10-301/601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

PAC Learning

+

The Big Picture

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Lecture 15

Oct. 18, 2021

Reminders

- **Homework 5: Neural Networks**
  - Out: Mon, Oct. 11
  - Due: Thu, Oct. 21 at 11:59pm

Q&A

Q: What is proof by contraposition?

A: $A \Rightarrow B \,,\; \neg B \Rightarrow \neg A$

- "If A, then B" is logically equivalent to "If not B then, not A"

- Ex: "if it's raining, I bring my umbrella" implies "if I don't bring my umbrella, it's not raining" and vice versa

Sample Complexity Results

Definition 0.1. The **sample complexity** of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

Four Cases we care about…

	Realizable	Agnostic
Finite $\lvert\mathcal{H}\rvert$	**Thm. 1** $N \geq \frac{1}{\epsilon}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.	
Infinite $\lvert\mathcal{H}\rvert$		

Example: Conjunctions

Question:

Suppose H = class of conjunctions over **x** in $\{0,1\}^M$

Example hypotheses:

$h(\mathbf{x}) = x_1 (1-x_3) x_5$

$h(\mathbf{x}) = x_1 (1-x_2) x_4 (1-x_5)$

If M = 10, ε = 0.1, δ = 0.01, how many examples suffice according to Theorem 1?

Answer:

A. $10*(2*\ln(10)+\ln(100)) \approx 92$
B. $10*(3*\ln(10)+\ln(100)) \approx 116$
C. $10*(10*\ln(2)+\ln(100)) \approx 116$
D. $10*(10*\ln(3)+\ln(100)) \approx 156$
E. $100*(2*\ln(10)+\ln(10)) \approx 691$
F. $100*(3*\ln(10)+\ln(10)) \approx 922$
G. $100*(10*\ln(2)+\ln(10)) \approx 924$
H. $100*(10*\ln(3)+\ln(10)) \approx 1329$

Thm. 1 $N \geq \frac{1}{\epsilon}\left[\log(|\mathcal{H}|) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.

Question 1

- A
- B
- C
- D
- E
- F
- G
- H

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Infinite $\lvert\mathcal{H}\rvert$		

1. Bound is **inversely linear in epsilon** (e.g. halving the error requires double the examples)
2. Bound is **only logarithmic in |H|** (e.g. quadrupling the hypothesis space only requires double the examples)

1. Bound is **inversely quadratic in epsilon** (e.g. halving the error requires 4x the examples)
2. Bound is **only logarithmic in |H|** (i.e. same as Realizable case)

	Realizable	Agnostic
Finite $\lvert\mathcal{H}\rvert$	**Thm. 1** $N \geq \frac{1}{\epsilon}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.	**Thm. 2** $N \geq \frac{1}{2\epsilon^2}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{2}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\lvert R(h) - \hat{R}(h)\rvert \leq \epsilon$.
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Sample Complexity Results

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Four Cases we care about…

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Infinite $\lvert\mathcal{H}\rvert$		

We need a new definition of "complexity" for a Hypothesis space for these results (see *VC Dimension*)

Sample Complexity Results

Definition 0.1. The **sample complexity** of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

Four Cases we care about…

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Infinite $\lvert\mathcal{H}\rvert$	**Thm. 3** $N = O(\frac{1}{\epsilon}\left[\mathrm{VC}(\mathcal{H})\log(\frac{1}{\epsilon}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.	**Thm. 4** $N = O(\frac{1}{\epsilon^2}\left[\mathrm{VC}(\mathcal{H}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\lvert R(h) - \hat{R}(h)\rvert \leq \epsilon$.

VC-DIMENSION

Labelings & Shattering

Def: A hypothesis h applied to some dataset S generates a **labeling** of S.

Def: Let $\mathcal{H}[S]$ be the set of all (distinct) labelings of S generated by hypotheses $h \in \mathcal{H}$.

$\mathcal{H}$ **shatters** S if $|\mathcal{H}[S]| = 2^{|S|}$

Equivalently, the hypotheses in $\mathcal{H}$ can generate every possible labeling of S.

Labelings & Shattering

Whiteboard:

– Shattering example: binary classification

VC-dimension

Def: The **VC-dimension** (or Vaporik-Chervonenkis dimension) of $\mathcal{H}$ is the cardinality of the largest set S such that $\mathcal{H}$ can shatter S.

