



Introduction to Statistical Machine Learning; MLE and MAP

STAT5241 Section 2

Statistical Machine Learning

Xiaofei Shi



Basic administrative details:

- All up-to-date information is on Courseworks
- Lectures are intended to be self-contained. For supplementary readings:
 - Pattern Recognition and Machine Learning, Christopher Bishop.
 - Machine Learning: A probabilistic perspective, Kevin Murphy.
 - The Elements of Statistical Learning: Data Mining, Inference and Prediction, Trevor Hastie, Robert Tibshirani, Jerome Friedman.
 - Machine Learning, Tom Mitchell.





Basic administrative details:

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Tentative Evaluation Plan

Course grade = 40% Homework + 40% Project + 20% Participation

- (40%) Homework: 4 homework in total;
- (40%) Project
- (20%) Final: See school schedule;



What is machine learning:

- The study of computer algorithms that improve automatically through experience



What is machine learning:

- The study of computer algorithms that improve automatically through experience
- Tom Mitchell:

“A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T , as measured by P , improves with experience E .”

 - experience E : training data
 - task T : improve decision in prediction, classification, clustering etc
 - performance measure P : loss function



What is machine learning:

- The study of computer algorithms that improve automatically through experience

-



What is machine learning:

- The study of computer algorithms that improve automatically through experience

-



- What is its relationship with AI, Data Science, Data Mining and Statistics?



While there is overlap, there are differences

- Statistics: the goal is the understanding of the data at hand
- Artificial Intelligence: the goal is to build an intelligent agent
- Data Mining: the goal is to extract patterns from large-scale data
- Data Science: the science encompassing collection, analysis, and interpretation of data



Learning tasks:

ACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAACGCTGAGCAATTCGATAGCAATTC
GATAACGCTGAGCAATTCGGATAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAACG
CTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATATCGATAGCAATTCGATAAATC
GGATAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAACGCTGAGCAATTCGATAGC
AATTCGATAACGCTGAGCAATTCGGATATCGATAGCAATTCGATAACGCTGAGCAACGCTGAGCA
ATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATAACGCTGAGCAATTCGATAGCAATTCGAT
AACGCTGAGCAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATAACGCTG
AGCAATTCGATAGCAATTCGATAACGCTGAGCTGAGCAATTCGATAGCAATTCGATAACGCTGA
GCAATTCGGATAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGATAACGCTGA
GATAGCAATTCGATAGCAATTCGATAGCAATTCGATAACGCTGAGCAACGCTGAGCAATTCGAT
AGCAATTCGATAACGCTGAGCAATTCGGATAACGCTGAGCAATTCGATAGCAATTCGATAACGCT
GAGCAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATATCGATAGCAATT
CGATAACGCTGAGCAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATAAC
GCTGAGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGATAACGCTGAGCAATTC
CTGATAGCAATTCGATAACGCTGAGCAACGCTGAGCAACGCTGAGCAACGCTGAGCAACGCTGAGCA
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ACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATAACGCTGAGCAATTCGAT
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ATCGGATAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGATAGCAATTCGAT
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TTCGATAGCAATTCGATAGCAATTCGATAGCAATTCGATAACGCTGAGCAACGCTGAGCAATTC
GATAGCAATTCGATAACGCTGAGCAATTCGGATAACGCTGAGCAATTCGATAGCAATTCGATAAC
GCTGAGCAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGATATCGATAGCA
ATTTCGATAACGCTGAGCAACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCAATTCGGAT
AACGCTGAGCAATTCGATAGCAATTCGATAACGCTGAGCTGAGCAATTCGATAGCAATTCGATA

Which part is the gene?

Supervised and
unsupervised learning (can
also use active learning)

Learning tasks:

Predict stock price

Help making trading decisions!

