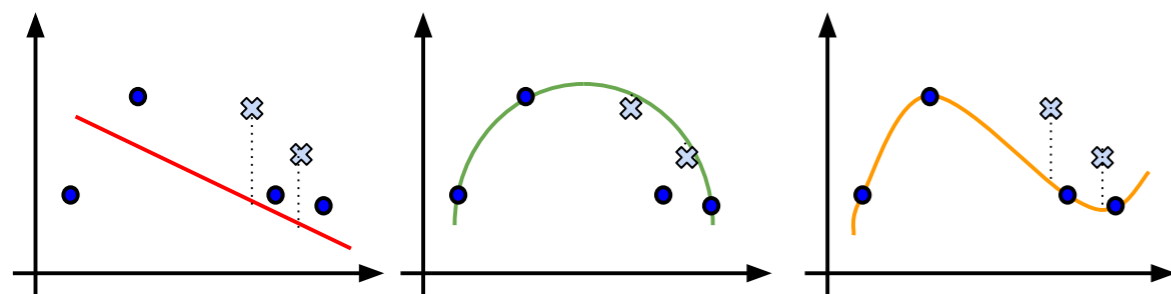
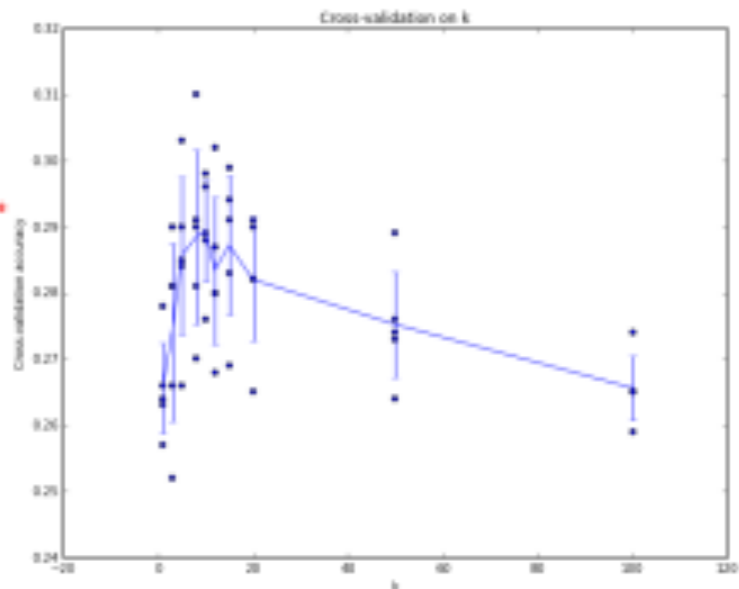
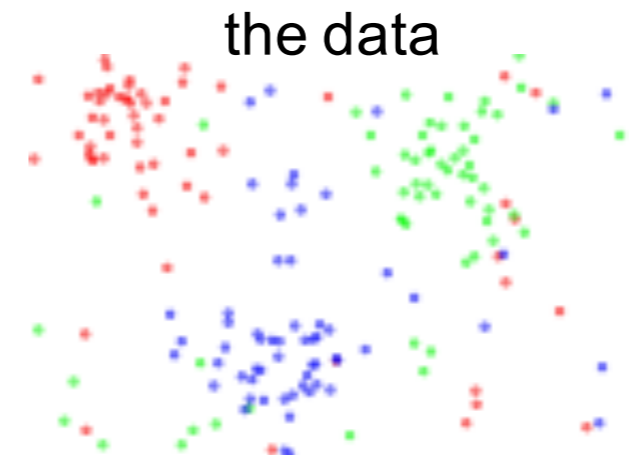
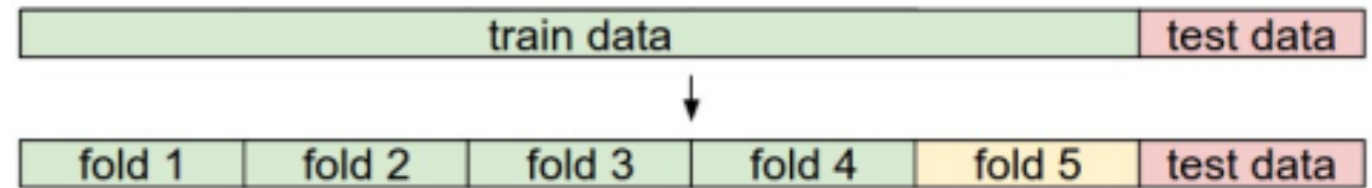
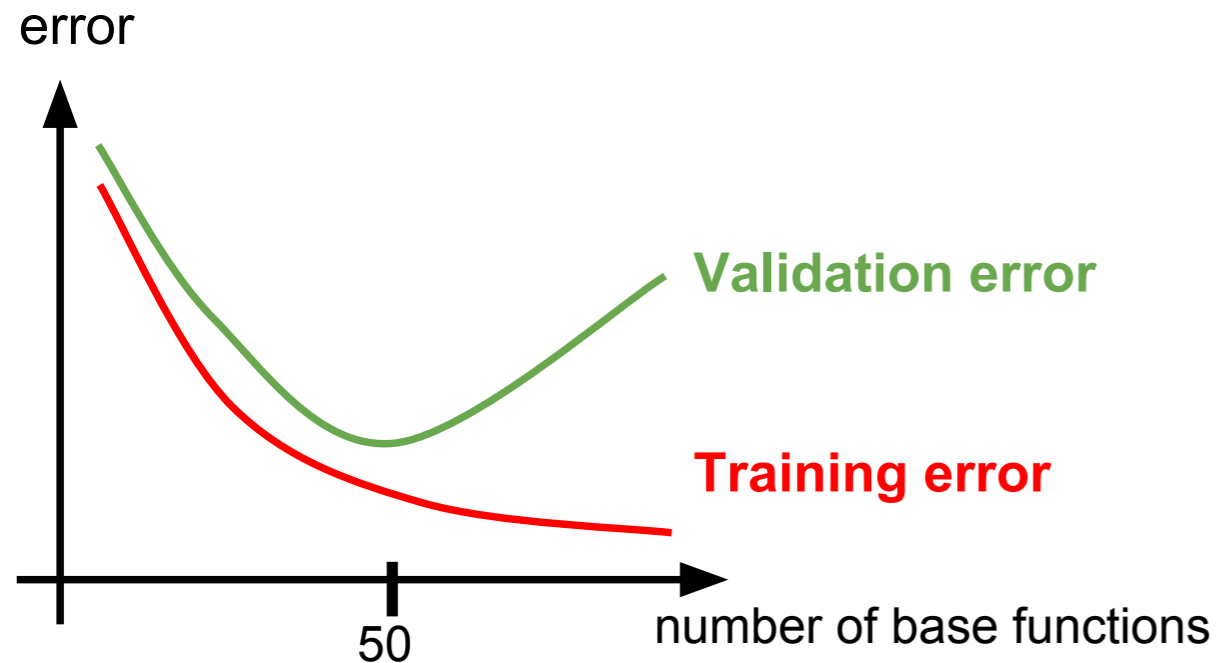


AIN311

Fundamentals of Machine Learning

Lecture 6:
Learning theory
Probability Review

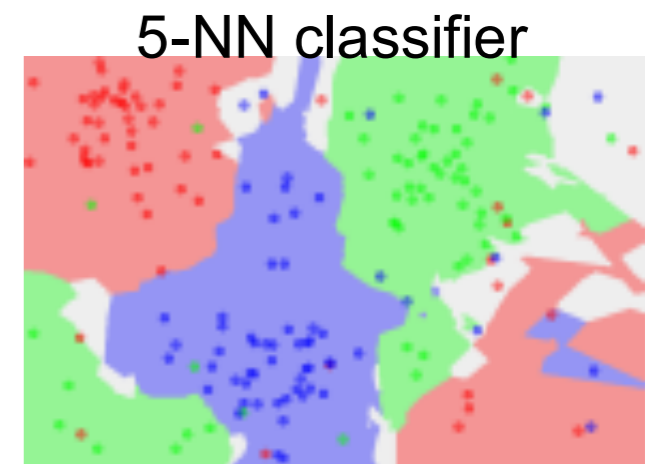
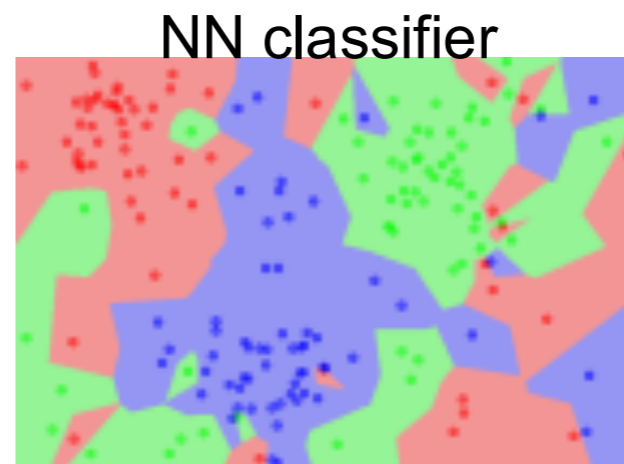
Last time... Regularization, Cross-Validation



- Underfitting**
- large training error
 - large validation error

- Just Right**
- small training error
 - small validation error

- Overfitting**
- small training error
 - large validation error



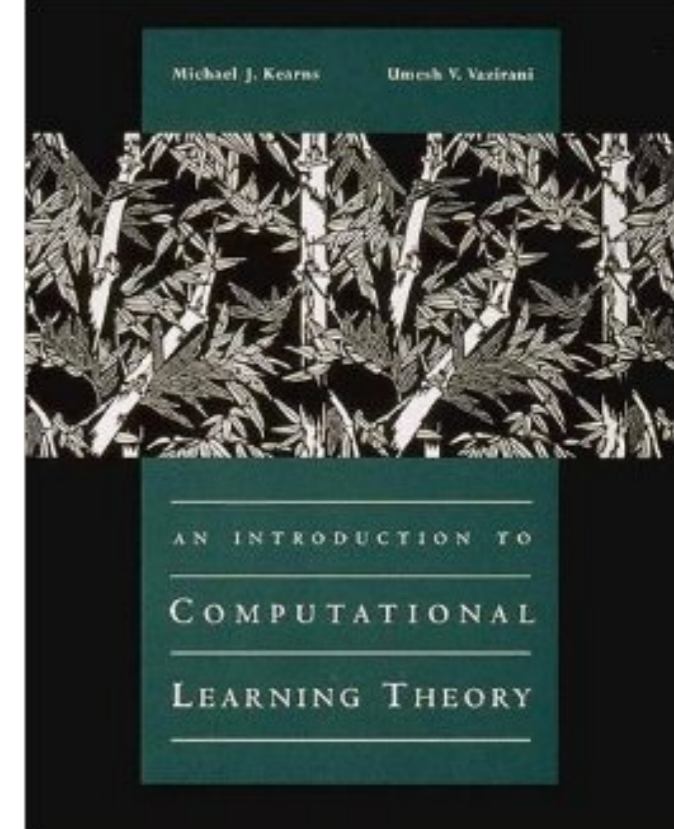
Today

- Learning Theory
- Probability Review

Learning Theory: Why ML Works

Computational Learning Theory

- Entire subfield devoted to the mathematical analysis of machine learning algorithms
- Has led to several practical methods:
 - PAC (probably approximately correct) learning
 - boosting
 - VC (Vapnik–Chervonenkis) theory
 - support vector machines



Annual conference: [Conference on Learning Theory \(COLT\)](#)

The Role of Theory

- Theory can serve two roles:
 - It can justify and help understand why common practice works.
theory after
 - It can also serve to suggest new algorithms and approaches that turn out to work well in practice.
theory before

Often, it turns out to be a mix!