If $\mathcal{H}$ can shatter arbitrarily large finite sets, then the VC-dimension of $\mathcal{H}$ is infinity

VC-dimension

Whiteboard:

- VC-dimension Example: linear separators
- Proof sketch of VC-dimension for linear separators in 2D

∃ vs. ∀

VC-dimension

– Proving **VC-dimension** requires us to show that **there exists** (∃) a dataset of size d that can be shattered and that **there does not exist** (∄) a dataset of size d+1 that can be shattered

Shattering

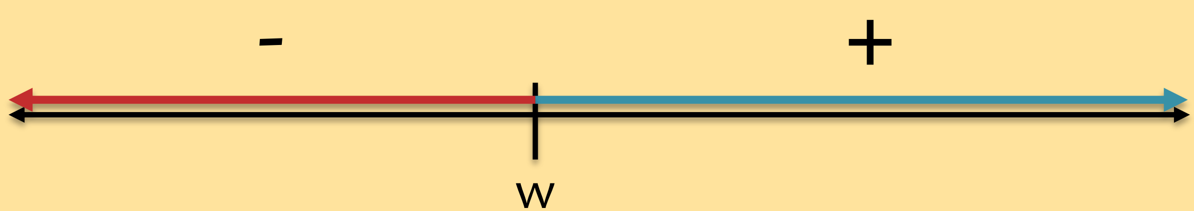
– Proving that a particular dataset can be **shattered** requires us to show that **for all** (∀) labelings of the dataset, our hypothesis class contains a hypothesis that can correctly classify it

VC-dimension Examples

- *Definition*: If VC(H) = d, then **there exists** (∃) a dataset of size d that can be shattered and that **there does not exist** (∄) a dataset of size d+1 that can be shattered

Question:

What is the VC-dimension of H = **1D positive rays.** That is for a threshold w, everything to the right of w is labeled as +1, everything else is labeled -1.



Answer:

When poll is active, respond at **pollev.com/10301601polls**

Question 2

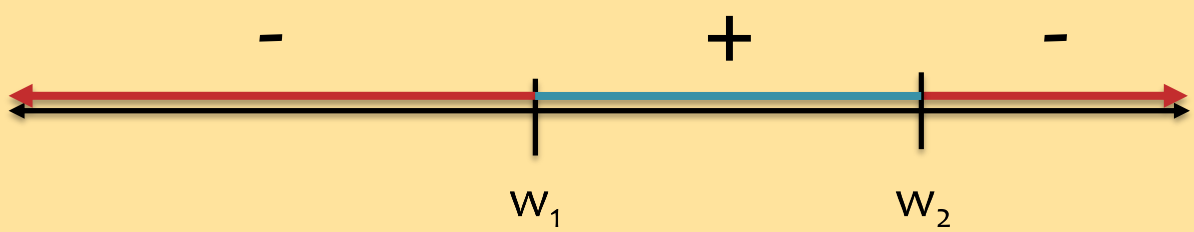
- A
- B
- C
- D
- E

VC-dimension Examples

- *Definition*: If VC(H) = d, then **there exists** (∃) a dataset of size d that can be shattered and that **there does not exist** (∄) a dataset of size d+1 that can be shattered

Question:

What is the VC-dimension of H = **1D positive intervals.** That is for an interval (w_1, w_2), everything inside the interval is labeled as +1, everything else is labeled -1.



Answer:

Question 3

A

B

C

D

E

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SLT-style Corollaries

Thm. 1 $N \geq \frac{1}{\epsilon}\left[\log(|\mathcal{H}|) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.

Solve the inequality in Thm.1 for epsilon to obtain Corollary 1

Corollary 1 (Realizable, Finite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for any h in $\mathcal{H}$ consistent with the training data (i.e. $\hat{R}(h) = 0$),

$$R(h) \leq \frac{1}{N}\left[\ln(|\mathcal{H}|) + \ln\left(\frac{1}{\delta}\right)\right]$$

We can obtain similar corollaries for each of the theorems…

SLT-style Corollaries

Corollary 1 (Realizable, Finite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for any h in $\mathcal{H}$ consistent with the training data (i.e. $\hat{R}(h) = 0$),

$$R(h) \leq \frac{1}{N}\left[\ln(|\mathcal{H}|) + \ln\left(\frac{1}{\delta}\right)\right]$$