Market Summary > Nasdaq Composite
INDEXNASDAQ: .IXIC

12,888.28 +18.28 (0.14%) ↑

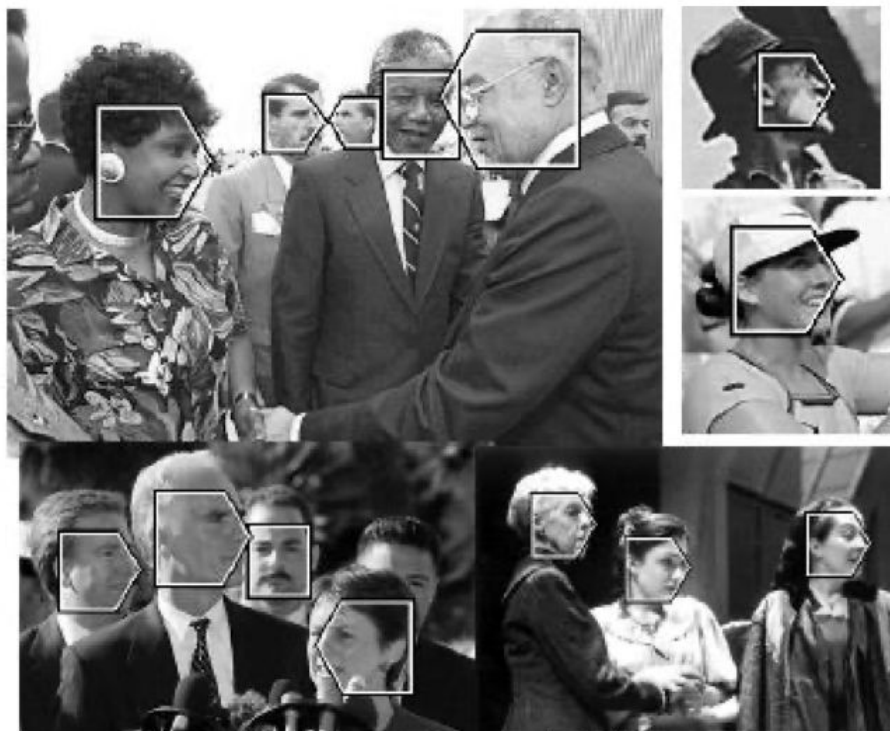
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1 day 5 days 1 month 6 months YTD 1 year 5 years Max



Supervised
learning

Learning tasks:



Learning tasks:

NELL: Never-Ending Language Learning

Can computers learn to read? We think so. "Read the Web" is a research project that attempts to create a computer system that learns over time to read the web. Since January 2010, our computer system called NELL (Never-Ending Language Learner) has been running continuously, attempting to perform two tasks each day:

- First, it attempts to "read," or extract facts from text found in hundreds of millions of web pages (e.g., `playsInstrument(George_Harrison, guitar)`).
- Second, it attempts to improve its reading competence, so that tomorrow it can extract more facts from the web, more accurately.





















So far, NELL has accumulated over 50 million candidate beliefs by reading the web, and it is considering these with high confidence. NELL has high confidence in 3,938,530 of these beliefs — these are displayed on this website. It is not perfect, but NELL is learning. You can track NELL's progress below or [@cmunell on Twitter](#), browse and download its [knowledge base](#), read more about our [technical approach](#), or join the [discussion group](#).



semi supervised learning

Recently-Learned Facts

Refresh

Instance	iteration	date learned	confidence
glass_window_restoration is a household item	1069	03-aug-2017	97.5  
bracelets_curb is a kind of clothing	1069	03-aug-2017	90.9  
hillsborough_lista_d_attesa_crea_un_gruppo_meetup is a visualizable thing	1069	03-aug-2017	99.1  
parison Levitra Viagra Cialis is a drug	1069	03-aug-2017	97.7  
the_democratic_daily is a newspaper	1069	03-aug-2017	100.0  
barcelona_international_airport is an airport in the city barcelona	1073	22-aug-2017	100.0  
john003 has brother james	1073	22-aug-2017	100.0  
omaha_world_herald is a newspaper in the city new york	1073	22-aug-2017	93.8  
abc is a company headquartered in the city new york	1073	22-aug-2017	100.0  
arachnids001 is an arthropod as well as mites also is	1073	22-aug-2017	93.8  



Learning tasks:

- Speech recognition, Natural language processing
- Computer vision
- Web forensics
- Medical outcomes analysis Robotics
- Sensor networks
- Social networks
- ...
- Many, many more...