The Role of Theory

- Practitioners discover something that works surprisingly well.
- Theorists figure out why it works and prove something about it.
 - In the process, they make it better or find new algorithms.
- Theory can also help you understand **what's possible and what's not possible.**

Learning and Inference

The inductive inference process:

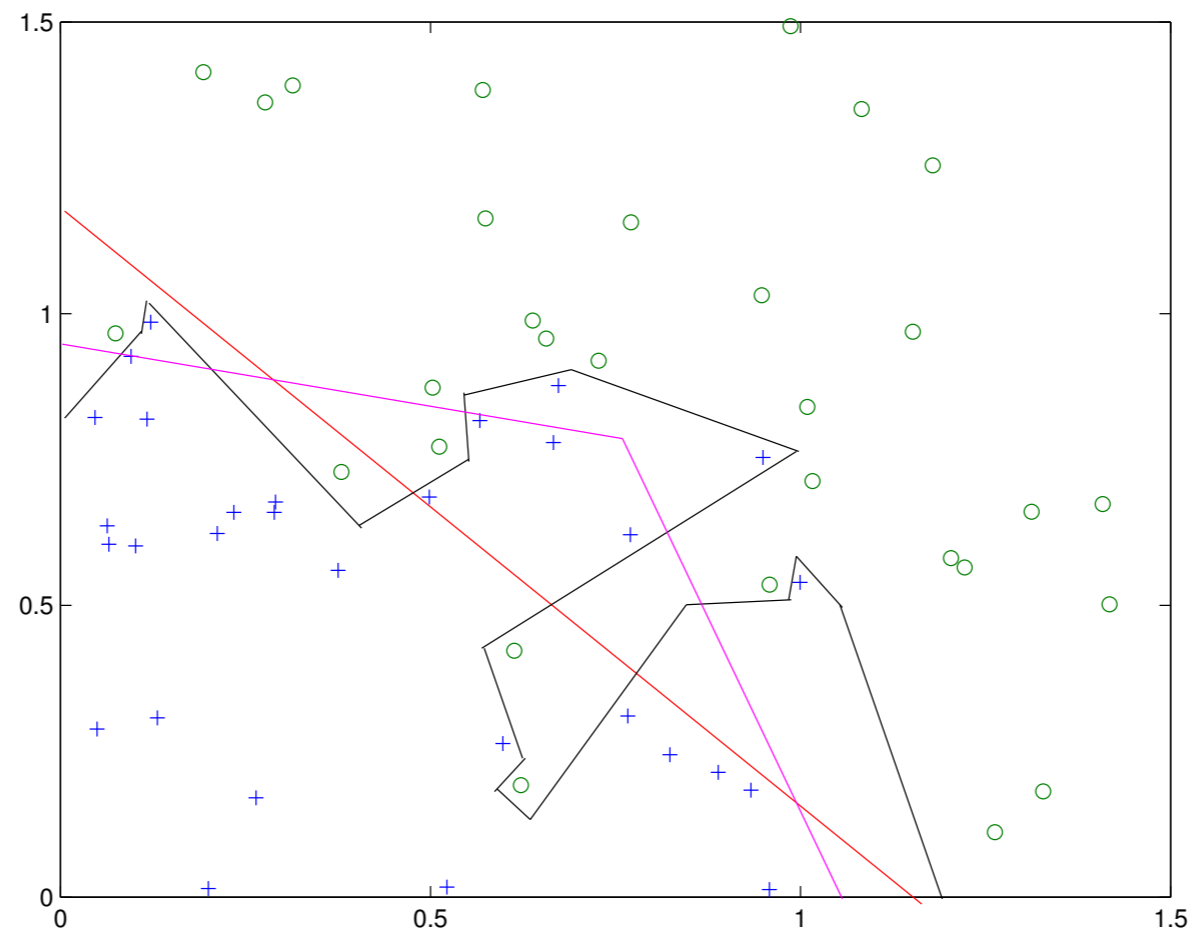
1. Observe a phenomenon
 2. Construct a model of the phenomenon
 3. Make predictions
- This is more or less the definition of natural sciences !
 - The goal of Machine Learning is to **automate** this process
 - The goal of Learning Theory is to **formalize** it.

Pattern recognition

- We consider here the **supervised learning** framework for pattern recognition:
 - Data consists of pairs (instance, label)
 - Label is +1 or -1
 - Algorithm constructs a function (instance \rightarrow label)
 - Goal: make few mistakes on future unseen instances

Approximation/Interpolation

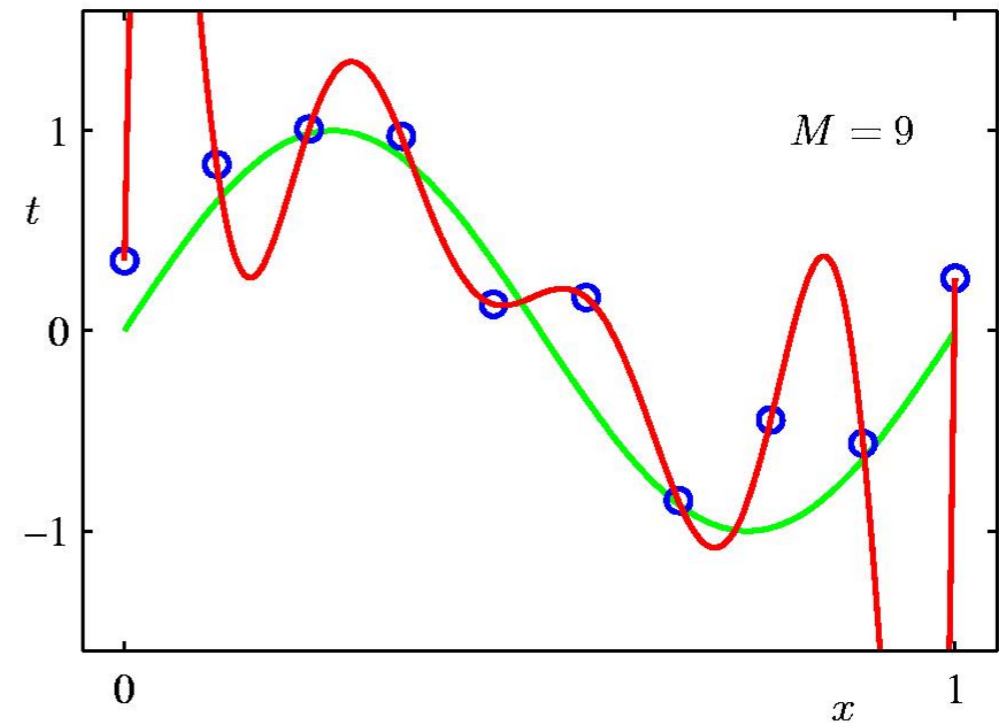
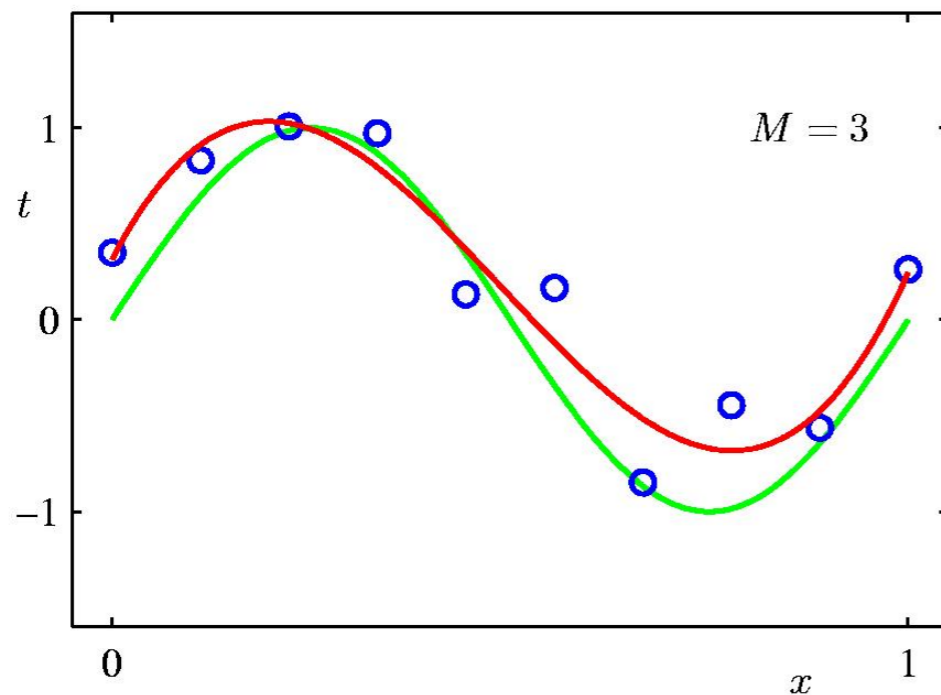
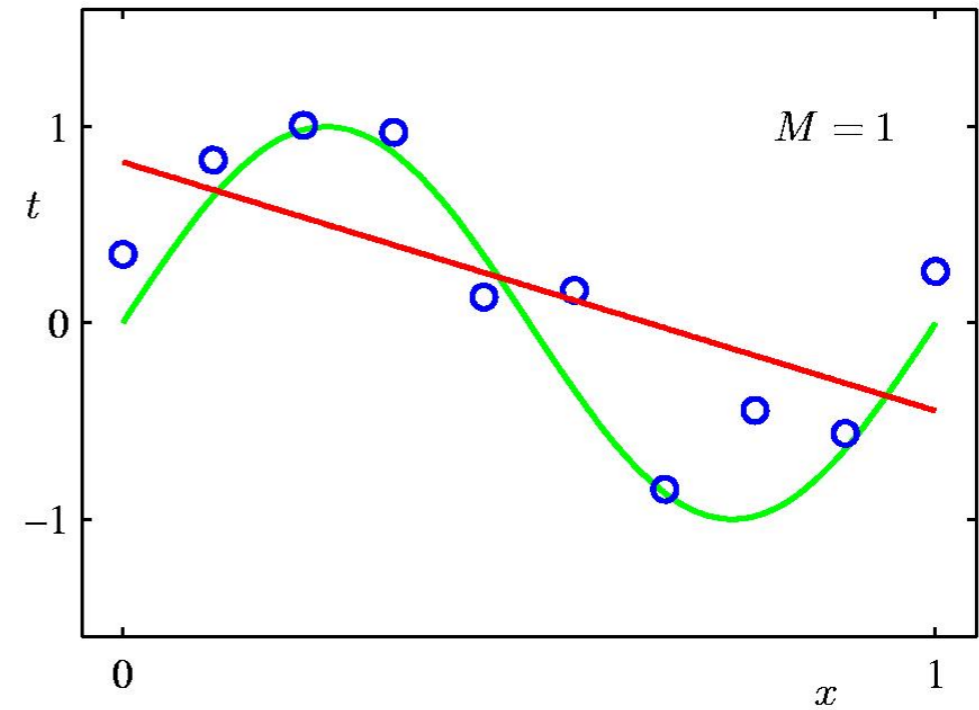
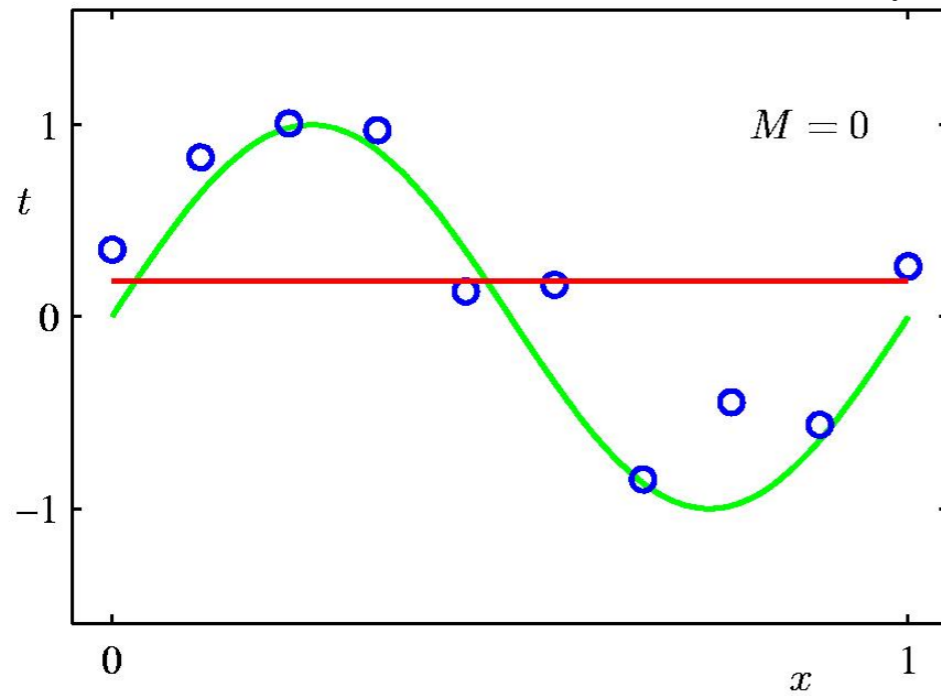
- It is always possible to build a function that fits exactly the data.



