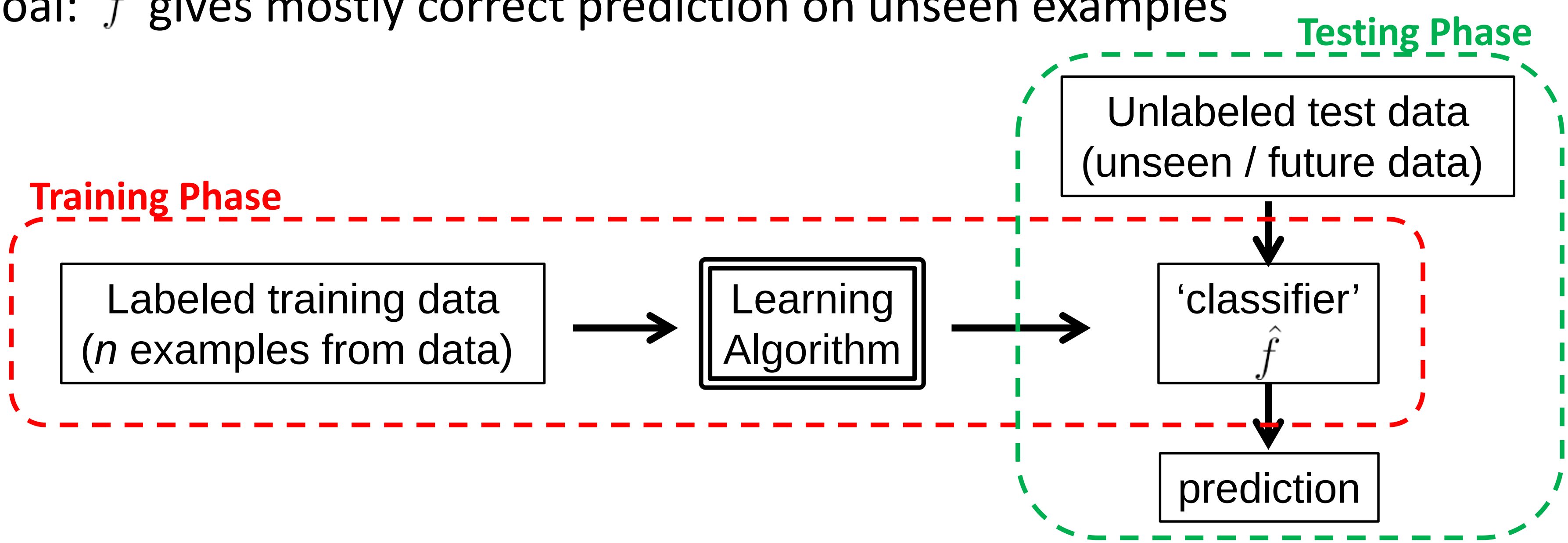
Supervised learning

Data: $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots \in \mathcal{X} \times \mathcal{Y}$

Assumption: there is a (relatively simple) function $f^* : \mathcal{X} \to \mathcal{Y}$
such that $f^*(\vec{x}_i) = y_i$ for most *i*

Learning task: given *n* examples from the data, find an approximation $\hat{f} \approx f^*$

Goal: $\hat{f}$ gives mostly correct prediction on unseen examples



Machine Learning: the basics…

Unsupervised learning

Data: $\vec{x}_1, \vec{x}_2, \ldots \in \mathcal{X}$

Assumption: there is an underlying structure in $\mathcal{X}$

Learning task: discover the structure given *n* examples from the data

Goal: come up with the summary of the data using the discovered structure

More later in the course…

Supervised Machine Learning

Statistical modeling approach:

Labeled training data
(*n* examples from data) → Learning Algorithm → ‘classifier’ $\hat{f}$

$$(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$$

drawn **independently** from
a fixed underlying distribution
(also called the *i.i.d.* assumption)

select $\hat{f}$ from…?

from a pool of ***models*** $\mathcal{F}$

that **maximizes**
label agreement of the
training data

How to select $\hat{f} \in \mathcal{F}$?