Data

- Observations:
 - fully observed
 - partially observed: censored data, hidden states, etc...
 - designed experiments
 - actively collected data



Task

- Supervised learning, or also called prediction:
 - Regression - given input, estimate output
 - Classification - given input, estimate category
- Unsupervised learning:
 - Data only contains inputs, but no “supervision” in data as to the descriptive outputs
 - density estimation
 - clustering
 - dimensionality reduction

Supervised learning:

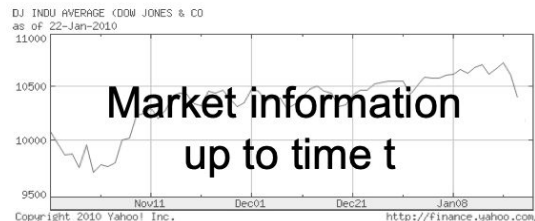
Feature Space \mathcal{X}



Label Space \mathcal{Y}



"Sports"
"News"
"Science"
...

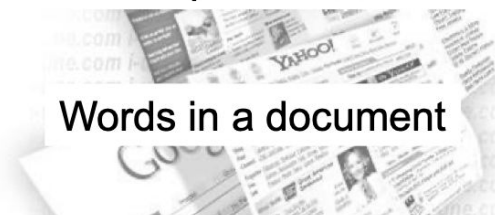


Share Price
"\$ 24.50"

Task: Given $X \in \mathcal{X}$, predict $Y \in \mathcal{Y}$.

Supervised learning:

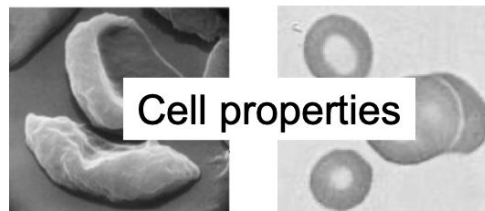
Feature Space \mathcal{X}



Label Space \mathcal{Y}



"Sports"
"News"
"Science"
...

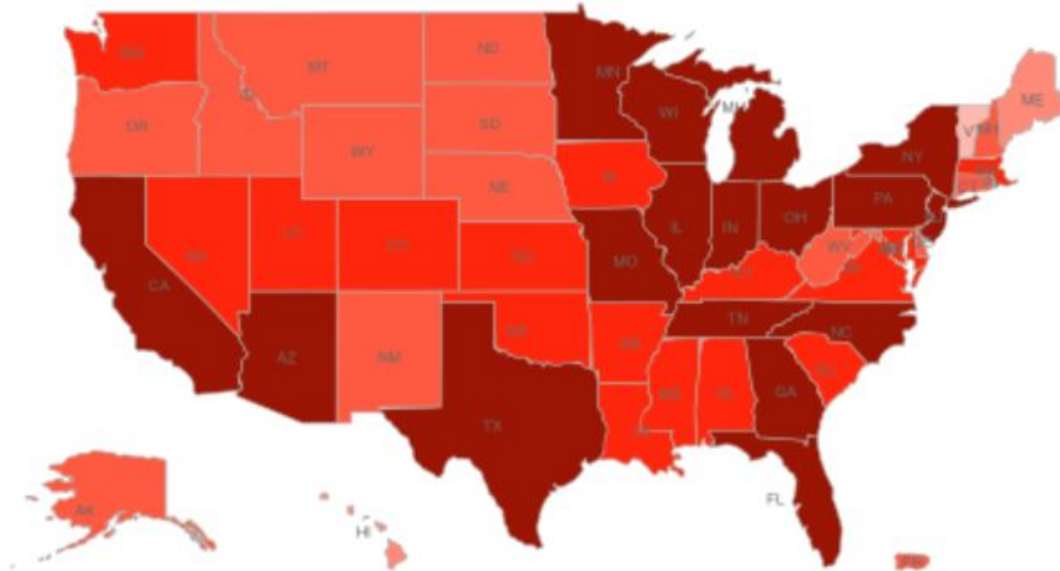


"Anemic cell"
"Healthy cell"

Task: Given $X \in \mathcal{X}$, predict $Y \in \mathcal{Y}$.