Corollary 2 (Agnostic, Finite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for all hypotheses h in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + \sqrt{\frac{1}{2N}\left[\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right)\right]}$$

SLT-style Corollaries

Corollary 3 (Realizable, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for any hypothesis h in $\mathcal{H}$ consistent with the data (i.e. with $\hat{R}(h) = 0$),

$$R(h) \leq O\left(\frac{1}{N}\left[\mathsf{VC}(\mathcal{H})\ln\left(\frac{N}{\mathsf{VC}(\mathcal{H})}\right) + \ln\left(\frac{1}{\delta}\right)\right]\right) \tag{1}$$

Corollary 4 (Agnostic, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for all hypotheses h in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + O\left(\sqrt{\frac{1}{N}\left[\mathsf{VC}(\mathcal{H}) + \ln\left(\frac{1}{\delta}\right)\right]}\right) \tag{2}$$

SLT-style Corollaries

Corollary 3 (Realizable, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for any hypothesis h in $\mathcal{H}$ consistent with the data (i.e. with $\hat{R}(h) = 0$),

$$R(h) \leq O\left(\frac{1}{N}\left[\text{VC}(\mathcal{H}) \ln\left(\frac{N}{\text{VC}(\mathcal{H})}\right) + \ln\left(\frac{1}{\delta}\right)\right]\right) \tag{1}$$

Corollary 4 (Agnostic, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1-\delta)$, for all hypotheses h in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + O\left(\sqrt{\frac{1}{N}\left[\text{VC}(\mathcal{H}) + \ln\left(\frac{1}{\delta}\right)\right]}\right) \tag{2}$$

Should these corollaries inform how we do model selection?

Generalization and Overfitting

Whiteboard:

- Model Selection
- Empirical Risk Minimization
- Structural Risk Minimization
- Motivation for Regularization

Questions For Today

1. Given a classifier with zero training error, what can we say about generalization error? (Sample Complexity, Realizable Case)

2. Given a classifier with low training error, what can we say about generalization error? (Sample Complexity, Agnostic Case)

3. Is there a theoretical justification for regularization to avoid overfitting? (Structural Risk Minimization)

Learning Theory Objectives

You should be able to…

- Identify the properties of a learning setting and assumptions required to ensure low generalization error
- Distinguish true error, train error, test error
- Define PAC and explain what it means to be approximately correct and what occurs with high probability
- Apply sample complexity bounds to real-world learning examples
- Distinguish between a large sample and a finite sample analysis
- Theoretically motivate regularization

THE BIG PICTURE

ML Big Picture

Learning Paradigms:

What data is available and when? What form of prediction?

- supervised learning
- unsupervised learning
- semi-supervised learning
- reinforcement learning
- active learning
- imitation learning
- domain adaptation
- online learning
- density estimation
- recommender systems
- feature learning
- manifold learning
- dimensionality reduction
- ensemble learning
- distant supervision
- hyperparameter optimization

Problem Formulation:

What is the structure of our output prediction?

boolean	Binary Classification
categorical	Multiclass Classification
ordinal	Ordinal Classification
real	Regression
ordering	Ranking
multiple discrete	Structured Prediction
multiple continuous	(e.g. dynamical systems)
both discrete & cont.	(e.g. mixed graphical models)

Application Areas

Key challenges?

NLP, Speech, Computer Vision, Robotics, Medicine, Search

Theoretical Foundations:

What principles guide learning?

- ❑ probabilistic
- ❑ information theoretic
- ❑ evolutionary search
- ❑ ML as optimization

Facets of Building ML Systems:

How to build systems that are robust, efficient, adaptive, effective?

1. *Data prep*
2. *Model selection*
3. *Training (optimization / search)*
4. *Hyperparameter tuning on validation data*
5. *(Blind) Assessment on test data*

Big Ideas in ML:

Which are the ideas driving development of the field?