- But is it reasonable?

Which Fit is Best?

from Bishop



Occam's Razor

- Idea: look for **regularities** in the observed phenomenon

These can be **generalized** from the observed past to the future

⇒ choose the simplest consistent model

- How to measure simplicity ?
 - Physics: number of constants
 - Description length
 - Number of parameters
 - ...



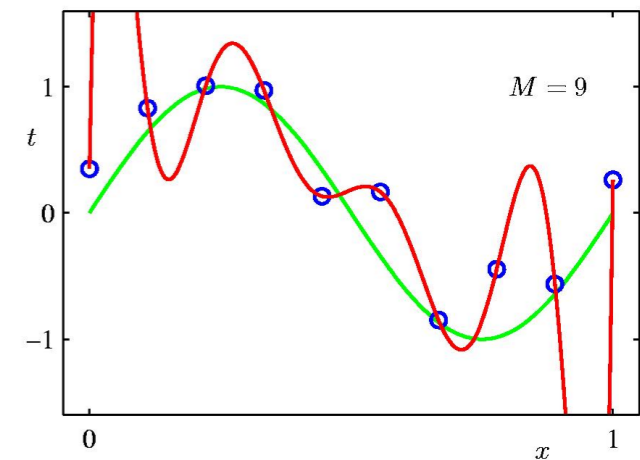
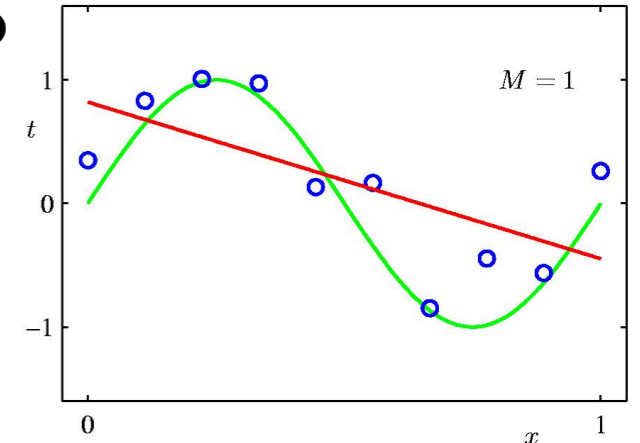
William of Occam
(c. 1288 – c. 1348)

No Free Lunch

- **No Free Lunch**
 - if there is no assumption on how the **past** is related to the future, prediction is impossible
 - if there is no **restriction** on the possible phenomena, generalization is impossible
- We need to make assumptions
- Simplicity is not absolute
- Data will never replace knowledge
- Generalization = data + knowledge

Recall from last week... Some key concepts

- Data fits – is linear model best (**model selection**)?
 - Simplest models do not capture all the important variations (signal) in the data: **underfit**
 - More complex model may **overfit** the training data (fit not only the signal but also the **noise** in the data), especially if not enough data to constrain model
- One method of assessing fit:
 - test **generalization** = model's ability to predict the held out data

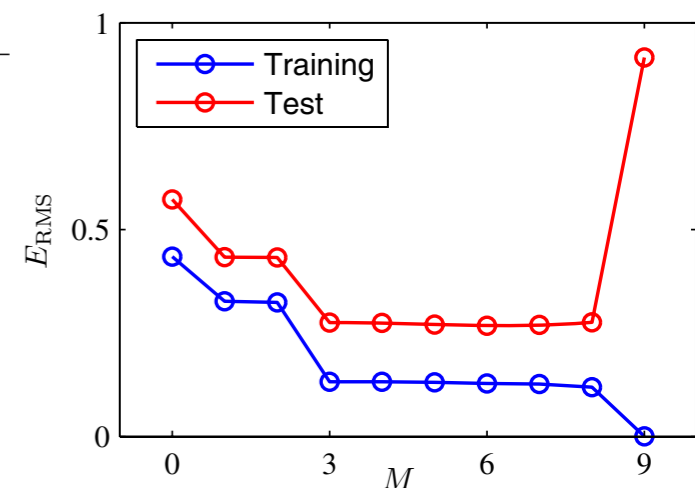


Regularization

$$\tilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

$$\|\mathbf{w}\|^2 \equiv \mathbf{w}^T \mathbf{w} = w_0^2 + w_1^2 + \dots + w_M^2$$

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
w_0^*	0.35	0.35	0.13
w_1^*	232.37	4.74	-0.05
w_2^*	-5321.83	-0.77	-0.06
w_3^*	48568.31	-31.97	-0.05
w_4^*	-231639.30	-3.89	-0.03
w_5^*	640042.26	55.28	-0.02
w_6^*	-1061800.52	41.32	-0.01
w_7^*	1042400.18	-45.95	-0.00
w_8^*	-557682.99	-91.53	0.00
w_9^*	125201.43	72.68	0.01



Probably Approximately Correct (PAC) Learning

- A formalism based on the realization that the best we can hope of an algorithm is that
 - It does a good job most of the time (**probably approximately correct**)

Probably Approximately Correct (PAC) Learning

- Consider a hypothetical learning algorithm
 - We have 10 different binary classification data sets.
 - For each one, it comes back with functions f_1, f_2, \dots, f_{10} .
 - ♦ For some reason, whenever you run f_4 on a test point, it crashes your computer. For the other learned functions, their performance on test data is always at most 5% error.
 - ♦ If this situation is guaranteed to happen, then this hypothetical learning algorithm is a PAC learning algorithm.
 - ❖ It satisfies **probably** because it only failed in one out of ten cases, and it's **approximate** because it achieved low, but non-zero, error on the remainder of the cases.

PAC Learning

Definitions 1. *An algorithm A is an (ϵ, δ) -PAC learning algorithm if, for all distributions \mathcal{D} : given samples from \mathcal{D} , the probability that it returns a “bad function” is at most δ ; where a “bad” function is one with test error rate more than ϵ on \mathcal{D} .*

PAC Learning

- Two notions of efficiency
 - **Computational complexity:** Prefer an algorithm that runs quickly to one that takes forever
 - **Sample complexity:** The number of examples required for your algorithm to achieve its goals

Definition: An algorithm \mathcal{A} is an **efficient (ϵ, δ) -PAC learning algorithm** if it is an (ϵ, δ) -PAC learning algorithm whose runtime is polynomial in $\frac{1}{\epsilon}$ and $\frac{1}{\delta}$.

In other words, to let your algorithm to achieve 4% error rather than 5%, the runtime required to do so should not go up by an exponential factor!

Example: PAC Learning of Conjunctions

- Data points are binary vectors, for instance $\mathbf{x} = \langle 0, 1, 1, 0, 1 \rangle$
- Some Boolean conjunction defines the true labeling of this data (e.g. $x_1 \wedge x_2 \wedge x_5$)
- There is some distribution \mathcal{D}_X over binary data points (vectors)
 $\mathbf{x} = \langle x_1, x_2, \dots, x_D \rangle$.
- There is a fixed concept conjunction c that we are trying to learn.
- There is no noise, so for any example x , its true label is simply $y = c(\mathbf{x})$

- **Example:**

- Clearly, the true formula cannot include the terms $x_1, x_2, \neg x_3, \neg x_4$

y	x_1	x_2	x_3	x_4
+1	0	0	1	1
+1	0	1	1	1
-1	1	1	0	1

Example: PAC Learning of Conjunctions

y	x_1	x_2	x_3	x_4
+1	0	0	1	1
+1	0	1	1	1
-1	1	1	0	1

$$f^0(\mathbf{x}) = x_1 \wedge \neg x_1 \wedge x_2 \wedge \neg x_2 \wedge x_3 \wedge \neg x_3 \wedge x_4 \wedge \neg x_4$$

$$f^1(\mathbf{x}) = \neg x_1 \wedge \neg x_2 \wedge x_3 \wedge x_4$$

$$f^2(\mathbf{x}) = \neg x_1 \wedge x_3 \wedge x_4$$

$$f^3(\mathbf{x}) = \neg x_1 \wedge x_3 \wedge x_4$$

- After processing an example, it is **guaranteed to classify that example correctly** (provided that there is no noise)
- **Computationally very efficient**
 - Given a data set of N examples in D dimensions, it takes $O(ND)$ time to process the data. This is linear in the size of the data set.