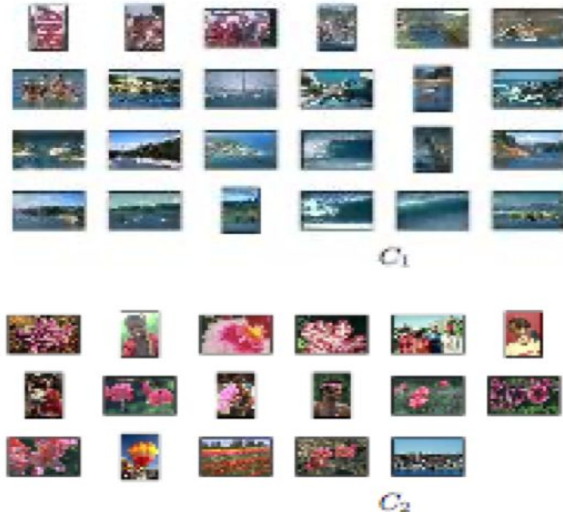
Unsupervised learning:



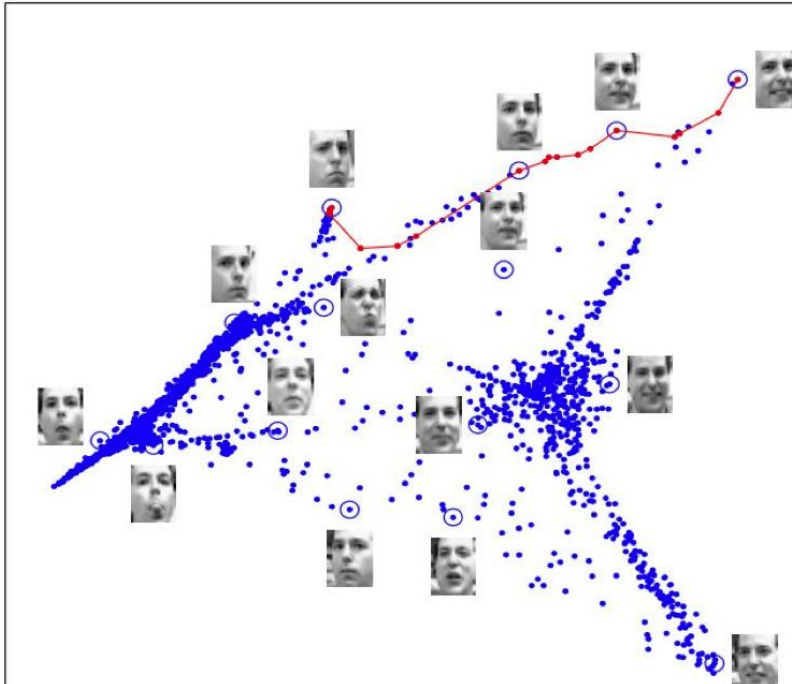
Unsupervised learning:

Group similar things e.g. images

[Goldberger et al.]



Unsupervised learning:



Facial recognition
dimensionality reduction

[Saul & Roweis '03]



Task

- Supervised learning:
Given a set of features and labels learn a model that will predict a label to a new feature set
- Unsupervised learning
Discover patterns in data
- Reasoning under uncertainty
Determine a model of the world either from samples or as you go along
- Active learning
Select not only model but also which examples to use



Algorithm



- Model-based methods
 - probabilistic model of the data
 - parametric models
 - non-parametric models
- Model-free methods

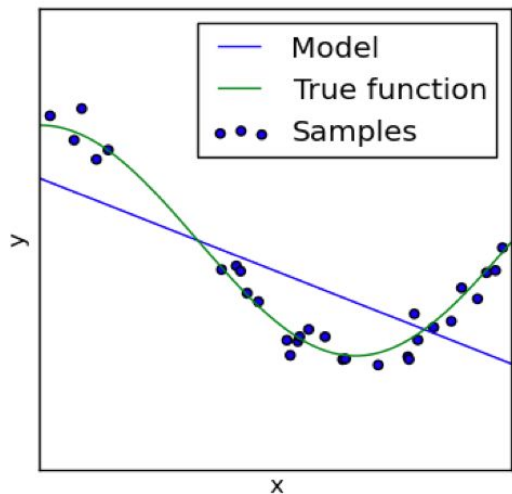
Model-based algorithm



- Learning: from data to model
 - build a model to summarize or to generate the data
 - get estimation on model parameters
 - thus know how to generate future data
- Inference: from model to data
 - Given the model, how can we answer questions relevant to us