- Maximum likelihood (best fits the data)
- Maximum a posteriori (best fits the data but incorporates prior assumptions)
- Optimization of ‘loss’ criterion (best discriminates the labels)
- …

Maximum Likelihood Estimation (MLE)

Given some data $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n \in \mathcal{X}$ i.i.d. *(Let's forget about the labels for now)*

Say we have a model class $\mathcal{P} = \{p_\theta \mid \theta \in \Theta\}$

ie, each model *p* can be described by a set of parameters θ

find the parameter settings θ that **best fits** the data.

If each model *p*, is a **probability model** then we can find the best fitting probability model via the ***likelihood estimation***!

Likelihood $\mathcal{L}(\theta|X) := P(X|\theta) = P(\vec{x}_1, \ldots, \vec{x}_n|\theta) \overset{\text{i.i.d.}}{=} \prod_{i=1}^{n} P(\vec{x}_i|\theta) = \prod_{i=1}^{n} p_\theta(\vec{x}_i)$

Interpretation: How **probable** (or how likely) is the data given the model p_θ?

Parameter setting θ that maximizes $\mathcal{L}(\theta|X)$

$$\arg\max_\theta \mathcal{L}(\theta|X) = \arg\max_\theta \prod_{i=1}^{n} p_\theta(\vec{x}_i)$$

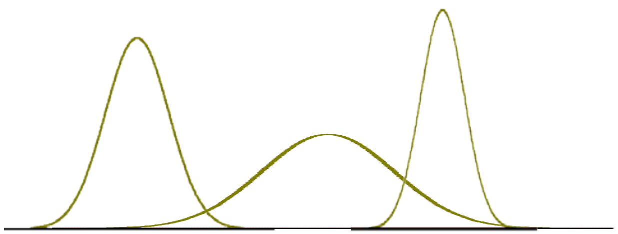
MLE Example

Fitting a statistical probability model to heights of females

Height data (in inches): 60, 62, 53, 58, … $\in \mathbf{R}$

$$x_1, x_2, \ldots x_n \in \mathcal{X}$$

Model class: Gaussian models in **R**



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

μ = mean parameter

σ^2 = variance parameter > 0

So, what is the MLE for the given data X ?

MLE Example (contd.)

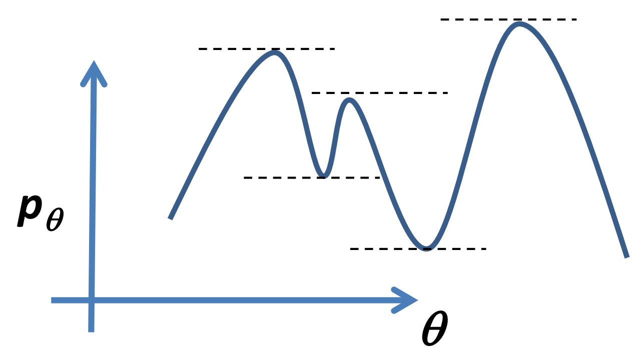
Height data (in inches): $x_1, x_2, \ldots x_n \in \mathcal{X}$ = **R**

Model class: Gaussian models in **R** $p_{\{\mu,\sigma^2\}}(x) := \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$

MLE: $$\arg\max_{\theta} \mathcal{L}(\theta|X) = \arg\max_{\mu,\sigma^2} \prod_{i=1}^{n} p_{\{\mu,\sigma^2\}}(x_i)$$ *Good luck!*

Trick #1: $$\arg\max_{\theta} \mathcal{L}(\theta|X) = \arg\max_{\theta} \log \mathcal{L}(\theta|X)$$ *"Log" likelihood*

Trick #2: finding max (or other extreme values) of a function is simply analyzing the '**stationary points**' of a function. That is, values at which the **derivative** of the function is zero !



