Probability, Decision Theory, and Loss Functions

CMSC 678

UMBC

A Terminology Buffet

Classification

Regression

Clustering

the task: what kind of problem are you solving?

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the task: what kind of problem are you solving?

Fully-supervised

Semi-supervised

Un-supervised

the data: amount of human input/number of labeled examples

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Classification

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the task: what kind of problem are you solving?

Fully-supervised

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Un-supervised

the data: amount of human input/number of labeled examples

Probabilistic Neural

Generative Memory-

based

Conditional

Exemplar

Spectral ...

the **approach**: how any data are being used

Outline

Review+Extension

Probability

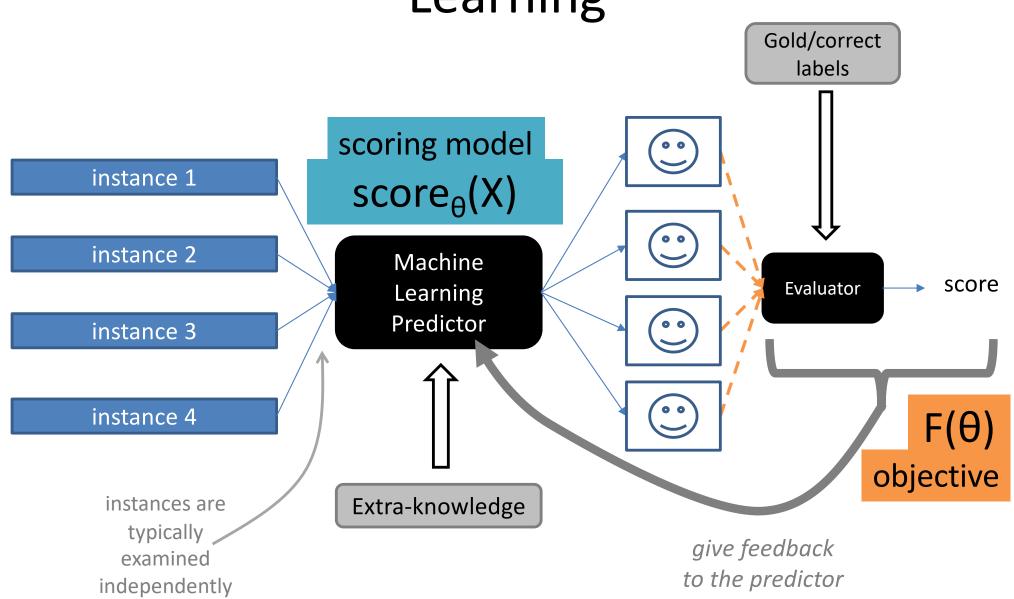
Decision Theory

Loss Functions

What does it mean to learn?

Generalization

Machine Learning Framework: Learning



Model, parameters and hyperparameters

Model: mathematical formulation of system (e.g., classifier)

Parameters: primary "knobs" of the model that are set by a learning algorithm



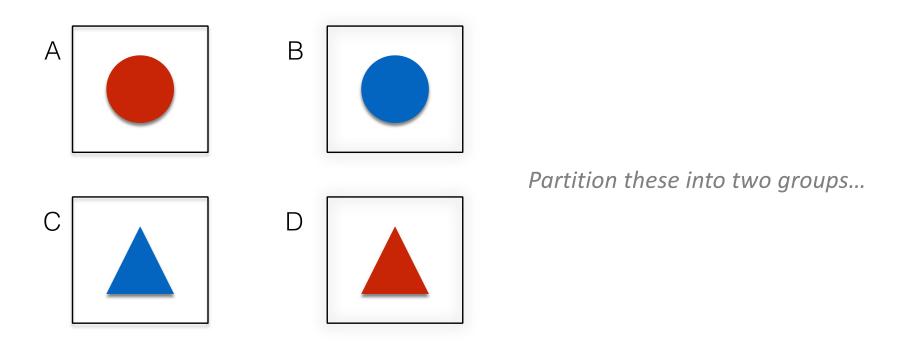
Hyperparameter: secondary "knobs"

Gradient Ascent

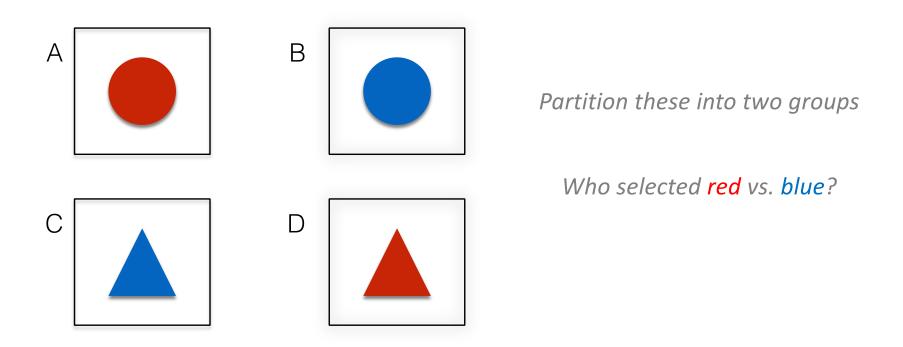
 $arg max F(\theta)$

General ML Consideration: Inductive Bias

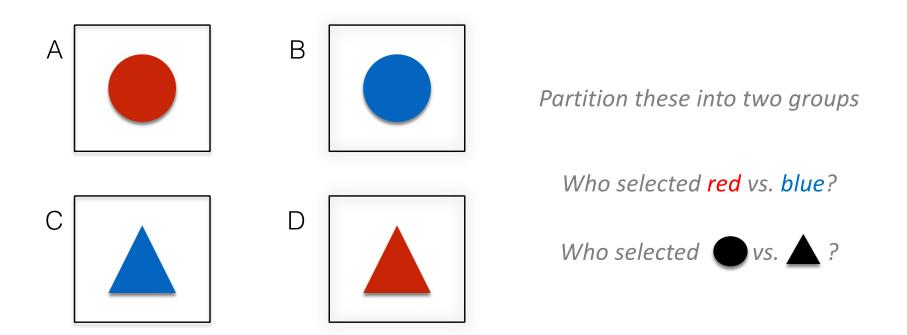
General ML Consideration: Inductive Bias



General ML Consideration: Inductive Bias

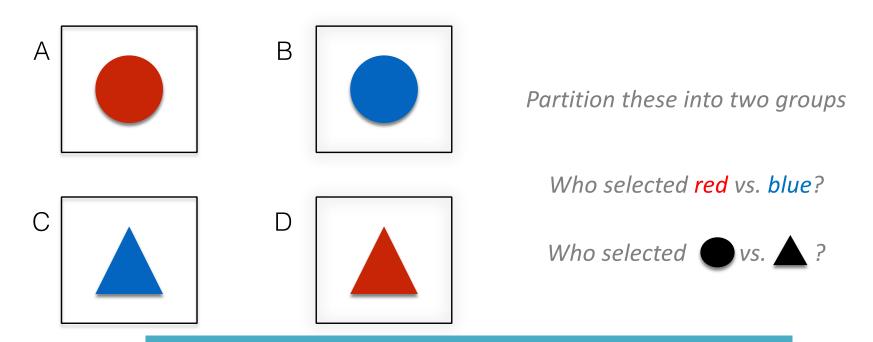


General ML Consideration: Inductive Bias



General ML Consideration: Inductive Bias

What do we know *before* we see the data, and how does that influence our modeling decisions?