Parametric model

- Fixed size model that the number of parameters does not grow with the data
- More data \rightarrow better fit of the model

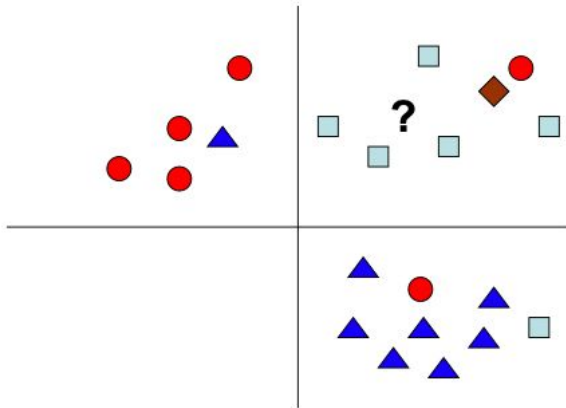


Fitting a simple line (2 params)
to a bunch of one-dim. samples

Model: data = point on line + noise

Non-parametric model

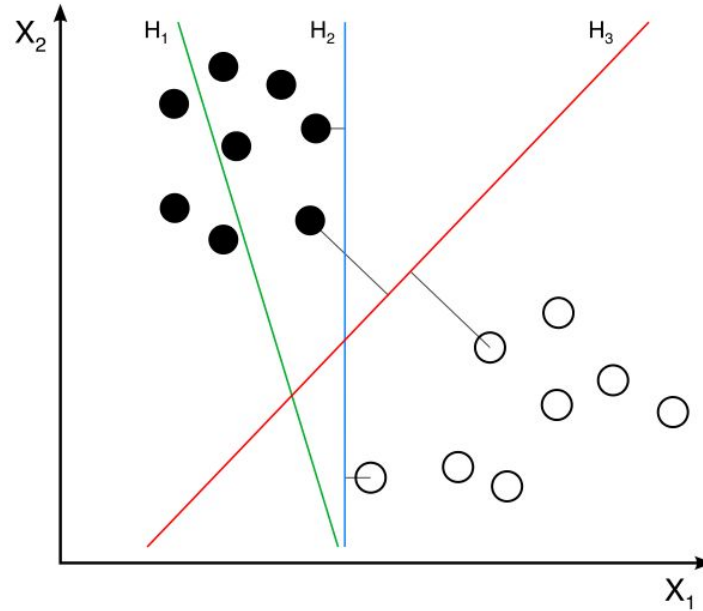
- The number of parameters grows with the data
- More data → a more complex model



- What is the class of the ?
Input
- Can use the other points (k nearest neighbors) but the number of points to search scales with the input data

Discriminative model

- Find the best line that separates black points from white points
- No generative assumption





Common topics

- Mathematical framework:
Well defined concepts based on explicit assumptions
- Representation:
How to encode/decode text? Images?
- Model selection
Which model should we use? How complex should it be?
- Use of prior knowledge
How do we take our beliefs into consideration? How much can we assume?



Theoretical foundation: probability

- In order to translate our task into formal mathematical problem, we need the language of

Probability : the study of uncertainty



A brief introduction to probability

- Random variables
refer to an event whose status is unknown:
 - A = “the stock price of google is going to increase by 0.1% tomorrow”: binary
 - A = “the app you use for food delivery” : discrete
 - A = “the chance of snow in NYC tomorrow” : continuous
- The set of all possible outcomes
 - All of the possible outcomes a random variable can take





Probability

A variety of useful facts can be derived from just three axioms:

1. $0 \leq P(A) \leq 1$
2. $P(\text{true}) = 1, P(\text{false}) = 0$
3. $P(A \cup B) = P(A) + P(B) - P(A \cap B)$