MLE Example (contd. 2)

Let's calculate the best fitting $\theta = \{\mu, \sigma^2\}$

$$\begin{aligned}
\arg\max_{\theta} \mathcal{L}(\theta|X) &= \arg\max_{\theta} \log \mathcal{L}(\theta|X) \\
&= \arg\max_{\mu,\sigma^2} \log\left(\prod_{i=1}^{n} p_{\{\mu,\sigma^2\}}(x_i)\right) \\
&= \arg\max_{\mu,\sigma^2} \sum_{i=1}^{n} \log\left(p_{\{\mu,\sigma^2\}}(x_i)\right) \\
&= \arg\max_{\mu,\sigma^2} \sum_{i=1}^{n} \left[\underbrace{-\frac{1}{2}\log(2\pi\sigma^2) - \frac{(x_i-\mu)^2}{2\sigma^2}}_{g_i(\mu,\sigma^2)}\right]
\end{aligned}$$

"Log" likelihood

i.i.d.

Maximizing μ :

$$0 = \nabla_\mu\left(\sum_{i=1}^{n} g_i(\mu,\sigma^2)\right) \implies \mu_{\mathrm{ML}} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Maximizing σ^2:

$$\sigma^2_{\mathrm{ML}} = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$$

MLE Example

So, the best fitting **Gaussian model** $p_{\{\mu,\sigma^2\}}(x) := \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(- \frac{(x-\mu)^2}{2\sigma^2} \right)$

Female height data: 60, 62, 53, 58, … ∈**R**

$$x_1, x_2, \ldots x_n \in \mathcal{X}$$

Is the one with parameters: $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$

What about other model classes?

Other popular probability models

Bernoulli model (coin tosses) *Scalar valued*

Multinomial model (dice rolls) *Scalar valued*

Poisson model (rare counting events) *Scalar valued*

Gaussian model (most common phenomenon) *Scalar valued*

Most machine learning data is vector valued!

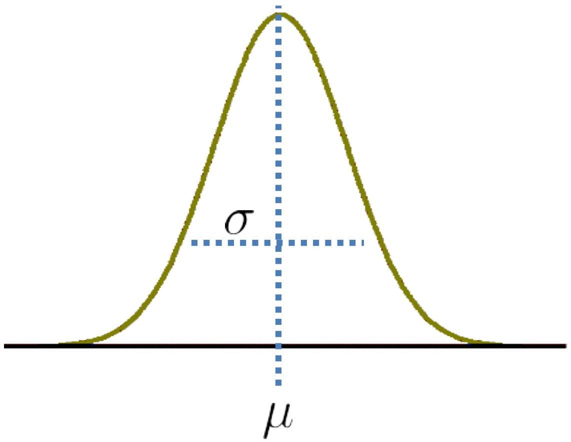
Multivariate Gaussian Model ***Vector valued***

Multivariate version available of other scalar valued models

Multivariate Gaussian

Univariate **R**

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

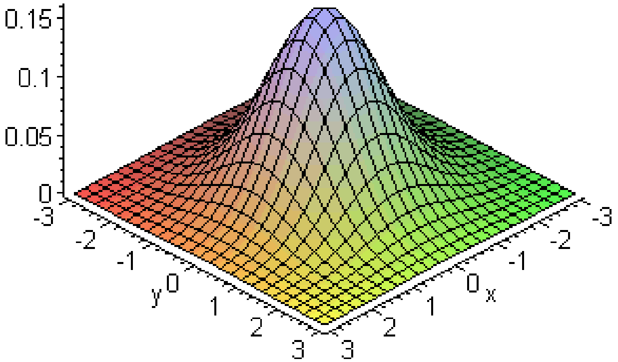


μ = mean parameter

σ^2 = variance parameter > 0

Multivariate **R**^{d}

$$p_{\{\vec{\mu},\Sigma\}}(\vec{x}) := \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^\mathsf{T}\Sigma^{-1}(\vec{x}-\vec{\mu}) \right)$$



$\vec{\mu}$ = mean vector

Σ = Covariance matrix (positive definite)

From MLE to Classification

MLE sounds great, how do we use it to do classification using **labelled** data?

$$\hat{f}(\vec{x}) = \arg\max_{y \in \mathcal{Y}} \; P[Y = y | X = \vec{x}]$$

Why? More later…

$$= \arg\max_{y \in \mathcal{Y}} \; \frac{P[X = \vec{x} | Y = y] \cdot P[Y = y]}{P[X = \vec{x}]}$$

Bayes rule

indep. of y

$$= \arg\max_{y \in \mathcal{Y}} \; P[X = \vec{x} | Y = y] \; \cdot \; P[Y = y]$$

Class conditional probability model

Class Prior

Class prior:

Simply the probability of data sample occurring from a category

Class conditional:

Use a separate probability model individual categories/class-type

We can find the appropriate parameters for the model using MLE!