Tip: Remember how your own biases/interpretation are influencing your approach

Today's Goals:

1. Remember Probability/Statistics

2.Understand Optimizing Empirical Risk

Outline

Review+Extension

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Decision Theory

Loss Functions

Probability Prerequisites

Basic probability axioms and definitions

Bayes rule

Joint probability

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Common distributions

Marginal probability

Expected Value (of a function) of a Random Variable

Definition of conditional probability

(Most) Probability Axioms

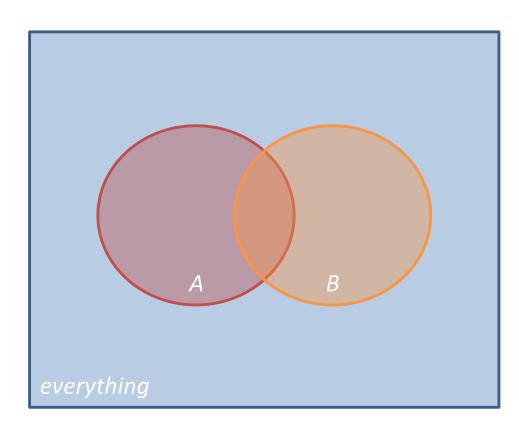
p(everything) = 1

$$p(\phi) = 0$$

 $p(A) \le p(B)$, when $A \subseteq B$

$$p(A \cup B) = p(A) + p(B),$$

when $A \cap B = \phi$



$$p(A \cup B) \neq p(A) + p(B)$$
$$p(A \cup B) = p(A) + p(B) - p(A \cap B)$$

Random variables: variables that represent the possible outcomes of some random "process"

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Example #1: A (weighted) coin that can come up heads or tails

X is a random variable denoting the possible outcomes

X=HEADS or X=TAILS

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Example #2: Measuring the amount of snow that fell in the last storm

Y is a random variable denoting the amount snow that fell, in inches

Y=0, or Y=0.5, or Y=1.0495928591, or Y=10, or ...

Random variables: variables that represent the possible outcomes of some random "process"

Example #1: A (weighted) coin that can come up heads or tails

X is a random variable denoting the possible outcomes

X=HEADS or X=TAILS

DISCRETE random variable

Example #2: Measuring the amount of snow that fell in the last storm

Y is a random variable denoting the amount snow that fell, in inches

Y=0, or Y=0.5, or Y=1.0495928591, or Y=10, or ...

CONTINUOUS random variable

	If X is a	
	Discrete random variable	Continuous random variable
The values k that X can take	Discrete: finite or countably	Continuous: uncountably
are	infinite (e.g., integers)	infinite (e.g., real values)

	If X is a	
	Discrete random variable	Continuous random variable
The values k that X can take are	Discrete: finite or countably infinite (e.g., integers)	Continuous: uncountably infinite (e.g., real values)
The function that gives the relative likelihood of a value p(X=k) is a	probability mass function (PMF)	probability density function (PDF)

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The values that PMF/PDF can take are	$0 \le p(X=k) \le 1$	$p(X=k) \ge 0$

	If X is a	
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We "add" with	Sums (∑)	Integrals (∫)

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The values that PMF/PDF can take are	$0 \le p(X=k) \le 1$	p(X=k) ≥ 0
We "add" with	Sums (∑)	Integrals (∫)
Our PMF/PDF satisfies p(everything)=1 by	$\sum_{k} p(X = k) = 1$	$\int p(x)dx = 1$

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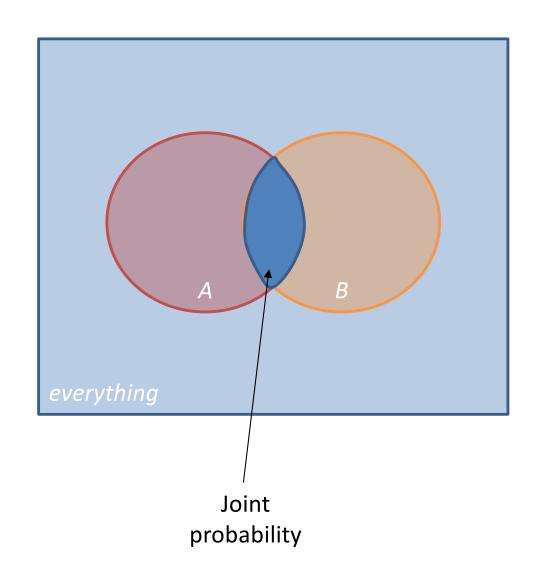
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Joint Probability

Probability that multiple things "happen together"

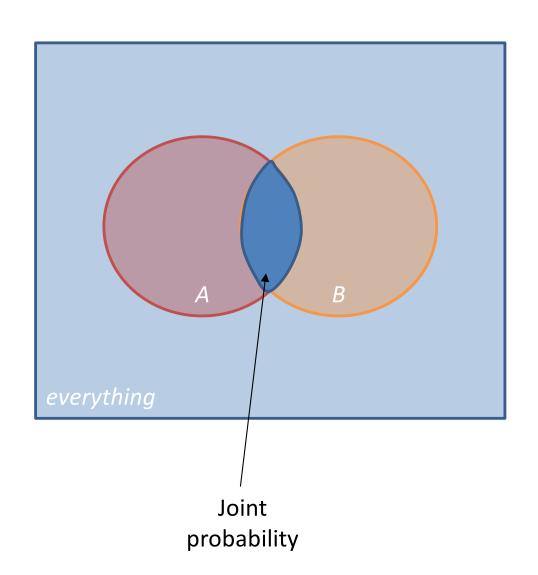


Joint Probability

Probability that multiple things "happen together"

p(x,y), p(x,y,z), p(x,y,w,z)

Symmetric: p(x,y) = p(y,x)



Joint Probability

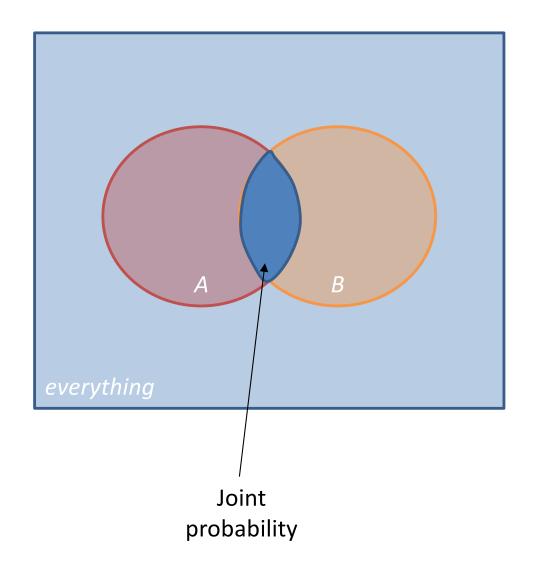
Probability that multiple things "happen together"