Joint probability

$P(A, B)$

If we assume independence, then $P(A, B) = P(A) P(B)$

Snow tomorrow	Snow today
1	1
0	0
1	0
1	1
0	1
1	1
0	0
0	0



Joint probability

$P(A, B)$

If we assume independence, then $P(A, B) = P(A) P(B)$

$P[\text{snow tomorrow}] = \frac{1}{2}$

$P[\text{snow today}] = \frac{1}{2}$

$P[\text{snow today and tomorrow}] = ?$

Snow tomorrow	Snow today
1	1
0	0
1	0
1	1
0	1
1	1
0	0
0	0



Joint probability

$P(A, B)$

If we assume independence, then $P(A, B) = P(A) P(B)$

$P[\text{snow tomorrow}] = \frac{1}{2}$

$P[\text{snow today}] = \frac{1}{2}$

$P[\text{snow today and tomorrow}] = \frac{3}{8}$

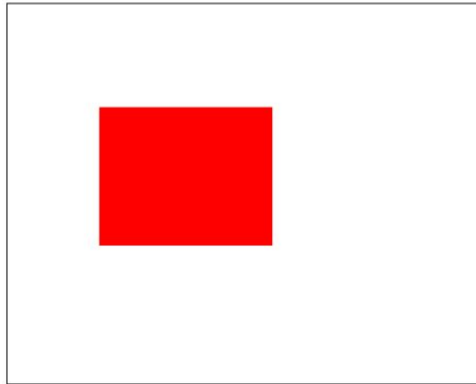
Snow tomorrow	Snow today
1	1
0	0
1	0
1	1
0	1
1	1
0	0
0	0



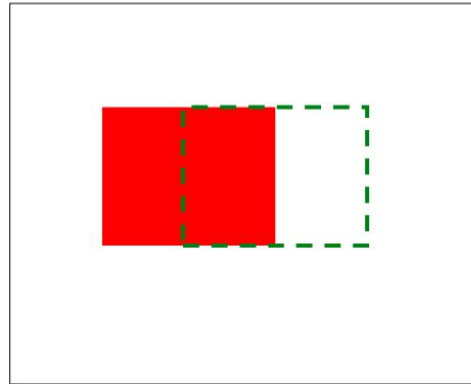
Conditional probability

$P(A | B)$: The fraction of cases where A is true if B is true

$P(A = 0.2)$



$P(A|B = 0.5)$





Conditional probability

- In some cases, given knowledge of one or more random variables we can improve upon our prior belief of another random variable
- $P[\text{snow tomorrow}] = \frac{1}{2}$
 $P[\text{snow tomorrow} \mid \text{snow today}] = \frac{3}{4}$
 $P[\text{no snow tomorrow} \mid \text{snow today}] = \frac{1}{4}$

Snow tomorrow	Snow today
1	1
0	0
1	0
1	1
0	1
1	1
0	0
0	0



Chain rule

- The joint probability can be calculated in terms of conditional probability:

$$P(A,B) = P(A|B) P(B)$$

- Together with Bayes rule (which is actually derived from it) this is one of the most powerful rules in probabilistic reasoning

Bayes rule

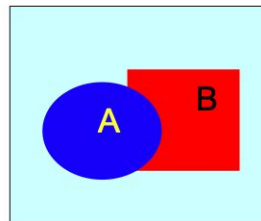
Often it would be useful to derive the rule a bit further:

- Derive from chain rule
- One of the most important rules for this class

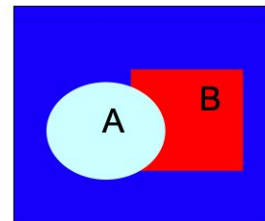
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{P(B|A)P(A)}{\sum_A P(B|A)P(A)}$$

This results from:
 $P(B) = \sum_A P(B,A)$

$P(B,A=1)$



$P(B,A=0)$



An example

- Suppose you have a coin, if I flip it, what's the probability it will fall with the head up?
- You might want to flip the coin several times