Classification via MLE Example

Task: learn a classifier to distinguish **`males`** from **`females`**

based on say height and weight measurements

Classifier: $$\hat{f}(\vec{x}) = \underset{y \in \{\text{male}, \text{female}\}}{\arg\max} \; P[X = \vec{x} | Y = y] \cdot P[Y = y]$$

Using **labelled** training data, learn all the parameters:

Learning **class priors**:

$P[Y = \text{male}] =$ fraction of training data labelled as male

$P[Y = \text{female}] =$ fraction of training data labelled as female

Learning **class conditionals**:

$$P[X | Y = \text{male}] = p_{\theta(\text{male})}(X)$$

$$P[X | Y = \text{female}] = p_{\theta(\text{female})}(X)$$

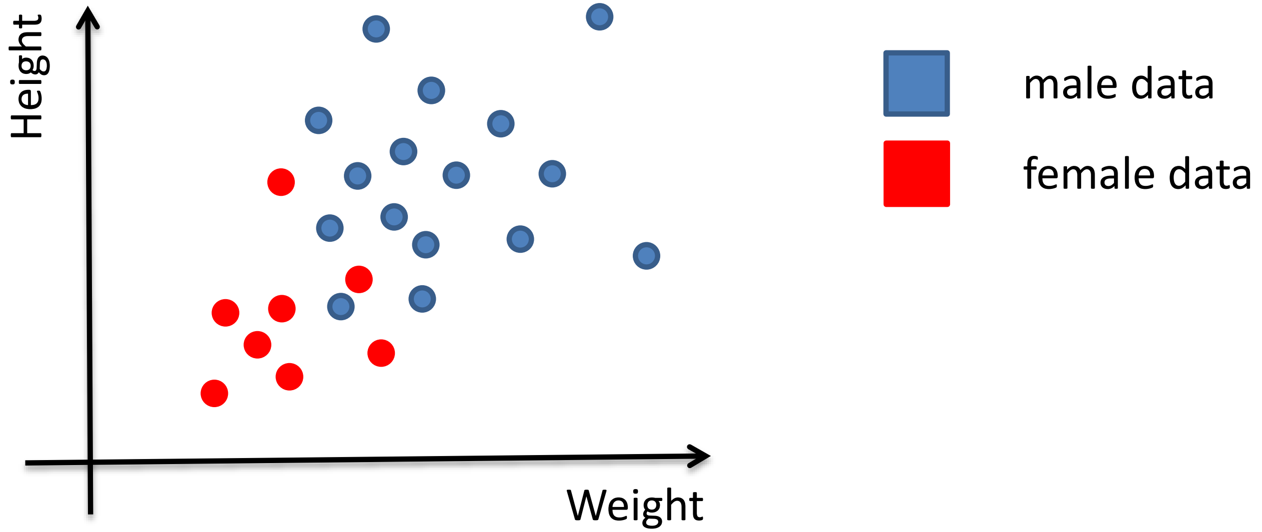
θ(male) = **MLE** using only male data

θ(female) = **MLE** using only female data

What are we doing geometrically?