- *inductive bias*
- *generalization / overfitting*
- *bias-variance decomposition*
- *generative vs. discriminative*
- *deep nets, graphical models*
- *PAC learning*
- *distant rewards*

ML Big Picture

Whiteboard

- Decision Rules / Models
- Objective Functions
- Regularization
- Optimization

PROBABILISTIC LEARNING

Probabilistic Learning

Function Approximation

Previously, we assumed that our output was generated using a **deterministic target function:**

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$
$$y^{(i)} = c^*(\mathbf{x}^{(i)})$$

Our goal was to learn a hypothesis h(**x**) that best approximates c^*(**x**)

Probabilistic Learning

Today, we assume that our output is **sampled** from a conditional **probability distribution:**

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$
$$y^{(i)} \sim p^*(\cdot|\mathbf{x}^{(i)})$$

Our goal is to learn a probability distribution p(y|**x**) that best approximates p^*(y|**x**)

PROBABILITY

Random Variables: Definitions

Discrete Random Variable	X	Random variable whose values come from a countable set (e.g. the natural numbers or {True, False})
Probability mass function (pmf)	$p(x)$	Function giving the probability that discrete r.v. X takes value x. $$p(x) := P(X = x)$$

Random Variables: Definitions

Continuous Random Variable	X	Random variable whose values come from an interval or collection of intervals (e.g. the real numbers or the range (3, 5))
Probability density function (pdf)	$f(x)$	Function the returns a nonnegative real indicating the relative likelihood that a continuous r.v. X takes value x

- For any continuous random variable: $P(X = x) = 0$
- Non-zero probabilities are only available to intervals:

$$P(a \leq X \leq b) = \int_a^b f(x)dx$$

Random Variables: Definitions

Cumulative distribution function	$F(x)$	Function that returns the probability that a random variable X is less than or equal to x: $$F(x) = P(X \leq x)$$

- For **discrete** random variables:

$$F(x) = P(X \leq x) = \sum_{x' < x} P(X = x') = \sum_{x' < x} p(x')$$

- For **continuous** random variables:

$$F(x) = P(X \leq x) = \int_{-\infty}^{x} f(x')dx'$$

Notational Shortcuts

A convenient shorthand:

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

$\Rightarrow$ For all values of a and b:

$$P(A=a|B=b) = \frac{P(A=a,B=b)}{P(B=b)}$$

Notational Shortcuts

But then how do we tell $P(E)$ apart from $P(X)$?

Event

Random Variable

Instead of writing:

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

We should write:

$$P_{A|B}(A|B) = \frac{P_{A,B}(A,B)}{P_B(B)}$$

…but only probability theory textbooks go to such lengths.

COMMON PROBABILITY DISTRIBUTIONS

Common Probability Distributions

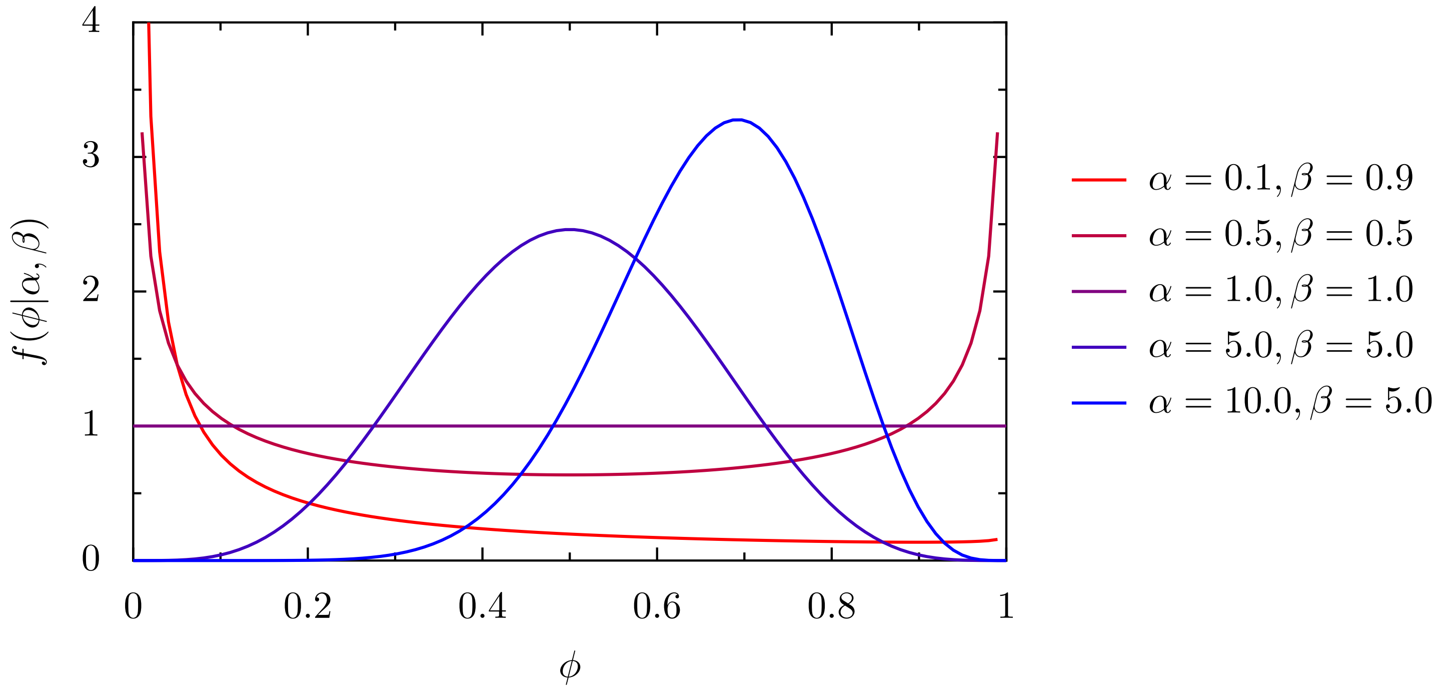
- For Discrete Random Variables:
  - Bernoulli
  - Binomial
  - Multinomial
  - Categorical
  - Poisson
- For Continuous Random Variables:
  - Exponential
  - Gamma
  - Beta
  - Dirichlet
  - Laplace
  - Gaussian (1D)
  - Multivariate Gaussian