Algorithm 30 BINARYCONJUNCTIONTRAIN(D)

```

1:  $f \leftarrow x_1 \wedge \neg x_1 \wedge x_2 \wedge \neg x_2 \wedge \dots \wedge x_D \wedge \neg x_D$  // initialize function
2: for all positive examples  $(x, +1)$  in  $D$  do
3:   for  $d = 1 \dots D$  do
4:     if  $x_d = 0$  then
5:        $f \leftarrow f$  without term " $x_d$ "
6:     else
7:        $f \leftarrow f$  without term " $\neg x_d$ "
8:     end if
9:   end for
10: end for
11: return  $f$ 

```

“Throw Out Bad Terms”

Example: PAC Learning of Conjunctions

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“Throw Out Bad Terms”

- Is this an efficient (ϵ, δ) -PAC learning algorithm?

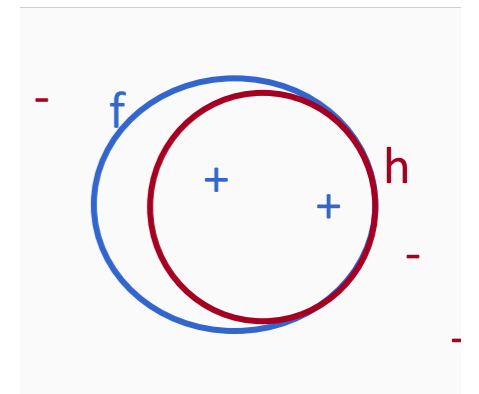
Learning Conjunctions: Analysis

$$f = x_2 \wedge x_3 \wedge x_4 \wedge x_5 \wedge x_{100}$$

$$h = x_1 \wedge x_2 \wedge x_3 \wedge x_4 \wedge x_5 \wedge x_{100}$$

- **Claim 1:** Any hypothesis consistent with the training data will only make mistakes on positive future examples. **Why?**

- A mistake will occur only if some literal z (in our example x_1) is present in h but not in f



- This mistake can cause a positive example to be predicted as negative by h . **Specifically:** $x_1 = 0, x_2 = 1, x_3 = 1, x_4 = 1, x_5 = 1, x_{100} = 1$
- The reverse situation can never happen
 - For an example to be predicted as positive in the training set, every relevant literal must have been present

Learning Conjunctions: Analysis

- **Theorem:** Suppose we are learning a conjunctive concept with n dimensional Boolean features using m training examples. If

$$m > \frac{n}{\epsilon} \left(\log(n) + \log \left(\frac{1}{\delta} \right) \right) \quad \boxed{\text{Poly in } n, 1/\delta, 1/\epsilon}$$

then, with probability $> 1 - \delta$, the error of the learned hypothesis $\text{err}_D(h)$ will be less than ϵ .

If we see these many training examples, then the algorithm will produce a conjunction that, with high probability, will make few errors

Learning Conjunctions: Analysis

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Let's prove this assertion

Proof Intuition

$$f = x_2 \wedge x_3 \wedge x_4 \wedge x_5 \wedge x_{100}$$

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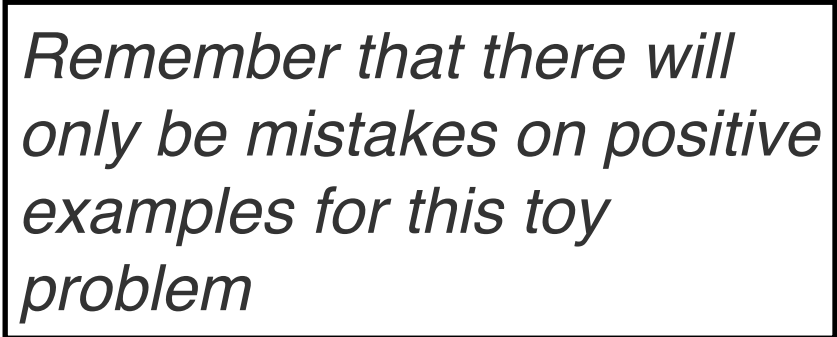
- What kinds of examples would drive a hypothesis to make a mistake?
- Positive examples, where x_1 is absent
 - f would say true and h would say false
- None of these examples appeared during training
 - Otherwise x_1 would have been eliminated
- If they never appeared during training, maybe their appearance in the future would also be rare!
 - Let's quantify our surprise at seeing such examples

Learning Conjunctions: Analysis

- Let $p(z)$ be the probability that, in an example drawn from D , the feature z is absent but the example has a positive label
 - That is, after training is done, $p(z)$ is the probability that in a randomly drawn example, the literal z causes a mistake
- For any z in the target function, $p(z) = 0$

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$$\langle (0, 1, 1, 1, 1, 0, \dots, 0, 1, 1), 1 \rangle$$

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$\langle (0, 1, 1, 1, 1, 0, \dots, 0, 1, 1), 1 \rangle$

$p(x_1)$: Probability that this situation occurs

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• We know that $err_D(h) \leq \sum_{z \in h} p(z)$

- via direct application of the union bound

Union bound

For a set of events, probability that at least one of them happens $<$ the sum of the probabilities of the individual events

Learning Conjunctions: Analysis

- Call a literal z *bad* if $p(z) > \frac{\epsilon}{n}$ n = dimensionality
- Intuitively, a bad literal is one that has a significant probability of not appearing with a positive example
 - (And, if it appears in all positive training examples, it can cause errors)

If there are no bad literals, then $\text{err}_D(h) < \epsilon$

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Let us try to see when this will not happen

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- Let z be a bad literal
- What is the probability that it will not be eliminated by one training example?

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$$\begin{aligned} Pr(z \text{ survives one example}) &= 1 - Pr(z \text{ is eliminated by one example}) \\ &\leq 1 - p(z) \\ &< 1 - \frac{\epsilon}{n} \end{aligned}$$

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There was one example of this kind
 $\langle (1, 1, 1, 1, 1, 0, \dots, 0, 1, 1), 1 \rangle$

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Learning Conjunctions: Analysis

- What we know so far:

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There are at most n bad literals. So

$$Pr(\text{Any bad literal survives } m \text{ examples}) < n \left(1 - \frac{\epsilon}{n}\right)^m$$

Learning Conjunctions: Analysis

$$\Pr(\text{Any bad literal survives } m \text{ examples}) < n \left(1 - \frac{\epsilon}{n}\right)^m$$

- We want this probability to be small
- Why? So that we can choose enough training examples so that the probability that any z survives all of them is less than some δ .

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- That is, we want $n \left(1 - \frac{\epsilon}{n}\right)^m < \delta$

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- Or equivalently, $m > \frac{n}{\epsilon} \left(\log(n) + \log\left(\frac{1}{\delta}\right) \right)$

Learning Conjunctions: Analysis

- To guarantee a probability of failure (i.e, error $> \epsilon$) that is less than δ , the number of examples we need is

$$m > \frac{n}{\epsilon} \left(\log(n) + \log\left(\frac{1}{\delta}\right) \right)$$

Poly in $n, 1/\delta, 1/\epsilon$

- That is, if m has this property, then
 - With probability $1 - \delta$, there will be no bad literals,
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- What does this mean:
 - If $\epsilon = 0.1$ and $\delta = 0.1$, then for $n = 100$, we need 6908 training examples

Learning Conjunctions: Analysis

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- What does this mean:
 - If $\epsilon = 0.1$ and $\delta = 0.1$, then for $n = 100$, we need 6908 training examples
 - If $\epsilon = 0.1$ and $\delta = 0.1$, then for $n = 10$, we need only 461 examples

Learning Conjunctions: Analysis

- To guarantee a probability of failure (i.e, error $> \epsilon$) that is less than δ , the number of examples we need is

$$m > \frac{n}{\epsilon} \left(\log(n) + \log\left(\frac{1}{\delta}\right) \right) \quad \boxed{\text{Poly in } n, 1/\delta, 1/\epsilon}$$

- That is, if m has this property, then
 - With probability $1 - \delta$, there will be no bad literals,
 - Or equivalently, with probability $1 - \delta$, we will have $\text{err}_D(h) < \epsilon$
- What does this mean:
 - If $\epsilon = 0.1$ and $\delta = 0.1$, then for $n = 100$, we need 6908 training examples
 - If $\epsilon = 0.1$ and $\delta = 0.1$, then for $n = 10$, we need only 461 examples
 - If $\epsilon = 0.1$ and $\delta = 0.01$, then for $n = 10$, we need 691 examples

Learning Conjunctions: Analysis

- To guarantee a probability of failure (i.e, error $> \epsilon$) that is less than δ , the number of examples we need is

$$m > \frac{n}{\epsilon} \left(\log(n) + \log\left(\frac{1}{\delta}\right) \right)$$

Poly in $n, 1/\delta, 1/\epsilon$

- That is, if m has this property, then
 - With probability $1 - \delta$, there will be no bad literals,
 - Or equivalently, with probability $1 - \delta$, we will have $\text{err}_D(h) < \epsilon$

What we have here is a PAC guarantee

*Our algorithm is **Probably Approximately Correct.***

Vapnik-Chervonenkis (VC) Dimension

- A classic measure of complexity of infinite hypothesis classes based on this intuition.
- The VC dimension is a very classification-oriented notion of complexity
 - The idea is to look at a finite set of unlabeled examples
 - no matter how these points were labeled, would we be able to find a hypothesis that correctly classifies them
- The idea is that as you add more points, being able to represent an arbitrary labeling becomes harder and harder.

Definitions 2. For data drawn from some space \mathcal{X} , the *VC dimension* of a hypothesis space \mathcal{H} over \mathcal{X} is the maximal K such that: *there exists a set $X \subseteq \mathcal{X}$ of size $|X| = K$, such that **for all** binary labelings of X , there exists a function $f \in \mathcal{H}$ that matches this labeling.*

How many points can a linear boundary classify exactly? (1-D)

- 2 points:

Yes!



- 3 points:

No!