Data geometry:

$$\mathcal{X} = \mathbf{R}^2 = \text{Weight} \times \text{Height}$$



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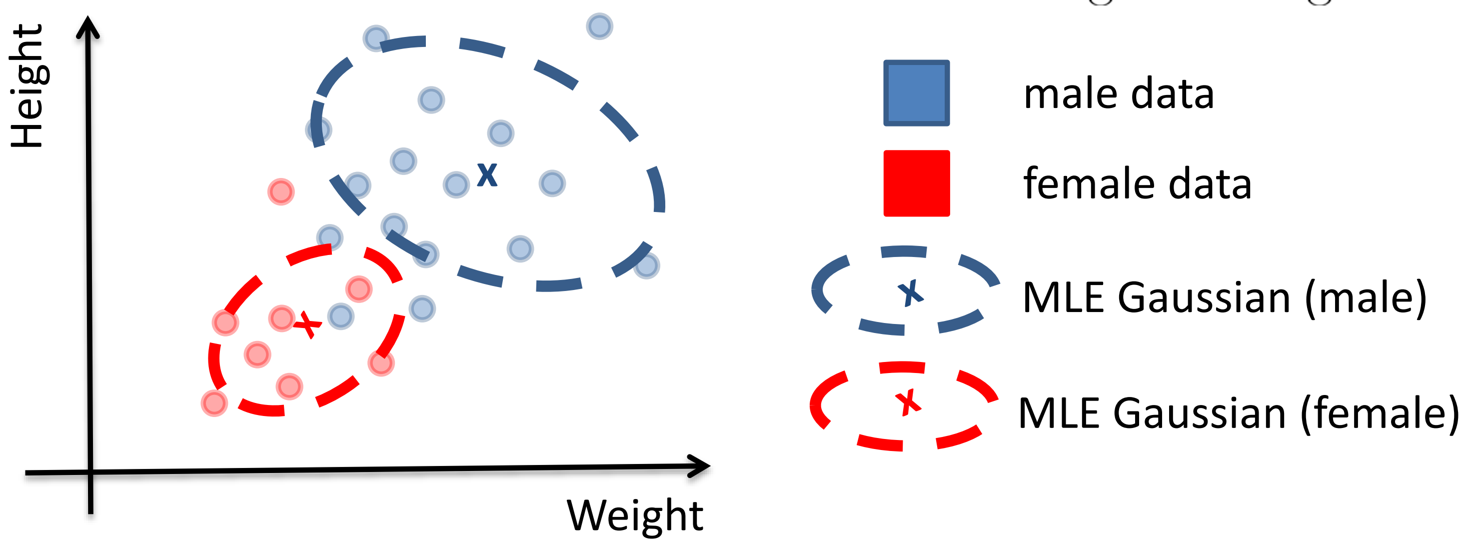

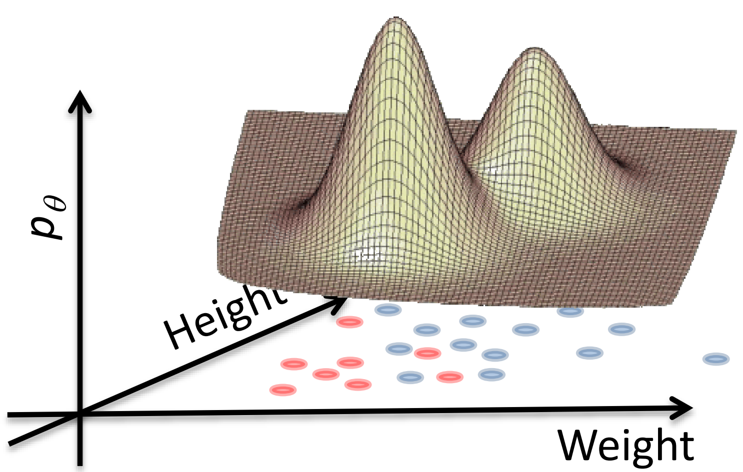

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$$P[X | Y = \text{female}] = p_{\theta(\text{female})}(X)$$

θ(male) = **MLE** using only male data

θ(female) = **MLE** using only female data

Classification via MLE Example

$\boxed{\text{We just made our first predictor } \hat{f} \text{ !}}$

But why: $\hat{f}(\vec{x}) = \arg\max_{y \in \mathcal{Y}} P[Y = y | X = \vec{x}]$

Why the particular f = argmax$_y$ P[Y|X] ?