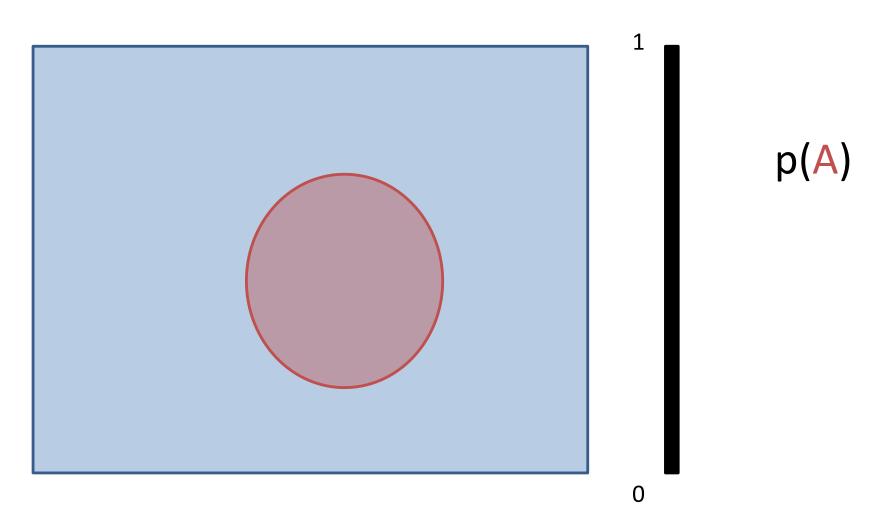
$$p(x,y)$$
, $p(x,y,z)$, $p(x,y,w,z)$

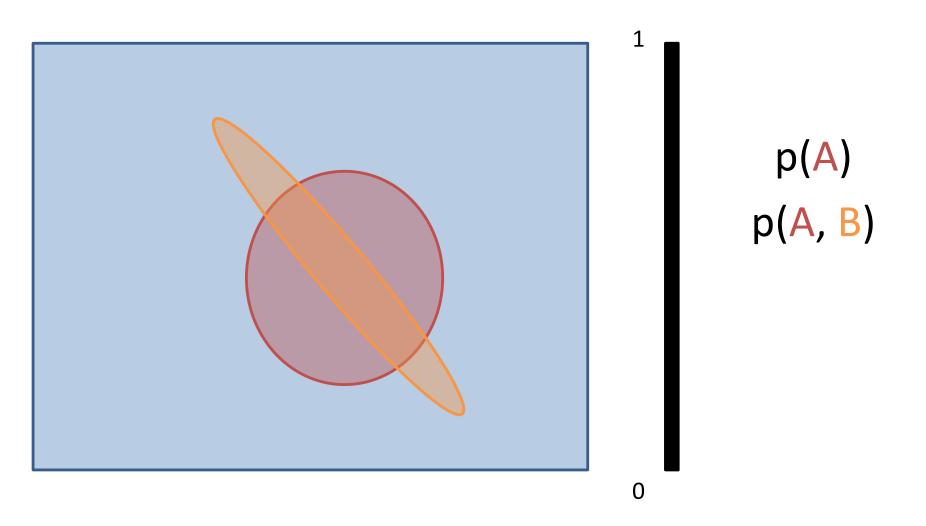
Symmetric: p(x,y) = p(y,x)

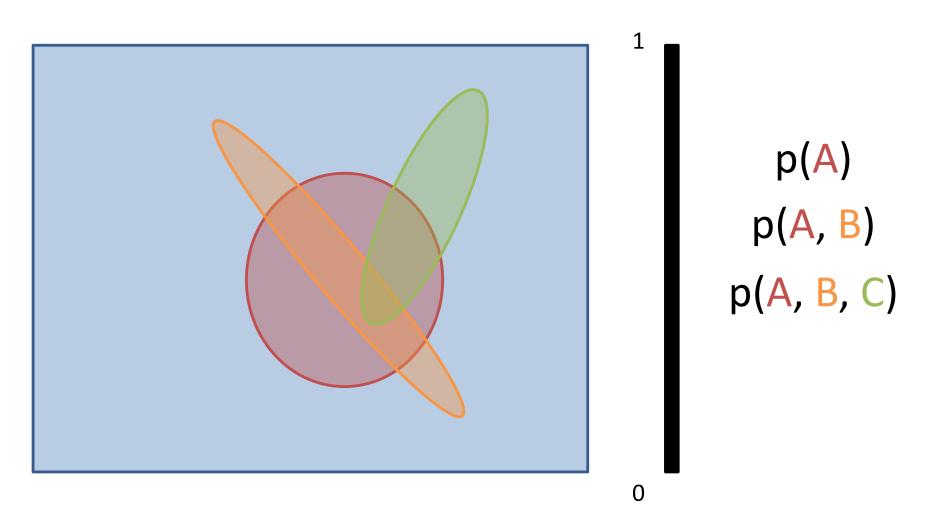
Form a table based of outcomes: sum across cells = 1

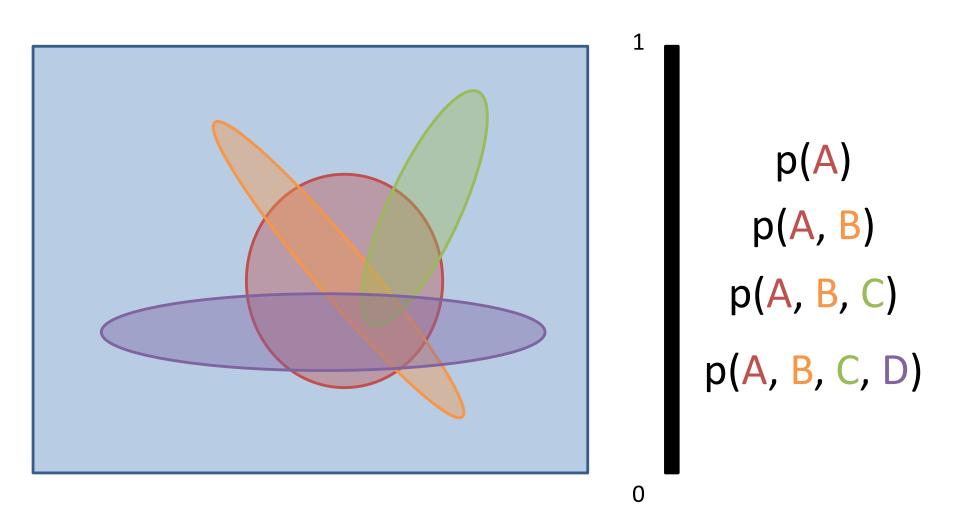
p(x,y)	Y=0	Y=1
X="cat"	.04	.32
X="dog"	.2	.04
X="bird"	.1	.1
X="human"	.1	.1

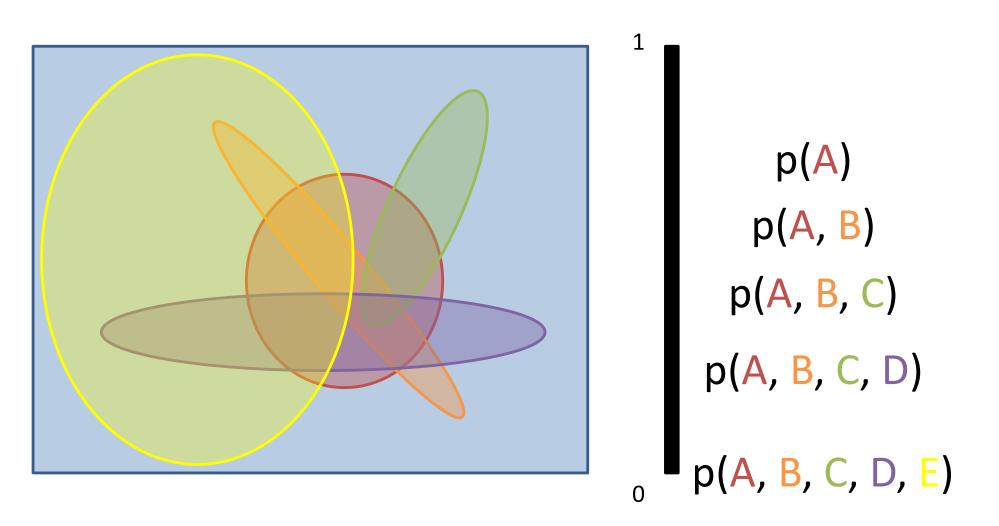












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Independence: when events can occur and not impact the probability of other events

Q: Are the results of flipping the same coin twice in succession independent?