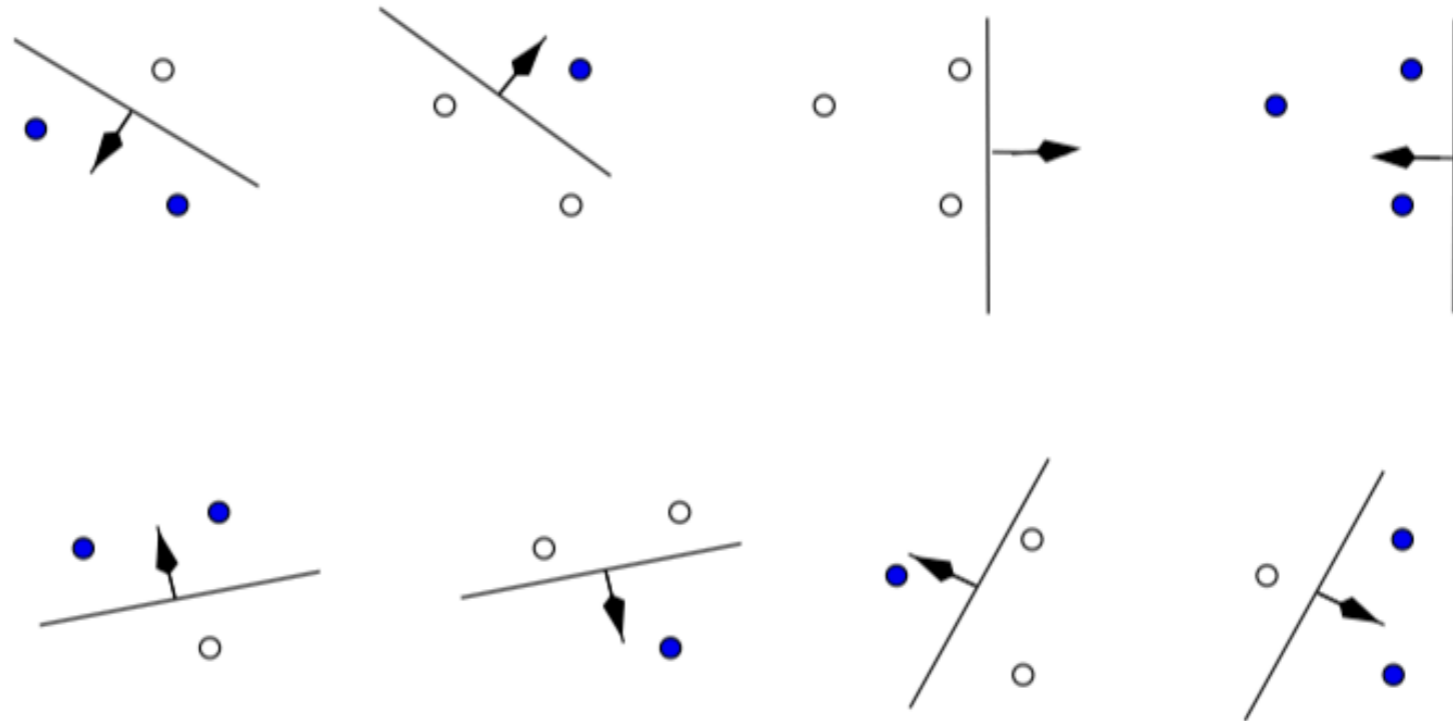
etc (8 total)

VC-dimension = 2

How many points can a linear boundary classify exactly? (2-D)

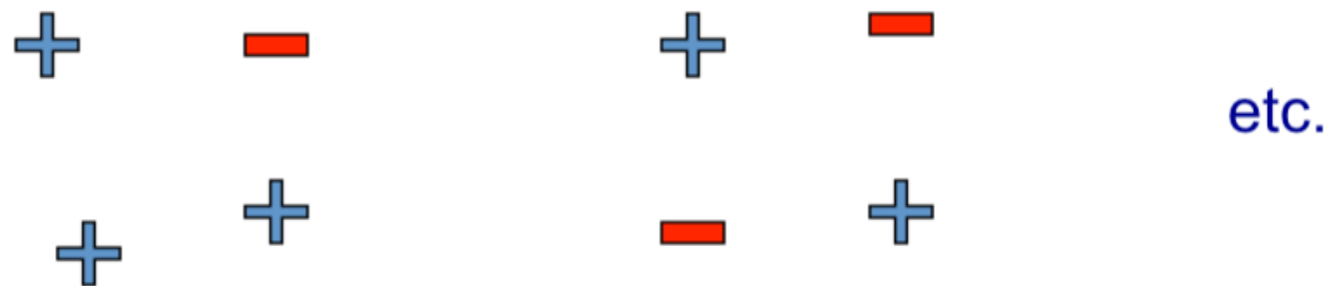
- 3 points:

Yes!



- 4 points:

No!



VC-dimension = 3

Basic Probability Review

Probability

- A is non-deterministic event
 - Can think of A as a boolean-valued variable
- Examples
 - A = your next patient has cancer
 - A = Max Verstappen wins United States Grand Prix 2023



Interpreting Probabilities

If I flip this coin, the probability that it will come up heads is 0.5

- **Frequentist Interpretation:** If we flip this coin many times, it will come up heads about half the time. *Probabilities are the expected frequencies of events over repeated trials.*
- **Bayesian Interpretation:** I believe that my next toss of this coin is equally likely to come up heads or tails. *Probabilities quantify subjective beliefs about single events.*
- Viewpoints play complementary roles in **machine learning:**
 - Bayesian view used to build models based on domain knowledge, and automatically derive learning algorithms
 - Frequentist view used to analyze worst case behavior of learning algorithms, in limit of large datasets
- From either view, basic mathematics is the same!



Axioms of Probability

- $0 \leq P(A) \leq 1$
- $P(\text{empty-set}) = 0$
- $P(\text{everything}) = 1$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

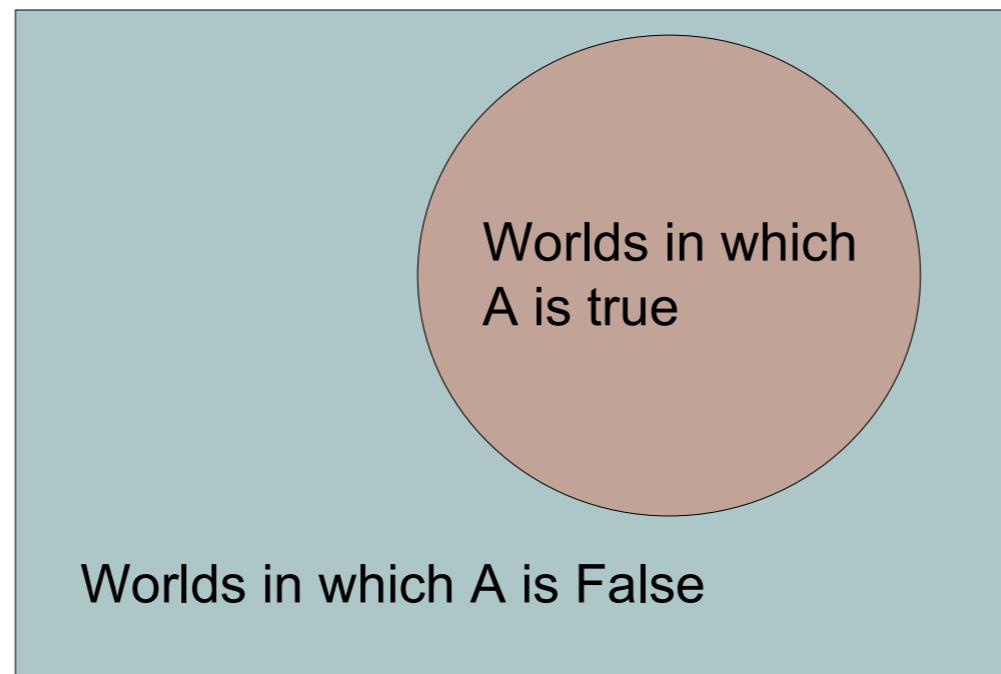
Interpreting the Axioms

- $0 \leq P(A) \leq 1$
- $P(\text{empty-set}) = 0$
- $P(\text{everything}) = 1$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

Event space of
all possible
worlds



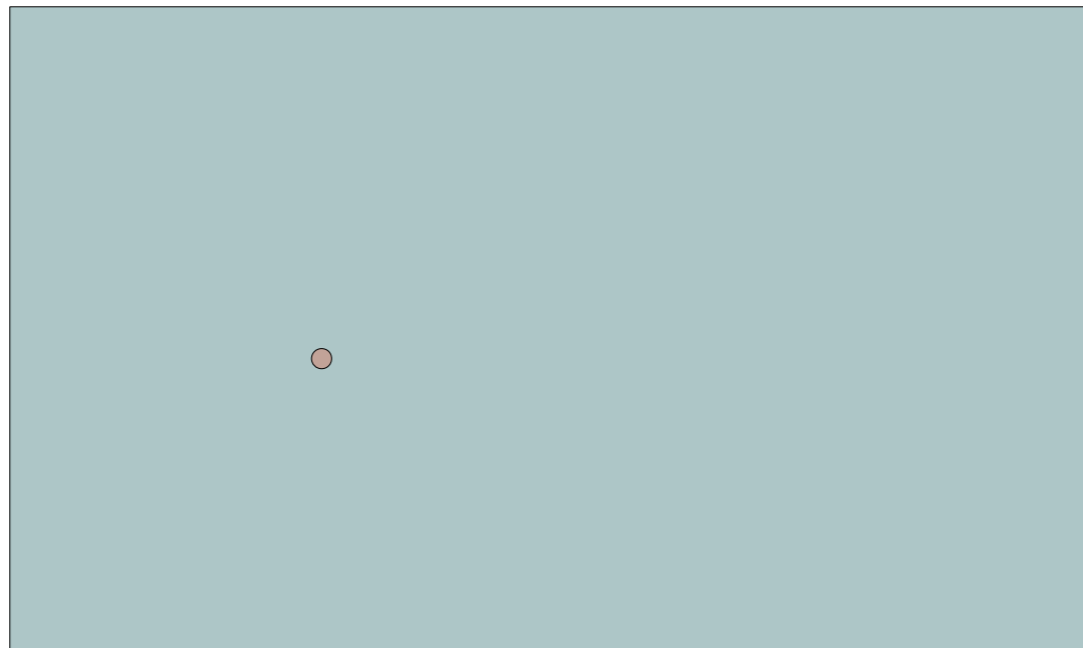
Its area is 1



$P(A) = \text{Area of reddish oval}$

Interpreting the Axioms

- $0 \leq P(A) \leq 1$
- $P(\text{empty-set}) = 0$
- $P(\text{everything}) = 1$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