An example

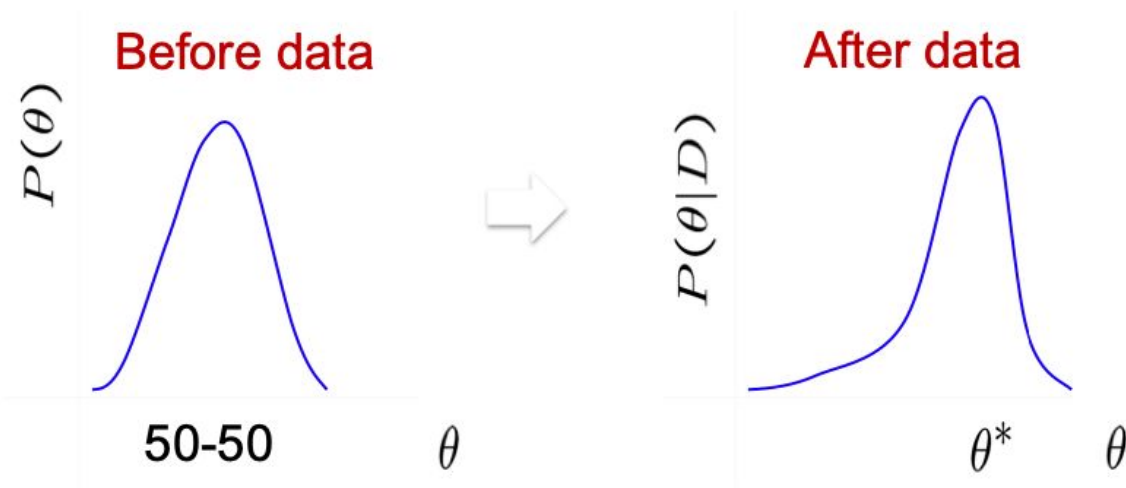
- Suppose you have a coin, if I flip it, what's the probability it will fall with the head up?
- You might want to flip the coin several times



- The probability is $\frac{3}{5}$ because frequency of heads in all flips
- Would you bet money on this estimation?

What about your prior knowledge?

- Rather than estimating a single parameter, we obtain a distribution over possible values of this parameter





Bayesian learning

- Use Bayes rule:

$$P(\theta \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \theta)P(\theta)}{P(\mathcal{D})}$$

- Or equivalently:

$$P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta)P(\theta)$$

posterior likelihood prior



Prior distribution

- Beliefs in an event in the absence of any other information
- Source of prior:
 - Represents expert knowledge (philosophical approach)
 - Simple posterior form (engineer's approach)
- Uninformative priors:
 - Uniform distribution
 - inappropriate distribution
- Conjugate priors:
 - closed-form representation of posteriors

Conjugate prior

Eg. 1 Coin flip problem

Likelihood given Bernoulli model:

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H} (1 - \theta)^{\alpha_T}$$



Conjugate prior

Eg. 1 Coin flip problem

Likelihood given Bernoulli model:

$$P(\mathcal{D} | \theta) = \theta^{\alpha_H} (1 - \theta)^{\alpha_T}$$

If prior is Beta distribution,

$$P(\theta) = \frac{\theta^{\beta_H-1} (1 - \theta)^{\beta_T-1}}{B(\beta_H, \beta_T)} \sim \text{Beta}(\beta_H, \beta_T)$$

Then posterior is Beta distribution

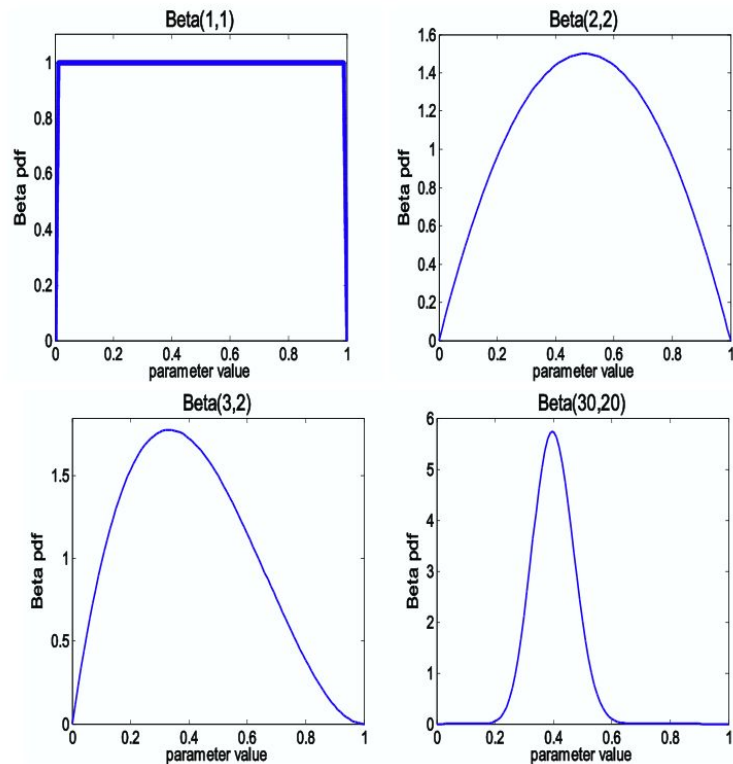
$$P(\theta | D) \sim \text{Beta}(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