Formally: p(x,y) = p(x)*p(y)

Generalizable to > 2 random variables

Independence: when events can occur and not impact the probability of other events

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Formally: p(x,y) = p(x)*p(y)

A: Yes (assuming no weird effects)

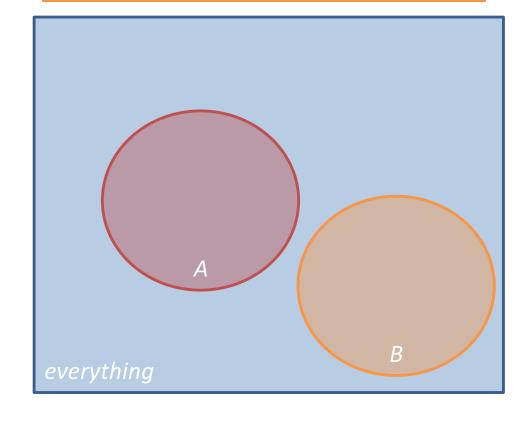
Generalizable to > 2 random variables

Independence: when events can occur and not impact the probability of other events

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Q: Are A and B independent?

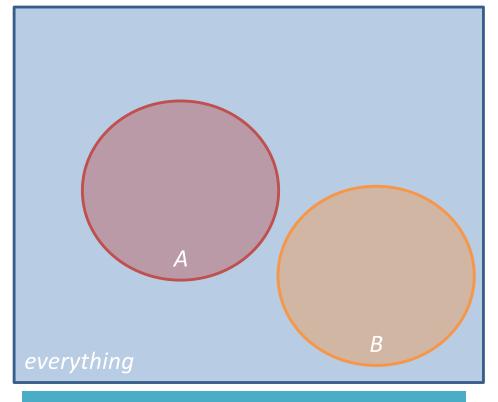


Independence: when events can occur and not impact the probability of other events

Formally: p(x,y) = p(x)*p(y)

Generalizable to > 2 random variables

Q: Are A and B independent?



A: No (work it out from p(A,B)) and the axioms

Independence: when events can occur and not impact the probability of other events

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Generalizable to > 2 random variables

Q: Are X and Y independent?

p(x,y)	Y=0	Y=1
X="cat"	.04	.32
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X="cat"	.04	.32
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A: No (find the marginal probabilities of p(x) and p(y))

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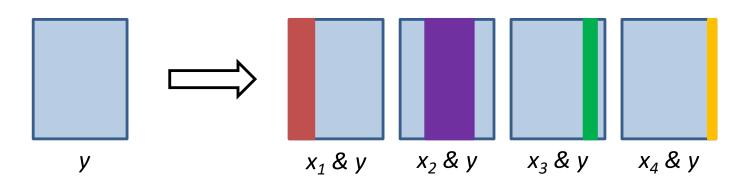
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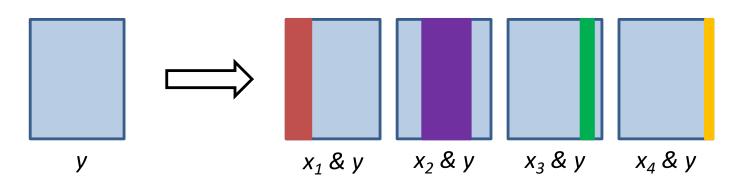
Marginal(ized) Probability: The Discrete Case



Consider the **mutually exclusive** ways that different values of x could occur with y

Q: How do write this in terms of joint probabilities?

Marginal(ized) Probability: The Discrete Case



Consider the **mutually exclusive** ways that different values of x could occur with y

$$p(y) = \sum_{x} p(x, y)$$

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Conditional Probability

$$p(X \mid Y) = \frac{p(X,Y)}{p(Y)}$$

Conditional Probabilities are Probabilities

Conditional Probability

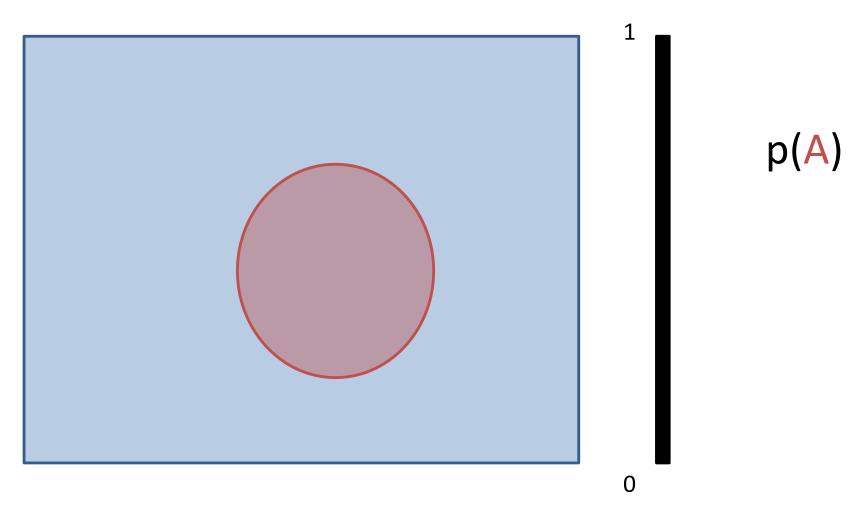
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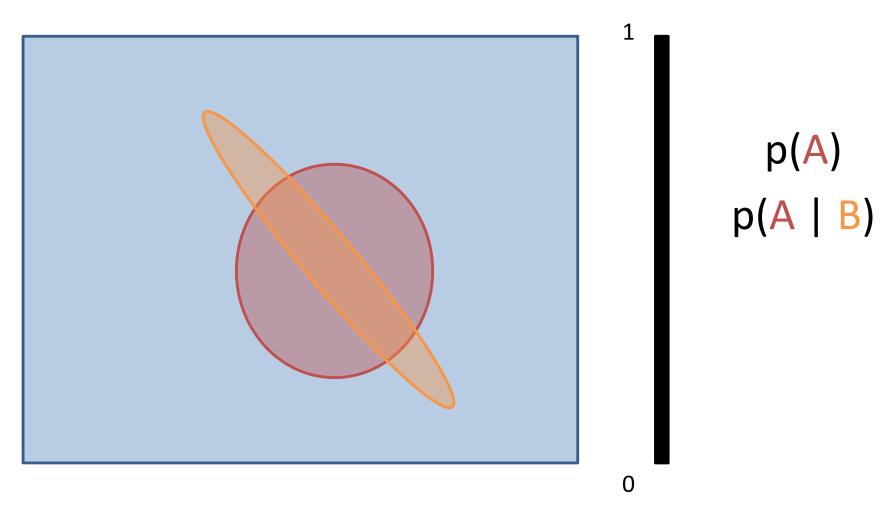
$$p(Y) = marginal probability of Y$$