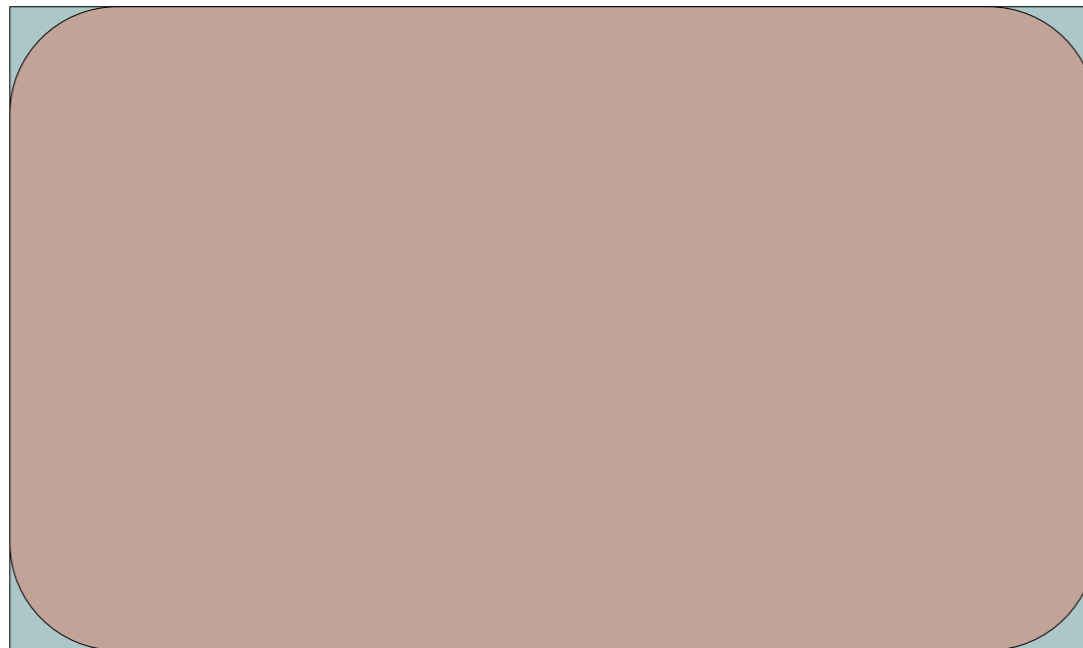


The area of A can't get any smaller than 0

And a zero area would mean no world could ever have A true

Interpreting the Axioms

- $0 \leq P(A) \leq 1$
- $P(\text{empty-set}) = 0$
- $P(\text{everything}) = 1$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

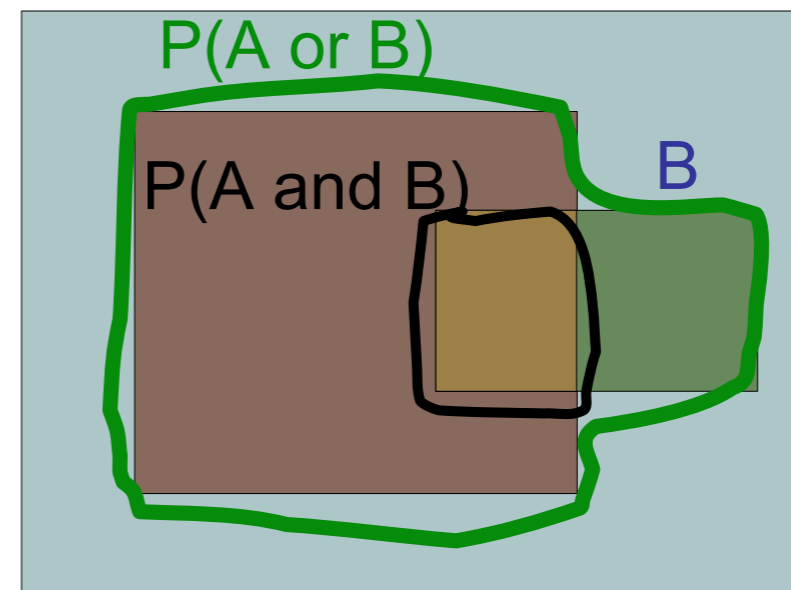
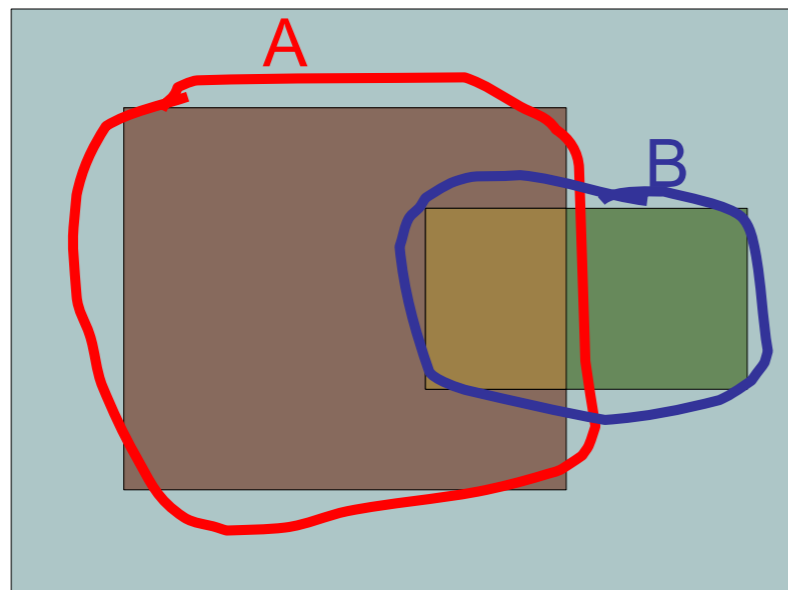


The area of A can't get any bigger than 1

And an area of 1 would mean all worlds will have A true

Interpreting the Axioms

- $0 \leq P(A) \leq 1$
- $P(\text{empty-set}) = 0$
- $P(\text{everything}) = 1$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$



Simple addition and subtraction

Discrete Random Variables

$X \longrightarrow$ discrete random variable

$\mathcal{X} \longrightarrow$ sample space of possible outcomes,
which may be finite or countably infinite

$x \in \mathcal{X} \longrightarrow$ outcome of sample of discrete random variable

Discrete Random Variables

X \longrightarrow discrete random variable

\mathcal{X} \longrightarrow sample space of possible outcomes,
which may be finite or countably infinite

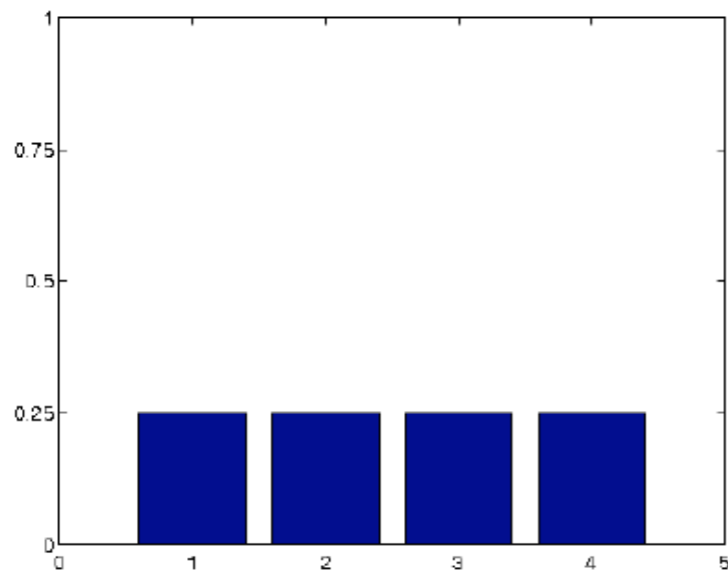
$x \in \mathcal{X}$ \longrightarrow outcome of sample of discrete random variable

$p(X = x)$ \longrightarrow probability distribution (probability mass function)

$p(x)$ \longrightarrow shorthand used when no ambiguity

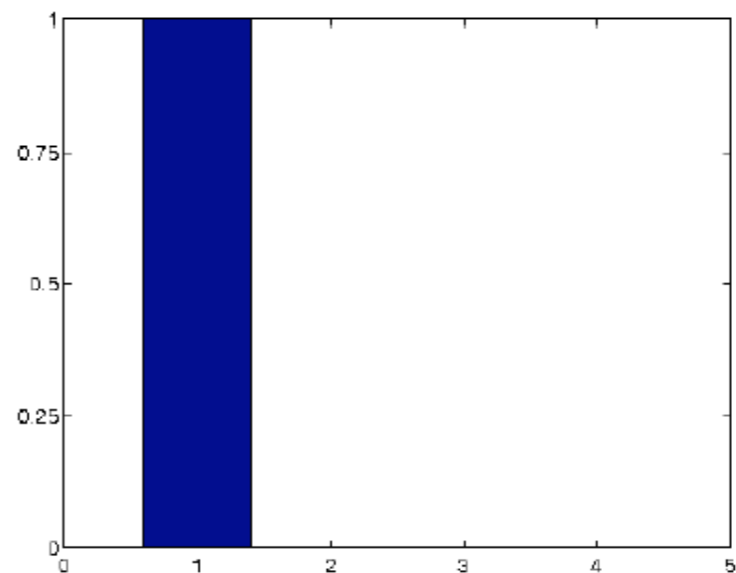
$0 \leq p(x) \leq 1$ for all $x \in \mathcal{X}$