Common Probability Distributions

Beta Distribution

probability density function:

$$f(\phi|\alpha,\beta) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

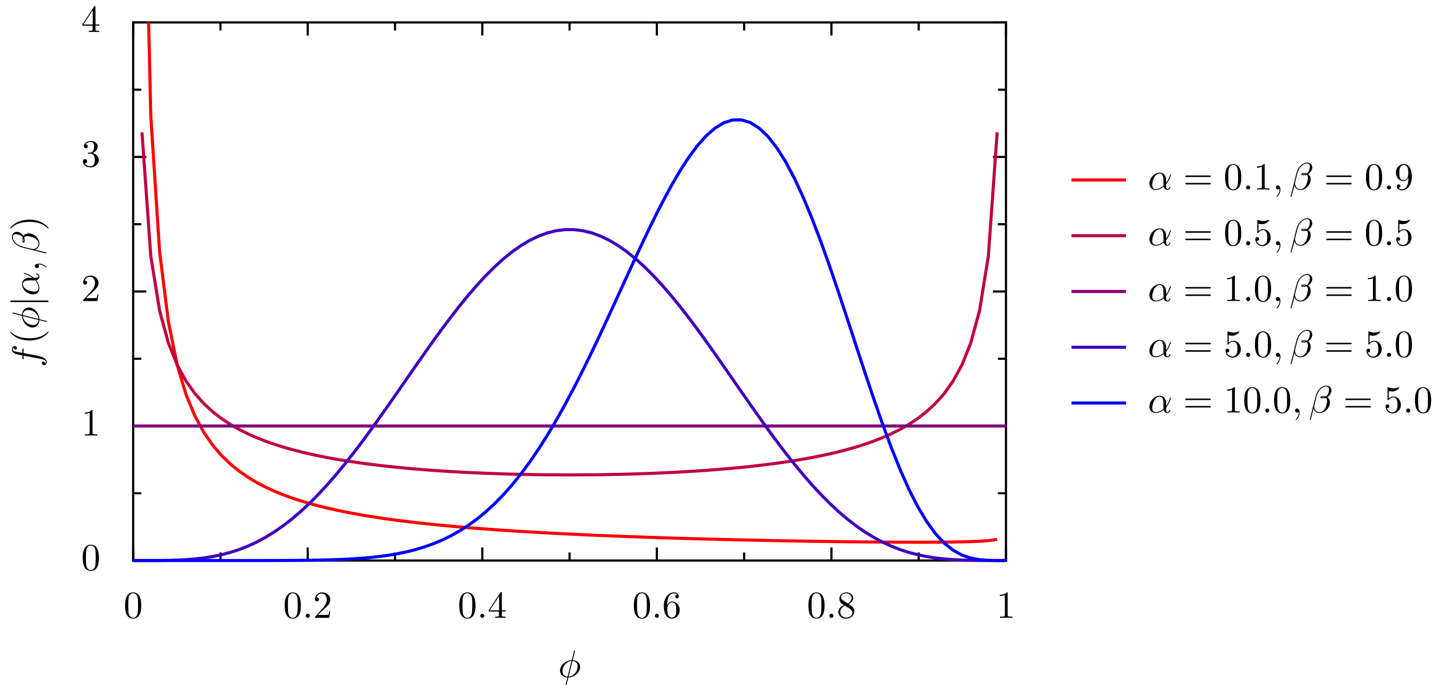


Common Probability Distributions

Dirichlet Distribution

probability density function:

$$f(\phi|\alpha,\beta) = \frac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

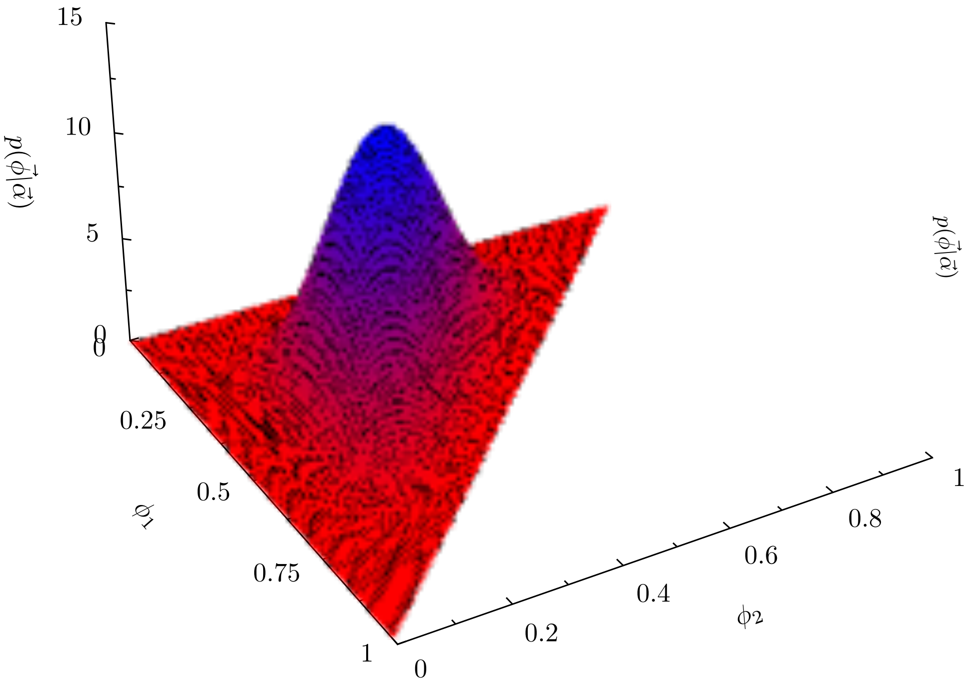


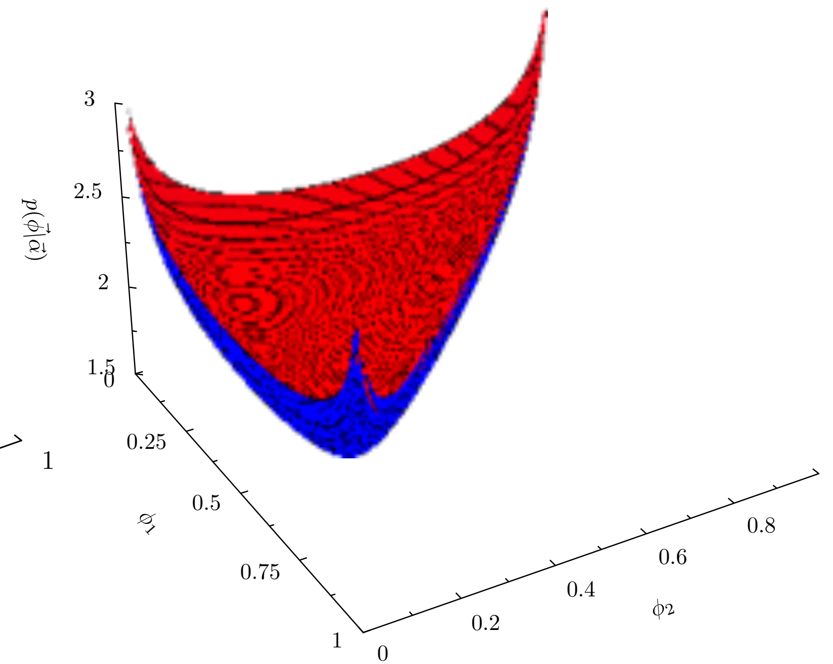
Common Probability Distributions

Dirichlet Distribution

probability density function:

$$p(\vec{\phi}|\boldsymbol{\alpha}) = \frac{1}{B(\boldsymbol{\alpha})}\prod_{k=1}^{K}\phi_k^{\alpha_k - 1} \quad \text{where } B(\boldsymbol{\alpha}) = \frac{\prod_{k=1}^{K}\Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^{K}\alpha_k)}$$





EXPECTATION AND VARIANCE

Expectation and Variance

The **expected value** of X is $E[X]$. Also called the mean.

- Discrete random variables:

  Suppose X can take any value in the set $\mathcal{X}$.

  $$E[X] = \sum_{x \in \mathcal{X}} x p(x)$$

- Continuous random variables:

  $$E[X] = \int_{-\infty}^{+\infty} x f(x) dx$$

Expectation and Variance

The **variance** of *X* is *Var(X)*.

$$Var(X) = E[(X - E[X])^2]$$

$$\mu = E[X]$$

- Discrete random variables:

$$Var(X) = \sum_{x \in \mathcal{X}} (x - \mu)^2 p(x)$$

- Continuous random variables:

$$Var(X) = \int_{-\infty}^{+\infty} (x - \mu)^2 f(x) dx$$

Joint probability

Marginal probability

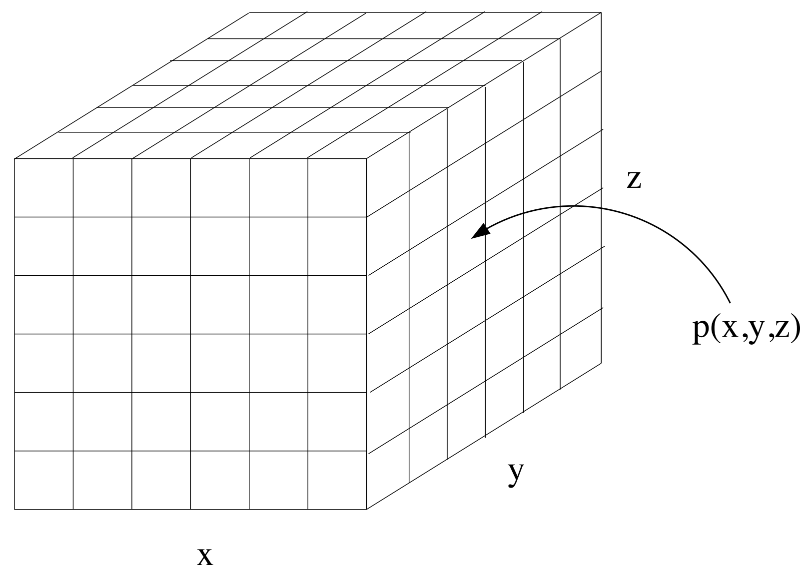
Conditional probability

MULTIPLE RANDOM VARIABLES

Joint Probability

- Key concept: two or more random variables may interact. Thus, the probability of one taking on a certain value depends on which value(s) the others are taking.
- We call this a joint ensemble and write

$$p(x, y) = \text{prob}(X = x \text{ and } Y = y)$$



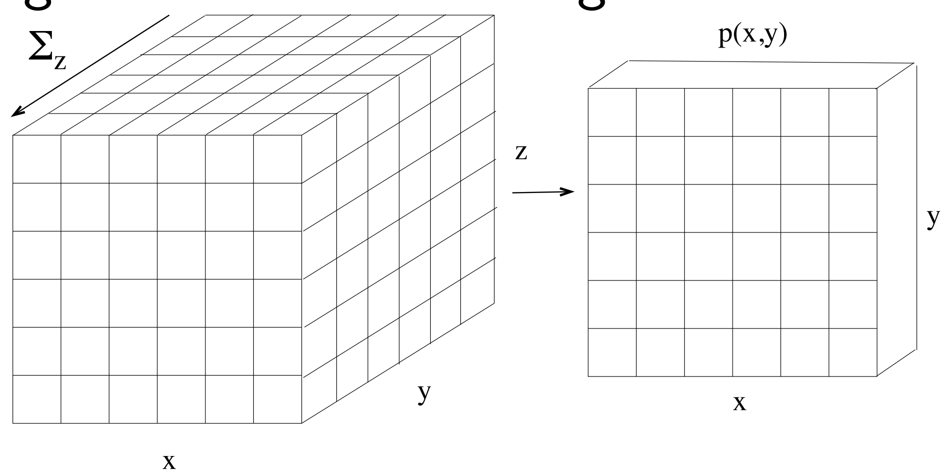
Slide from Sam Roweis (MLSS, 2005)