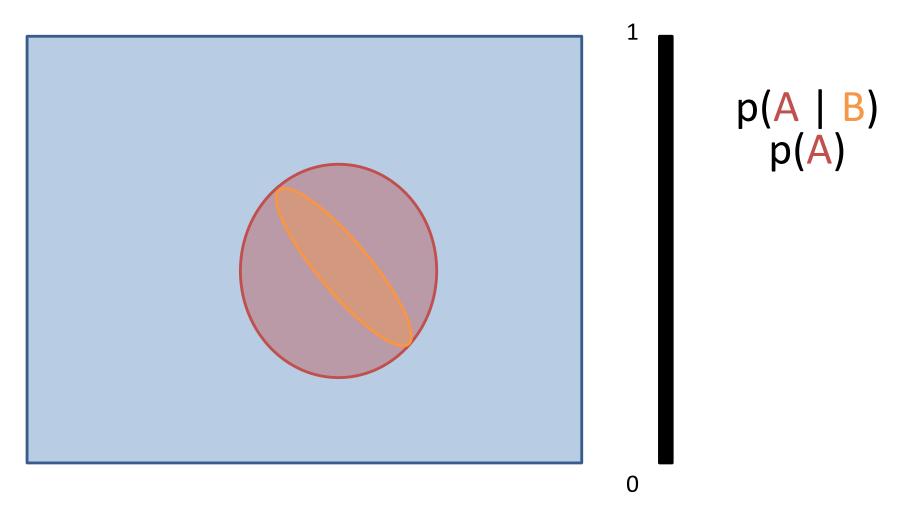
Conditional Probability

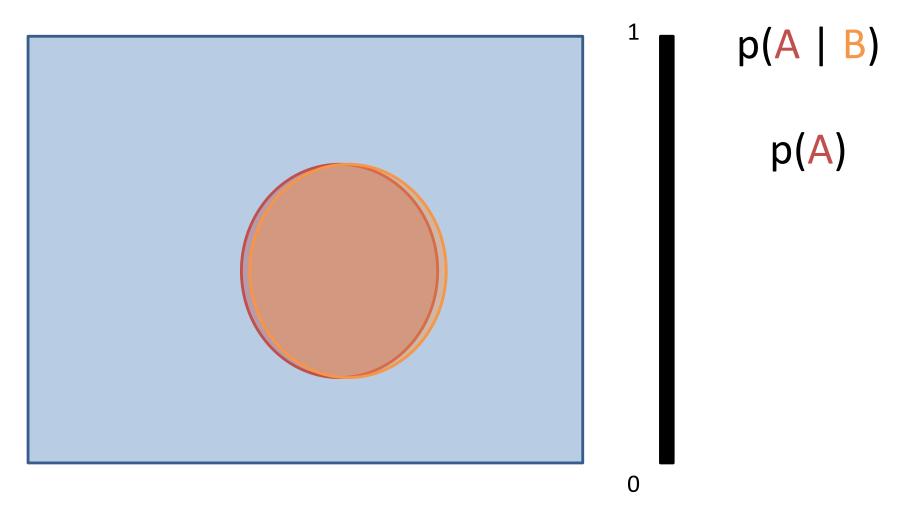
$$p(X \mid Y) = \frac{p(X,Y)}{p(Y)}$$

$$p(Y) = \int p(X,Y)dX$$

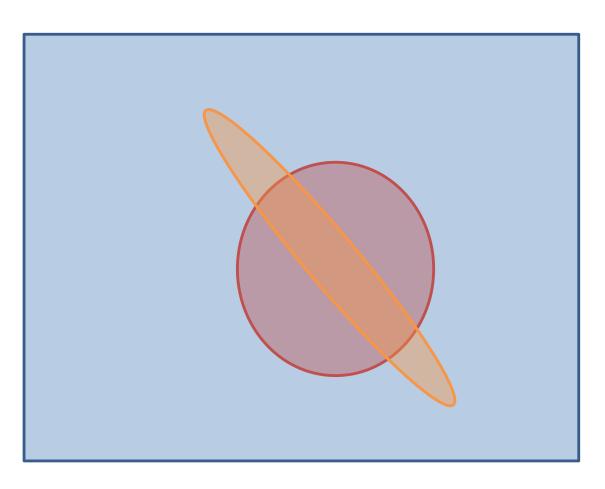








Conditional Probabilities

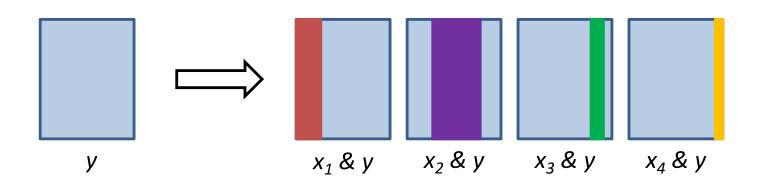


Bias vs. Variance

Lower bias: More specific to what we care about

Higher variance: For fixed observations, estimates become less reliable

Revisiting Marginal Probability: The Discrete Case



$$p(y) = \sum_{x} p(x,y)$$
$$= \sum_{x} p(x)p(y \mid x)$$

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Deriving Bayes Rule

Start with conditional p(X | Y)

Deriving Bayes Rule

$$p(X \mid Y) = \frac{p(X,Y)}{p(Y)}$$
 Solve for p(x,y)

Deriving Bayes Rule

$$p(X \mid Y) = \frac{p(X,Y)}{p(Y)}$$
 Solve for p(x,y)

$$p(X,Y) = p(X \mid Y)p(Y)$$
 p(x,y) = p(y,x)

$$p(X \mid Y) = \frac{p(Y \mid X) * p(X)}{p(Y)}$$

Bayes Rule

$$p(X \mid Y) = \frac{p(Y \mid X) * p(X)}{p(Y \mid X)}$$

posterior probability

prior probability

 $p(Y \mid X) * p(X)$

posterior probability

marginal likelihood
(probability)

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Probability Chain Rule

$$p(x_{1}, x_{2}, ..., x_{S}) =$$

$$p(x_{1})p(x_{2} | x_{1})p(x_{3} | x_{1}, x_{2}) \cdots p(x_{S} | x_{1}, ..., x_{i}) =$$

$$\prod_{i}^{S} p(x_{i} | x_{1}, ..., x_{i-1})$$
extension of Bayes rule

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Distribution Notation

If X is a R.V. and G is a distribution:

• $X \sim G$ means X is distributed according to ("sampled from") G

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- $X \sim G$ means X is distributed according to ("sampled from") G
- G often has parameters $\rho=(\rho_1,\rho_2,\dots,\rho_M)$ that govern its "shape"
- Formally written as $X \sim G(\rho)$

Distribution Notation

If X is a R.V. and G is a distribution:

- X ~ G means X is distributed according to ("sampled from") G
- G often has parameters $\rho=(\rho_1,\rho_2,\ldots,\rho_M)$ that govern its "shape"
- Formally written as $X \sim G(\rho)$

i.i.d. If $X_1, X_2, ..., X_N$ are all independently sampled from $G(\rho)$, they are independently and identically distributed

Bernoulli/Binomial

Categorical/Multinomial

Poisson

Normal

(Gamma)

Bernoulli: A single draw

- Binary R.V.: 0 (failure) or 1 (success)
- $X \sim \text{Bernoulli}(\rho)$
- $p(X = 1) = \rho, p(X = 0) = 1 \rho$
- Generally, $p(X = k) = \rho^k (1 p)^{1-k}$

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Binomial: Sum of N iid Bernoulli draws

- Values X can take: 0, 1, ..., N
- Represents number of successes
- $X \sim \text{Binomial}(N, \rho)$

•
$$p(X = k) = \binom{N}{k} \rho^k (1 - \rho)^{N-k}$$

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Categorical: A single draw

- Finite R.V. taking one of K values: 1, 2, ..., K
- $X \sim \operatorname{Cat}(\rho), \rho \in \mathbb{R}^K$
- $p(X = 1) = \rho_1, p(X = 2) = \rho_2, ... p(X = K) = \rho_K$
- Generally, $p(X = k) = \prod_j \rho_j^{\mathbf{1}[k=j]}$
- $1[c] = \begin{cases} 1, & c \text{ is true} \\ 0, & c \text{ is false} \end{cases}$