$$\sum_{x \in \mathcal{X}} p(x) = 1$$



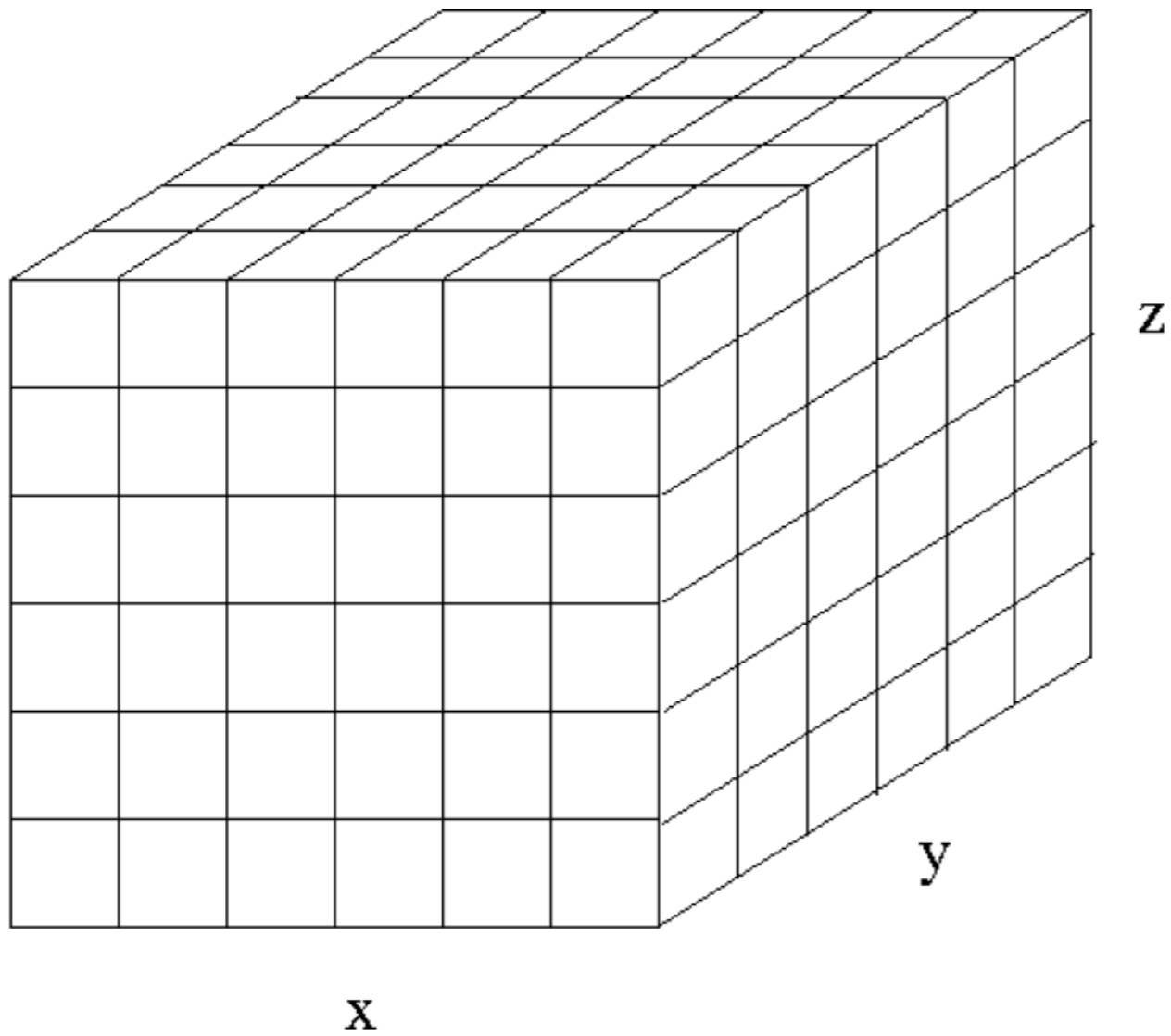
uniform distribution

$$\mathcal{X} = \{1, 2, 3, 4\}$$



degenerate distribution

Joint Distribution



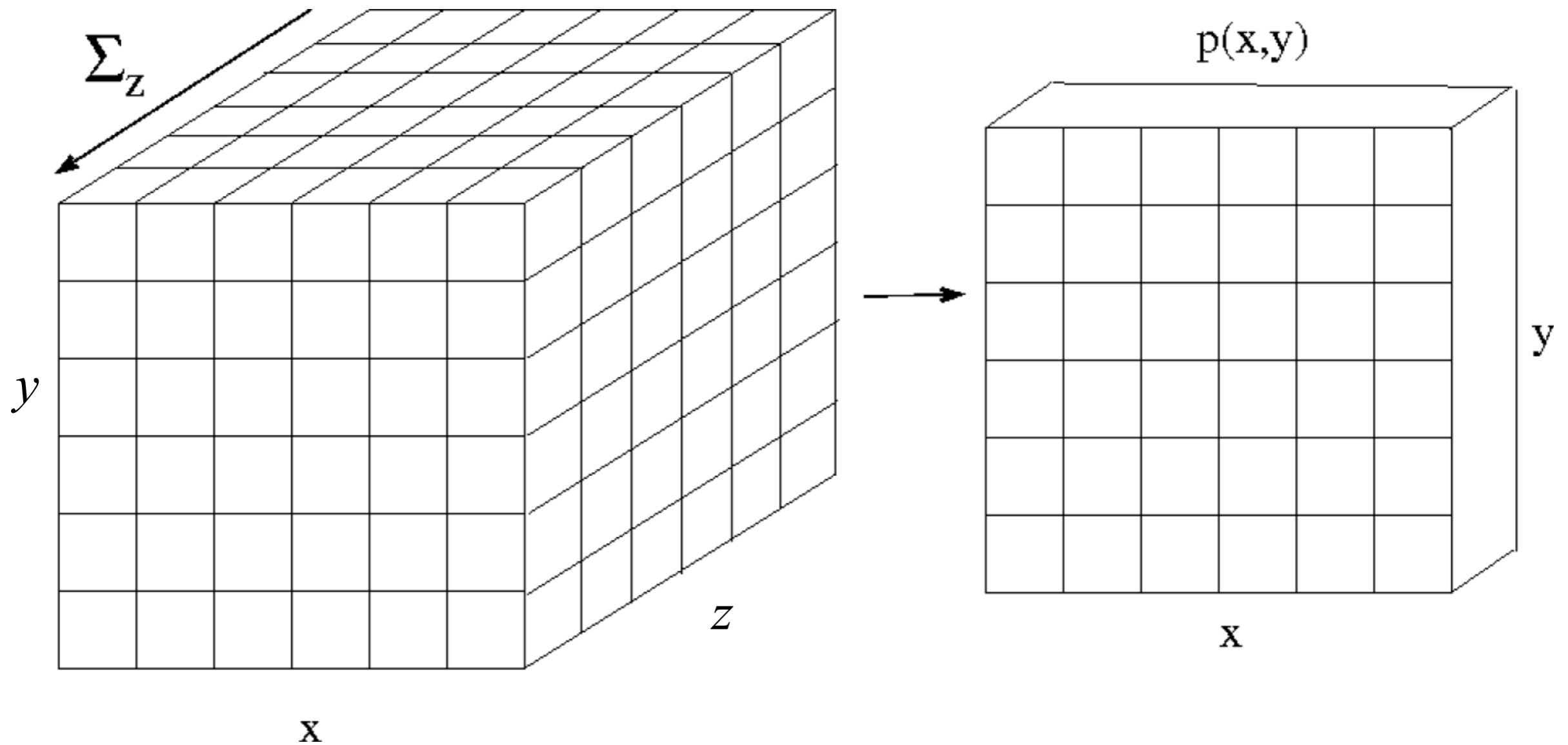
Marginalization

- Marginalization

- Events: $P(A) = P(A \text{ and } B) + P(A \text{ and not } B)$

- Random variables $P(X = x) = \sum_y P(X = x, Y = y)$

Marginal Distributions



$$p(x, y) = \sum_{z \in \mathcal{Z}} p(x, y, z)$$

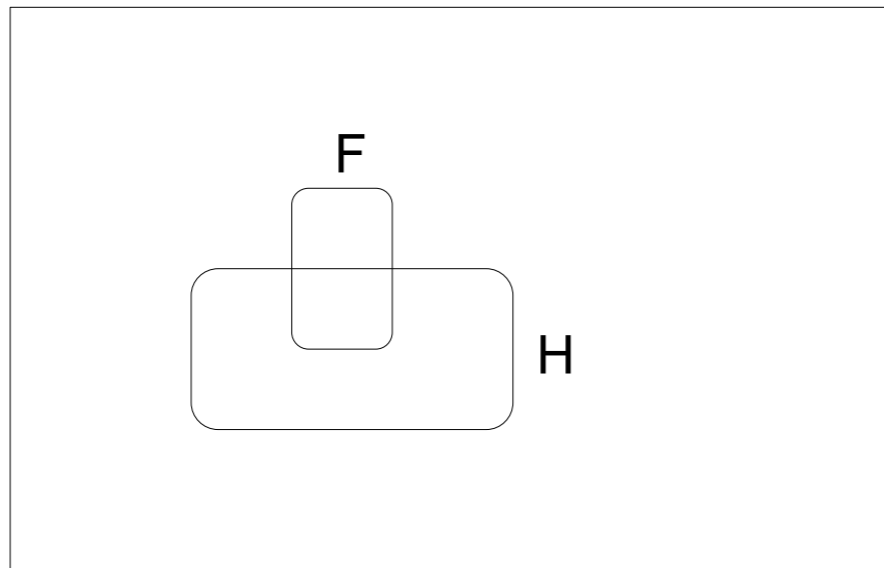
$$p(x) = \sum_{y \in \mathcal{Y}} p(x, y)$$

Conditional Probabilities

- $P(Y=y \mid X=x)$
- What do you believe about $Y=y$, if I tell you $X=x$?
- $P(\text{Max Verstappen winning the 2024 United States Grand Prix})?$
- What if I tell you:
 - He has won the Formula One World Champion title for 2021, 2022, and 2023.
 - He has won the United States Grand Prix 3/8 he has raced there.

Conditional Probabilities

- $P(A | B)$ = In worlds that where B is true, fraction where A is true
- Example
 - H: “Have a headache”
 - F: “Coming down with Flu”