Marginal Probabilities

- We can "sum out" part of a joint distribution to get the *marginal distribution* of a subset of variables:

$$p(x) = \sum_y p(x, y)$$

- This is like adding slices of the table together.



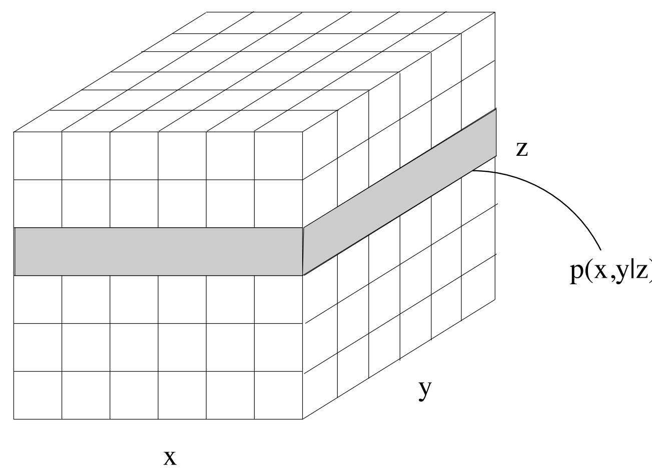
- Another equivalent definition: $p(x) = \sum_y p(x|y)p(y)$.

Slide from Sam Roweis (MLSS, 2005)

Conditional Probability

- If we know that some event has occurred, it changes our belief about the probability of other events.
- This is like taking a "slice" through the joint table.

$$\boxed{p(x|y) = p(x,y)/p(y)}$$

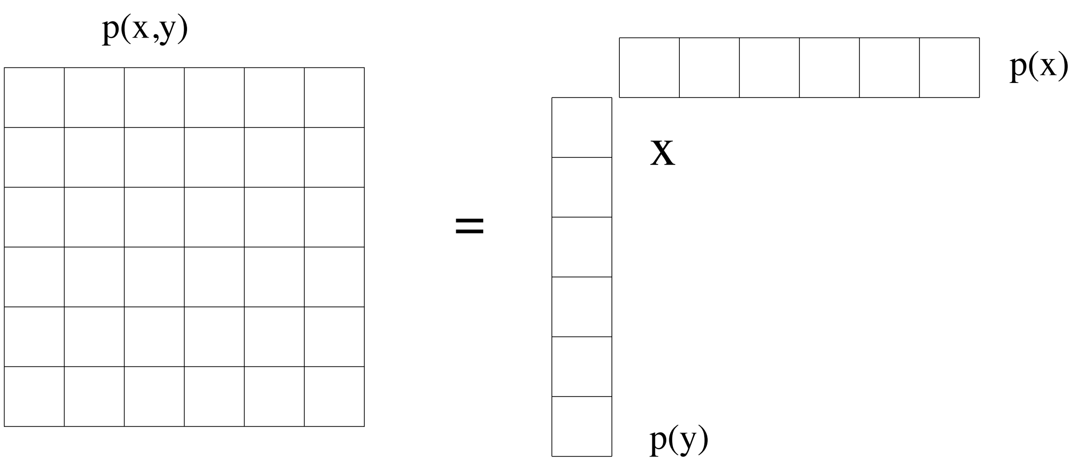


Slide from Sam Roweis (MLSS, 2005)

Independence and Conditional Independence

- Two variables are independent iff their joint factors:

$$p(x, y) = p(x)p(y)$$



- Two variables are conditionally independent given a third one if for all values of the conditioning variable, the resulting slice factors:

$$p(x, y|z) = p(x|z)p(y|z) \qquad \forall z$$

Slide from Sam Roweis (MLSS, 2005)