Multinomial: Sum of N iid Categorical draws

- Vector of size K representing how often value k was drawn
- $X \sim \text{Multinomial}(N, \rho), \rho \in \mathbb{R}^K$

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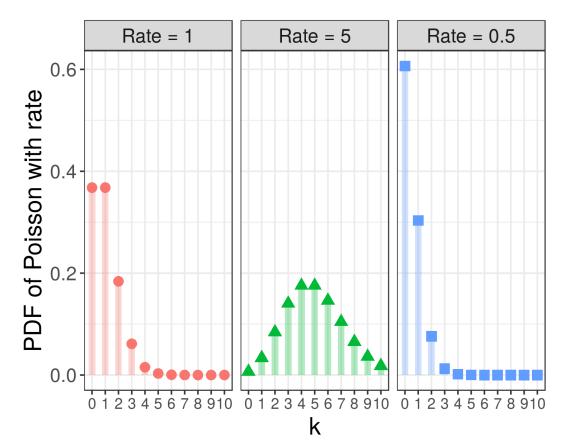
Normal

(Gamma)

Poisson

- Finite R.V. taking any integer that is >= 0
- $X \sim \text{Poisson}(\lambda), \lambda \in \mathbb{R}$ is the "rate"

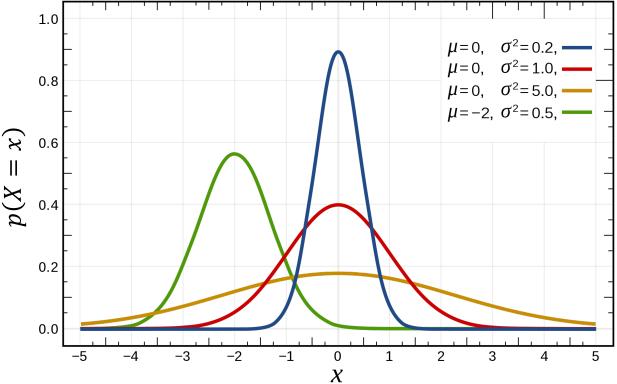
•
$$p(X = k) = \frac{\lambda^k \exp(-\lambda)}{k!}$$



Normal

- Real R.V. taking any real number
- $X \sim \text{Normal}(\mu, \sigma), \mu$ is the mean, σ is the standard deviation

•
$$p(X = x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(\frac{-(x-\mu)^2}{2\sigma^2})$$



https://upload.wikimedia.org/wikipedia/commons/thumb/7/74/Normal_Distribution_PDF.svg/192 0px-Normal_Distribution_PDF.svg.png

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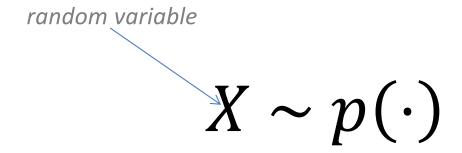
Common distributions

Marginal probability

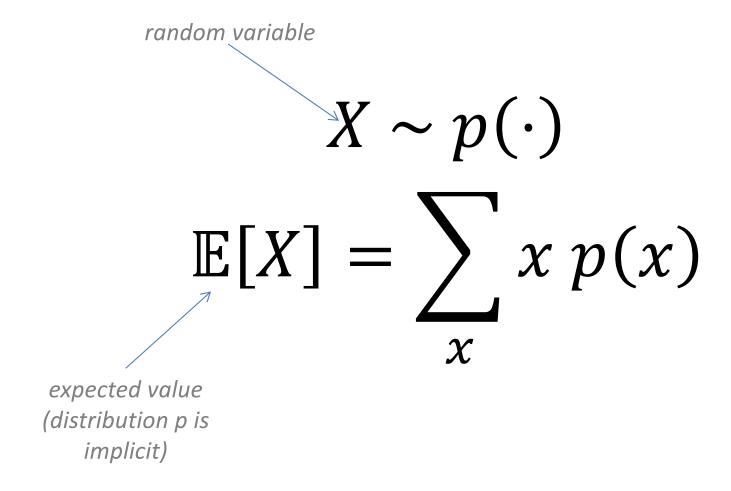
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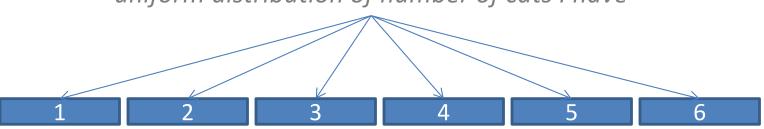
Expected Value of a Random Variable



Expected Value of a Random Variable



uniform distribution of number of cats I have



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

$$1/6 * 1 +$$

$$1/6 * 2 +$$

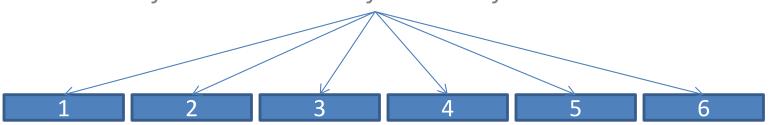
$$1/6 * 3 +$$

$$1/6 * 4 +$$

$$1/6 * 5 +$$

$$1/6 * 6$$

uniform distribution of number of cats I have



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

$$1/6 * 1 +$$

$$1/6 * 2 +$$

$$1/6 * 3 +$$

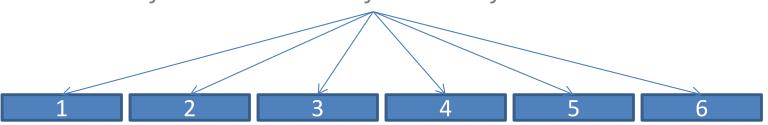
$$1/6 * 4 +$$

$$1/6 * 5 +$$

$$1/6 * 6$$

Q: What common distribution is this?

uniform distribution of number of cats I have



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

$$1/6 * 1 +$$

$$1/6 * 2 +$$

$$1/6 * 3 +$$

$$1/6 * 4 +$$

$$1/6 * 5 +$$

$$1/6 * 6$$

Q: What common distribution is this?

A: Categorical

non-uniform distribution of number of cats a normal cat person has

1 2 3 4 5 6

$$\mathbb{E}[X] = \sum_{x} x \, p(x)$$

$$1/2 * 1 + 1/10 * 2 + 1/10 * 3 + 1/10 * 4 + 1/10 * 5 + 1/10 * 6$$

Expected Value of a Function of a Random Variable

$$X \sim p(\cdot)$$

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

$$\mathbb{E}[f(X)] = ???$$

Expected Value of a Function of a Random Variable

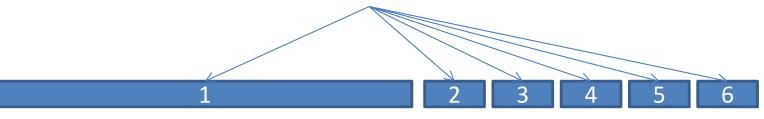
$$X \sim p(\cdot)$$

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

$$\mathbb{E}[f(X)] = \sum_{x} f(x) p(x)$$

Expected Value of Function: Example

non-uniform distribution of number of cats I start with



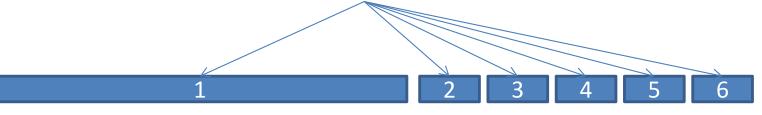
What if each cat magically becomes two?