Conjugate prior

Beta prior:

$Beta(\beta_H, \beta_T)$ More concentrated as values of β_H, β_T increase

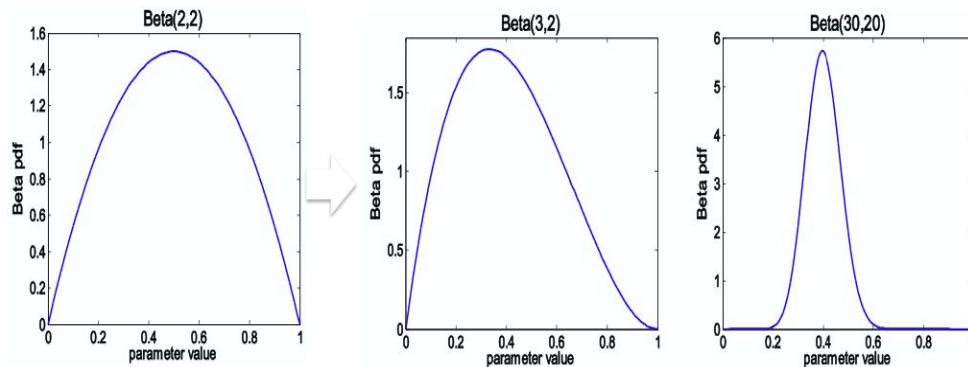


Conjugate prior

$$P(\theta) \sim \text{Beta}(\beta_H, \beta_T)$$

$$P(\theta|D) \sim \text{Beta}(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

Posterior:



As $n = \alpha_H + \alpha_T$
increases

As we get more samples, effect of prior is “washed out”



Conjugate prior:

- Gaussian prior + Gaussian sample distribution → Gaussian posterior
- Beta prior + Bernoulli sample distribution → Beta posterior
- Gamma prior + exponential sample distribution → Gamma posterior
- Dirichlet prior + multinomial sample distribution → Dirichlet posterior





Posterior distribution

- The approach seen so far is what is known as a Bayesian approach
- Prior information encoded as a distribution over possible values of parameter
- Using the Bayes rule, we can get an updated posterior distribution over parameters



Maximum likelihood principle (MLE)

Data likelihood: $P(D | M) = q^{n_1} (1 - q)^{n_2}$

We would like to find: $\arg \max_q q^{n_1} (1 - q)^{n_2}$

Or more generally, $\hat{P}(\text{dataset} | M) = \hat{P}(x_1 \wedge x_2 \dots \wedge x_n | M) = \prod_{k=1}^n \hat{P}(x_k | M)$

- Our goal is to determine the values for the parameters in M
- We can do this by maximizing the probability of generating the observed samples



An example: Coin flips



MLE v.s. MAP

- Maximum Likelihood estimation (MLE):

Choose value that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg \max_{\theta} P(D|\theta)$$

- Maximum a posteriori (MAP) estimation:

Choose value that is most probable given observed data and prior belief

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} P(\theta|D) \\ &= \arg \max_{\theta} P(D|\theta)P(\theta)\end{aligned}$$



MAP: Coin flips



References

- Tom Mitchell: Machine Learning, Chapter 6
- Kevin Murphy: Machine Learning: A probabilistic perspective, Chapter 1, 2, 5, 6
- Ziv Bar-Joseph, Tom Mitchell, Pradeep Ravikumar and Aarti Singh: CMU 10-701