Accuracy of a classifier f : $$P_{(\vec{x},y)}\left[f(\vec{x})=y\right] \quad = \quad \mathbb{E}_{(\vec{x},y)}\left[\mathbf{1}\left[f(\vec{x})=y\right]\right]$$

Assume binary classification (for simplicity) : $$\mathcal{Y}=\{0,1\}$$

Let: $$f(\vec{x})=\arg\max_{y\in\{0,1\}} \; P[Y=y|X=\vec{x}]$$ Bayes classifier

$$g(\vec{x})=\mathcal{X}\to\{0,1\}$$ any classifier

Theorem: $$P_{(\vec{x},y)}\left[g(\vec{x})=y\right] \quad \leq \quad P_{(\vec{x},y)}\left[f(\vec{x})=y\right]$$

!!! Bayes classifier is optimal !!!

Optimality of Bayes classifier

Theorem: $$P_{(\vec{x},y)}\left[g(\vec{x}) = y\right] \quad \leq \quad P_{(\vec{x},y)}\left[f(\vec{x}) = y\right]$$

Observation: For any classifier *h*

$$\begin{aligned}
P\left[h(\vec{x}) = y | X = \vec{x}\right] &= P\left[h(\vec{x}) = 0, Y = 0 | X = \vec{x}\right] + P\left[h(\vec{x}) = 1, Y = 1 | X = \vec{x}\right] \\
&= \mathbf{1}[h(\vec{x}) = 1] \cdot P[Y = 1 | X = \vec{x}] + \mathbf{1}[h(\vec{x}) = 0] \cdot P[Y = 0 | X = \vec{x}] \\
&= \mathbf{1}[h(\vec{x}) = 1]\eta(\vec{x}) + \mathbf{1}[h(\vec{x}) = 0]\big(1 - \eta(\vec{x})\big)
\end{aligned}$$

So:

$$\begin{aligned}
&P\left[f(\vec{x}) = y | X = \vec{x}\right] - P\left[g(\vec{x}) = y | X = \vec{x}\right] \\
&\quad = \eta(\vec{x})\Big[\mathbf{1}[f(\vec{x}) = 1] - \mathbf{1}[g(\vec{x}) = 1]\Big] + \big(1 - \eta(\vec{x})\big)\Big[\mathbf{1}[f(\vec{x}) = 0] - \mathbf{1}[g(\vec{x}) = 0]\Big] \\
&\quad = \big(2\eta(\vec{x}) - 1\big)\Big[\mathbf{1}[f(\vec{x}) = 1] - \mathbf{1}[g(\vec{x}) = 1]\Big] \\
&\quad \geq 0 \qquad \text{By the choice of } f
\end{aligned}$$

Integrate over X to remove the conditional

$\blacksquare$

So… is classification a solved problem?

We know that Bayes classifier is optimal.

So have we solved all classification problems?

$\boxed{\text{Not even close!}}$

Why?

$$f(\vec{x}) = \arg\max_{y \in \mathcal{Y}} \; P[Y = y | X = \vec{x}]$$

How to estimate P[Y|X] ?

$$= \arg\max_{y \in \mathcal{Y}} \; P[X = \vec{x} | Y = y] \cdot P[Y = y]$$

How to estimate P[X|Y] ?

- How good is the model class?
- Quality of estimation degrades with increase in the dimension of X!
- Active area of research!

Classification via Prob. Models: Variation

Naïve Bayes classifier:

$$\hat{f}(\vec{x}) = \arg\max_{y \in \mathcal{Y}} \quad P[X = \vec{x} | Y = y] \cdot P[Y = y]$$

$$= \arg\max_{y \in \mathcal{Y}} \quad \prod_{j=1}^{d} P[X^{(j)} = x^{(j)} | Y = y] \cdot P[Y = y]$$

$$\vec{x} = \begin{bmatrix} x^{(1)} \\ \vdots \\ x^{(d)} \end{bmatrix}$$

Naïve Bayes assumption: The individual features/measurements are **independent** given the class label

Advantages:

Computationally very simple model. Quick to code.

Disadvantages:

Does not properly capture the interdependence between features, giving bad estimates.

How to evaluate the quality of a classifier?

Your friend claims: “My classifier is better than yours”

How can you evaluate this statement?