$$f(k) = 2^k$$

$$\mathbb{E}[f(X)] = \sum_{x} f(x) p(x)$$

Expected Value of Function: Example

non-uniform distribution of number of cats I start with



What if each cat magically becomes two?

$$f(k) = 2^k$$

$$\mathbb{E}[f(X)] = \sum_{x} f(x) p(x) = \sum_{x} 2^{x} p(x)$$

$$1/2 * 2^{1} +$$
 $1/10 * 2^{2} +$
 $1/10 * 2^{3} +$
 $1/10 * 2^{4} +$
 $1/10 * 2^{5} +$
 $1/10 * 2^{6}$

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"Decision theory is trivial, apart from the computational details" – MacKay, ITILA, Ch 36

Input: x ("state of the world")

Output: a decision ŷ

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Output: a decision ŷ

Requirement 1: a decision (hypothesis) function h(x) to produce ŷ

"Decision theory is trivial, apart from the computational details" – MacKay, ITILA, Ch 36

Input: x ("state of the world")

Output: a decision ŷ

Requirement 1: a decision (hypothesis) function h(x) to produce ŷ

Requirement 2: a function $\ell(y, \hat{y})$ telling us how wrong we are

"Decision theory is trivial, apart from the computational details" – MacKay, ITILA, Ch 36

Input: x ("state of the world")

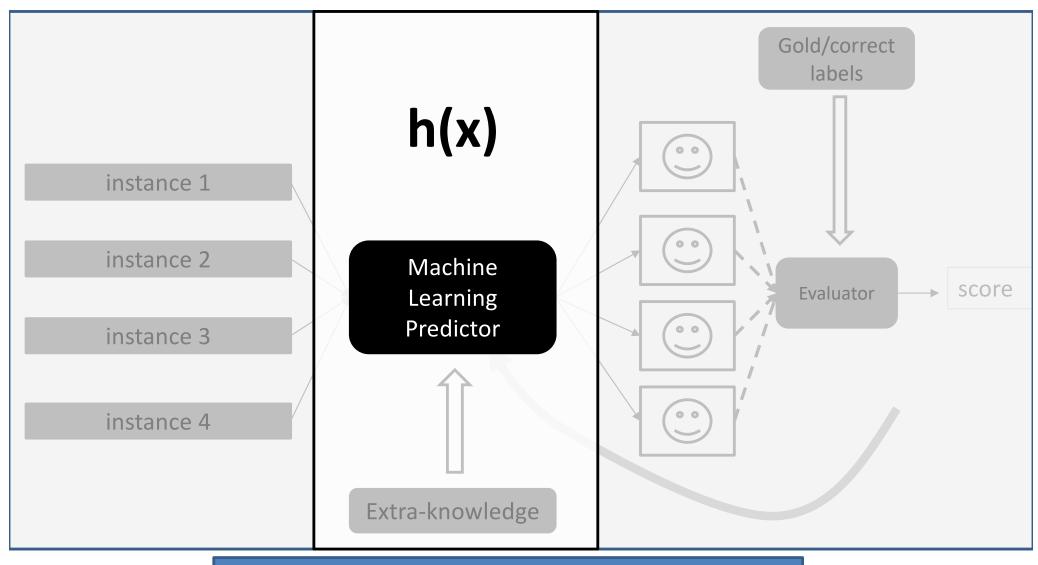
Output: a decision ŷ

Requirement 1: a decision (hypothesis) function h(x) to produce ŷ

Requirement 2: a loss function $\ell(y, \hat{y})$ telling us how wrong we are

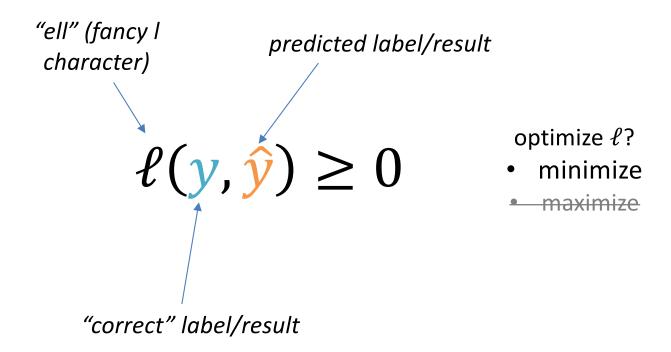
Goal: minimize our *expected* loss across any possible input

Requirement 1: Decision Function



h(x) is our predictor (classifier, regression model, clustering model, etc.)

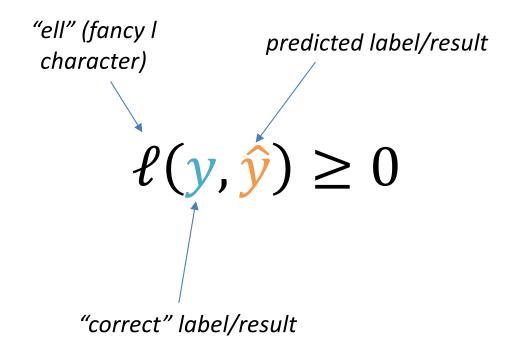
Requirement 2: Loss Function



loss: A function that tells you how much to penalize a prediction ŷ from the correct answer y

Requirement 2: Loss Function

Negative ℓ ($-\ell$) is called a *utility* or *reward* function



loss: A function that tells you how much to penalize a prediction ŷ from the correct answer y

minimize expected loss across any possible input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y,\hat{y})]$$

Risk Minimization

minimize expected loss across any possible input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y, \hat{y})] = \arg\min_{h} \mathbb{E}[\ell(y, h(x))]$$

a *particular*, unspecified input pair (**x**,y)... but we want any possible pair

minimize expected loss across any possible input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y, \hat{y})] = \arg\min_{h} \mathbb{E}[\ell(y, h(x))] = \arg\min_{h} \mathbb{E}_{(x,y)\sim P}[\ell(y, h(x))]$$

Assumption: there exists *some* true (but likely unknown) distribution *P* over inputs **x** and outputs **y**

Risk Minimization

minimize expected loss across any possible input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y,\hat{y})] =$$

$$\arg\min_{h} \mathbb{E}[\ell(y,h(x))] =$$

$$\arg\min_{h} \mathbb{E}_{(x,y)\sim P}[\ell(y,h(x))] =$$

$$\arg\min_{h} \int \ell(y,h(x))P(x,y)d(x,y)$$

Risk Minimization

minimize expected loss across any possible input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y, \hat{y})] =$$

$$\arg\min_{h} \mathbb{E}[\ell(y, h(x))] =$$

$$\underset{h}{\operatorname{argmin}} \mathbb{E}_{(x,y)\sim P} [\ell(y,h(x))] =$$

$$\underset{h}{\operatorname{argmin}} \int \ell(y, h(x)) P(x, y) d(x, y)$$

we don't know this distribution*!