Given a classifier *f* , we essentially need to compute:

$$P_{(\vec{x},y)}\left[f(\vec{x}) = y\right] \quad = \quad \mathbb{E}_{(\vec{x},y)}\left[\mathbf{1}\left[f(\vec{x}) = y\right]\right]$$

Accuracy of *f*

But… we **don’t know** the underlying distribution

We can use **training data** to estimate…

$$\frac{1}{n}\sum_{i=1}^{n}\mathbf{1}[f(\vec{x}_i) = y_i]$$

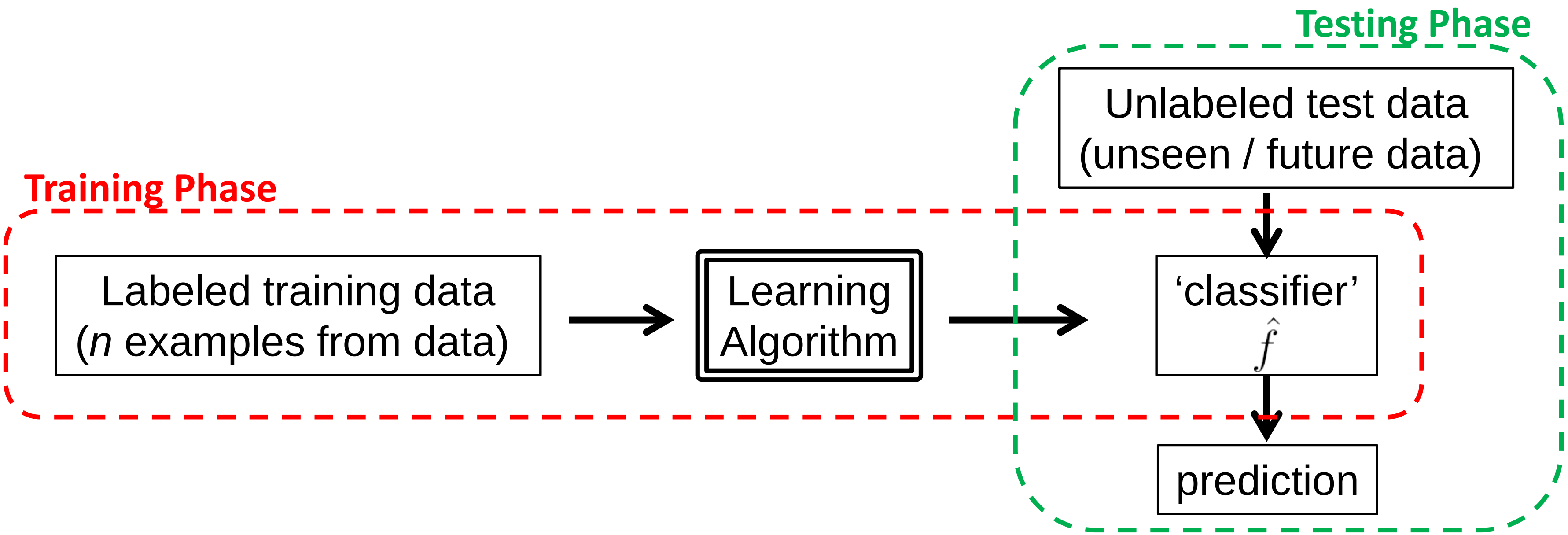
Severely overestimates the accuracy!

Why? Training data is already used to construct *f*, so it is NOT an unbiased estimator

How to evaluate the quality of a classifier?

General strategy:

- Divide the labelled data into **training** and **test** FIRST
- Only use the training data for learning f
- Then the test data can be used as an **unbiased estimator** for gauging the predictive accuracy of f



What we learned…

- Why machine learning
- Basics of Supervised Learning
- Maximum Likelihood Estimation
- Learning a classifier via probabilistic modelling
- Optimality of Bayes classifier
- Naïve Bayes classifier
- How to evaluate the quality of a classifier

Questions?

Next time…

Direct ways of finding the discrimination boundary

Remember

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  http://www.cs.columbia.edu/~verma/classes/sp18/coms4771/
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