Empirical Risk Minimization

minimize expected loss across our observed input

$$\arg\min_{\hat{y}} \mathbb{E}[\ell(y, \hat{y})] =$$

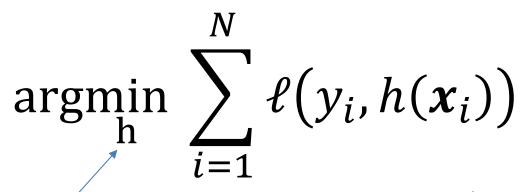
$$\arg\min_{h} \mathbb{E}[\ell(y, h(x))] =$$

$$\arg\min_{h} \mathbb{E}_{(x,y)\sim P}[\ell(y, h(x))] \approx$$

$$\underset{h}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, h(x_i))$$

Empirical Risk Minimization

minimize expected loss across our observed input



our classifier/predictor

controlled by our parameters θ

change $\theta \rightarrow$ change the behavior of the classifier

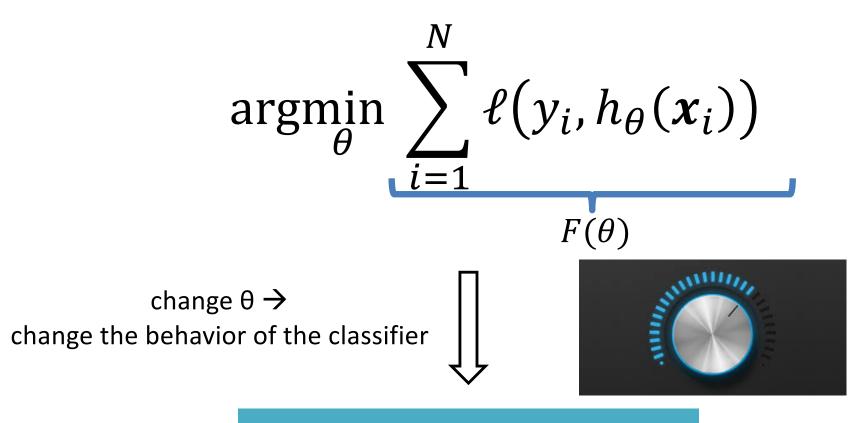


$$\underset{h}{\operatorname{argmin}} \sum_{i=1}^{N} \ell(y_i, h_{\theta}(x_i))$$

change $\theta \rightarrow$ change the behavior of the classifier



$$\underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{N} \ell(y_i, h_{\theta}(x_i))$$



How? Use Gradient Descent on $F(\theta)$!

$$\underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{N} \ell(y_i, h_{\theta}(x_i))$$

change $\theta \rightarrow$ change the behavior of the classifier



$$\nabla_{\theta} F = \sum_{i} \frac{\partial \ell(y_{i}, \hat{y} = h_{\theta}(\boldsymbol{x}_{i}))}{\partial \hat{y}} \nabla_{\theta} h_{\theta}(\boldsymbol{x}_{i})$$

differentiating might not always work: "... apart from the computational details"

$$\underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{N} \ell(y_i, h_{\theta}(\boldsymbol{x}_i))$$

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Step 1: compute the gradient of the loss wrt the predicted value

$$\underset{\theta}{\operatorname{argmin}} \sum_{i=1}^{N} \ell(y_i, h_{\theta}(\boldsymbol{x}_i))$$

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$$\nabla_{\theta} F = \sum_{i} \frac{\partial \ell(y_{i}, \hat{y} = h_{\theta}(x_{i}))}{\partial \hat{y}} \nabla_{\theta} h_{\theta}(x_{i})$$
Step 2: compute

Step 1: compute the gradient of the loss wrt the predicted value

Step 2: compute the gradient of the predicted value wrt θ.

differentiating might not always work: "... apart from the computational details"

Outline

Review+Extension

Probability

Decision Theory

Loss Functions

Loss Functions Serve a Task

Classification

Regression

Clustering

the task: what kind of problem are you solving?

Fully-supervised

Semi-supervised

Un-supervised

the **data**: amount of human input/number of labeled examples

Probabilistic Neural

Generative Memorybased

Conditional

Exemplar

Spectral ...

the **approach**: how any data are being used

Classification: Supervised Machine Learning

Assigning subject categories, topics, or genres
Spam detection
Authorship identification

Age/gender identification
Language Identification
Sentiment analysis

. . .

Input:

an instance da fixed set of classes $C = \{c_1, c_2, ..., c_J\}$ A training set of m hand-labeled instances $(d_1, c_1), ..., (d_m, c_m)$

Output:

a learned classifier γ that maps instances to classes

y learns to associate certain *features* of instances with their labels

Classification Example: Face Recognition

Class	Image	Class	Image
Avrim		Tom	

$$\ell(y, \hat{y}) = \begin{cases} 0, & \text{if } y = \hat{y} \\ 1, & \text{if } y \neq \hat{y} \end{cases}$$

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Solution 1: is the data linearly separable? Perceptron (next class) can work

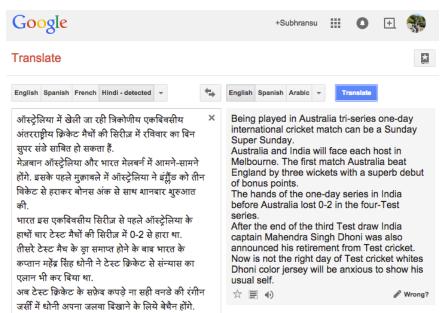
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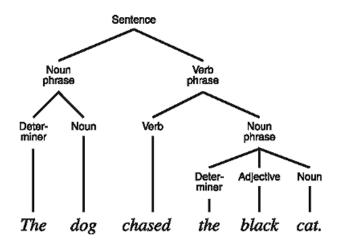
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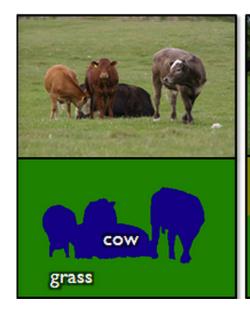
Solution 1: is the data linearly separable? Perceptron (next class) can work

Solution 2: is h(x) a conditional distribution $p(y \mid x)$? Maximize that probability (a couple classes)

Structured Classification: Sequence & Structured Prediction









Structured Classification Loss Function Example: 0-1 Loss?

$$\ell(y, \hat{y}) = \begin{cases} 0, & \text{if } y = \hat{y} \\ 1, & \text{if } y \neq \hat{y} \end{cases}$$

Problem 1: not differentiable wrt \hat{y} (or θ)

Solution 1: is the data linearly separable? Perceptron (next class) can work

Solution 2: is h(x) a conditional distribution $p(y \mid x)$? Use MAP

Problem 2: too strict.
Structured Prediction
involves many individual
decisions

Solution 1: Specialize 0-1 to the structured problem at hand

Regression

Like classification, but real-valued

Regression Example: Stock Market Prediction



Regression Loss Function Examples

squared loss/MSE (Mean squared error)

$$\ell(y, \hat{y}) = (y - \hat{y})^2$$

 \hat{y} is a real value \rightarrow nicely differentiable (generally) \odot

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absolute loss

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Absolute value is mostly differentiable

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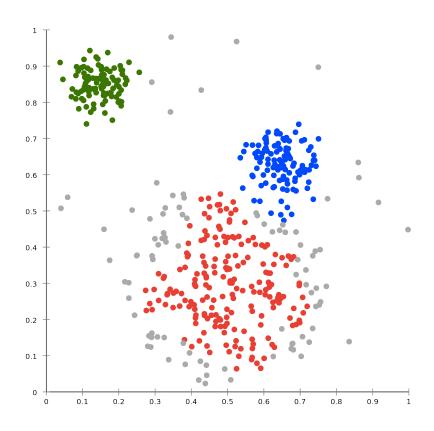
absolute loss

$$\ell(y, \hat{y}) = |y - \hat{y}|$$

Absolute value is mostly differentiable

These loss functions prefer different behavior in the predictions (hint: look at the gradient of each)... we'll get back to this

Unsupervised learning: Clustering



We'll return to clustering loss functions later

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