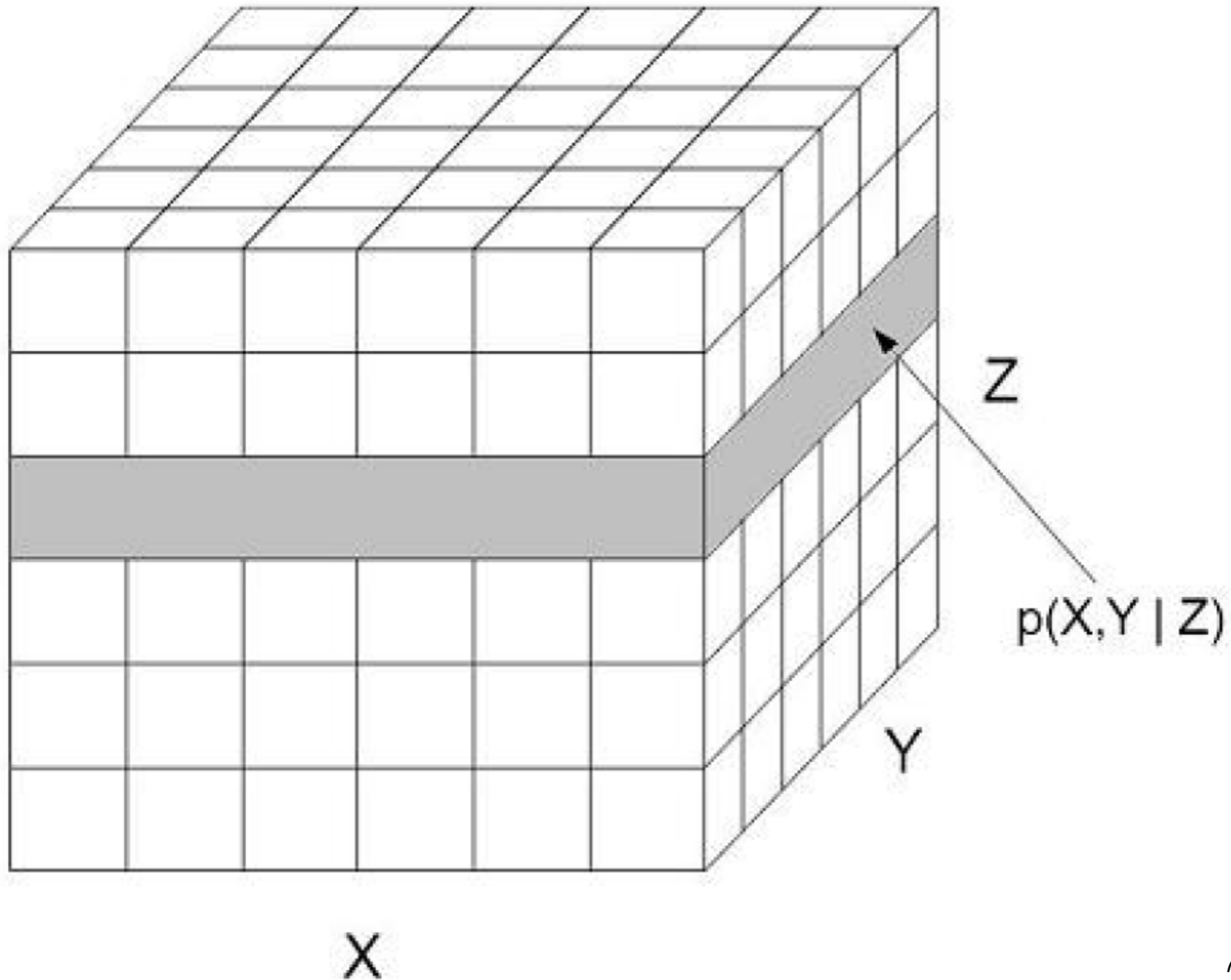
$$P(H) = 1/10$$

$$P(F) = 1/40$$

$$P(H|F) = 1/2$$

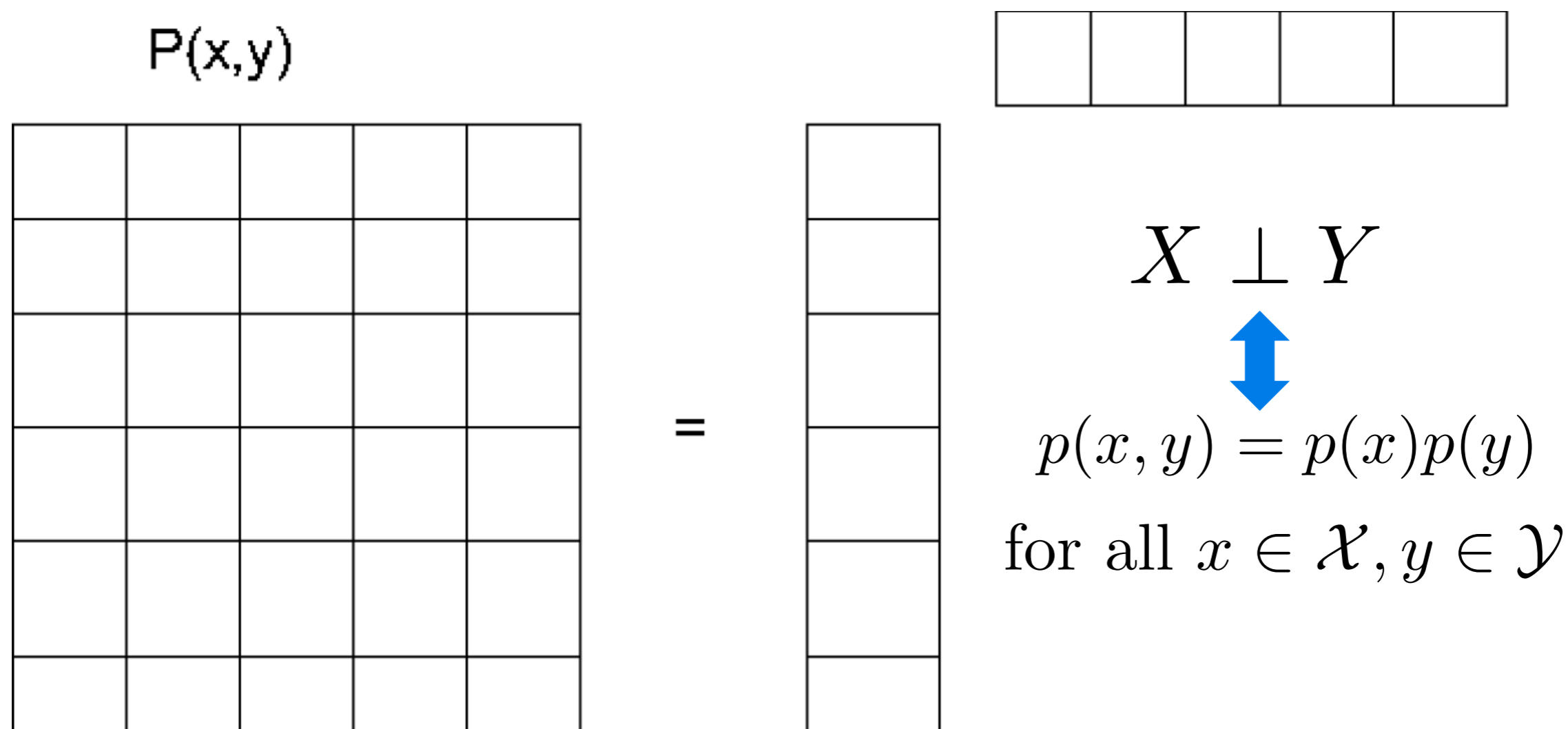
Headaches are rare and flu is rarer, but if you're coming down with flu there's a 50-50 chance you'll have a headache.

Conditional Distributions



$$p(x, y | Z = z) = \frac{p(x, y, z)}{p(z)}$$

Independent Random Variables



Equivalent conditions on conditional probabilities:

$$p(x \mid Y = y) = p(x) \text{ and } p(y) > 0 \text{ for all } y \in \mathcal{Y}$$

$$p(y \mid X = x) = p(y) \text{ and } p(x) > 0 \text{ for all } x \in \mathcal{X}$$

Bayes Rule (Bayes Theorem)

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

$$p(y | x) = \frac{p(x, y)}{p(x)} = \frac{p(x | y)p(y)}{\sum_{y' \in \mathcal{Y}} p(y')p(x | y')} \\ \propto p(x | y)p(y)$$



- A basic identity from the definition of conditional probability
- Used in ways that have no thing to do with Bayesian statistics!
- Typical application to learning and data analysis:

Y	\longrightarrow	unknown parameters we would like to infer
$X = x$	\longrightarrow	observed data available for learning
$p(y)$	\longrightarrow	prior distribution (domain knowledge)
$p(x y)$	\longrightarrow	likelihood function (measurement model)
$p(y x)$	\longrightarrow	posterior distribution (learned information)

Binary Random Variables

- **Bernoulli Distribution:** Single toss of a (possibly biased) coin

$$\mathcal{X} = \{0, 1\}$$

$$0 \leq \theta \leq 1$$

$$\text{Ber}(x \mid \theta) = \theta^{\delta(x,1)} (1 - \theta)^{\delta(x,0)}$$



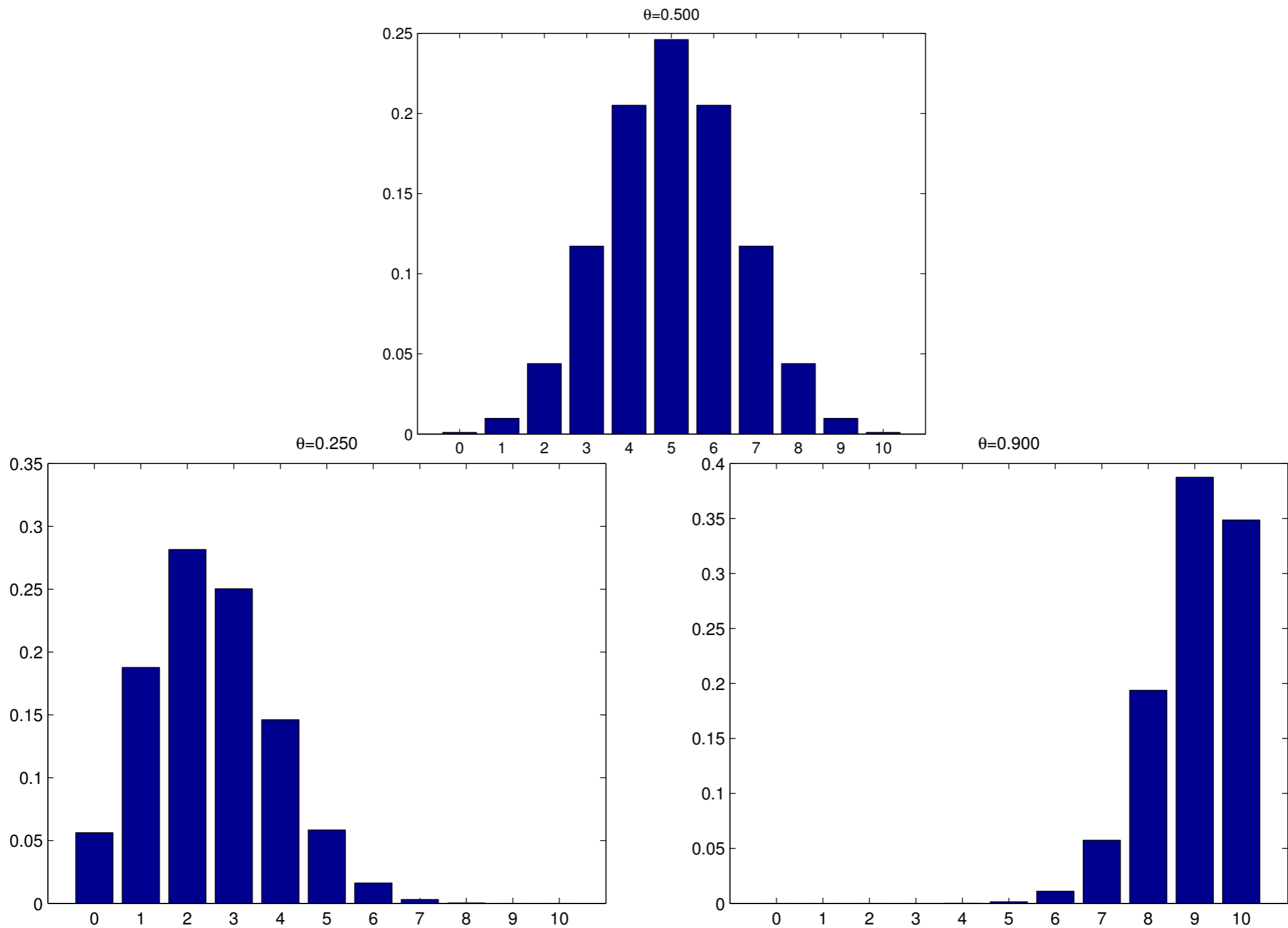
- **Binomial Distribution:** Toss a single (possibly biased) coin n times, and report the number k of times it comes up

$$\mathcal{K} = \{0, 1, 2, \dots, n\}$$

$$0 \leq \theta \leq 1$$

$$\text{Bin}(k \mid n, \theta) = \binom{n}{k} \theta^k (1 - \theta)^{n-k} \quad \binom{n}{k} = \frac{n!}{(n-k)!k!}$$

Binomial Distributions



Bean Machine (Sir Francis Galton)



http://en.wikipedia.org/wiki/Bean_machine

Categorical Random Variables

- **Multinoulli Distribution:** Single roll of a (possibly biased) die

$$\mathcal{X} = \{0, 1\}^K, \sum_{k=1}^K x_k = 1 \quad \text{binary vector encoding}$$

$$\theta = (\theta_1, \theta_2, \dots, \theta_K), \theta_k \geq 0, \sum_{k=1}^K \theta_k = 1$$

$$\text{Cat}(x | \theta) = \prod_{k=1}^K \theta_k^{x_k}$$

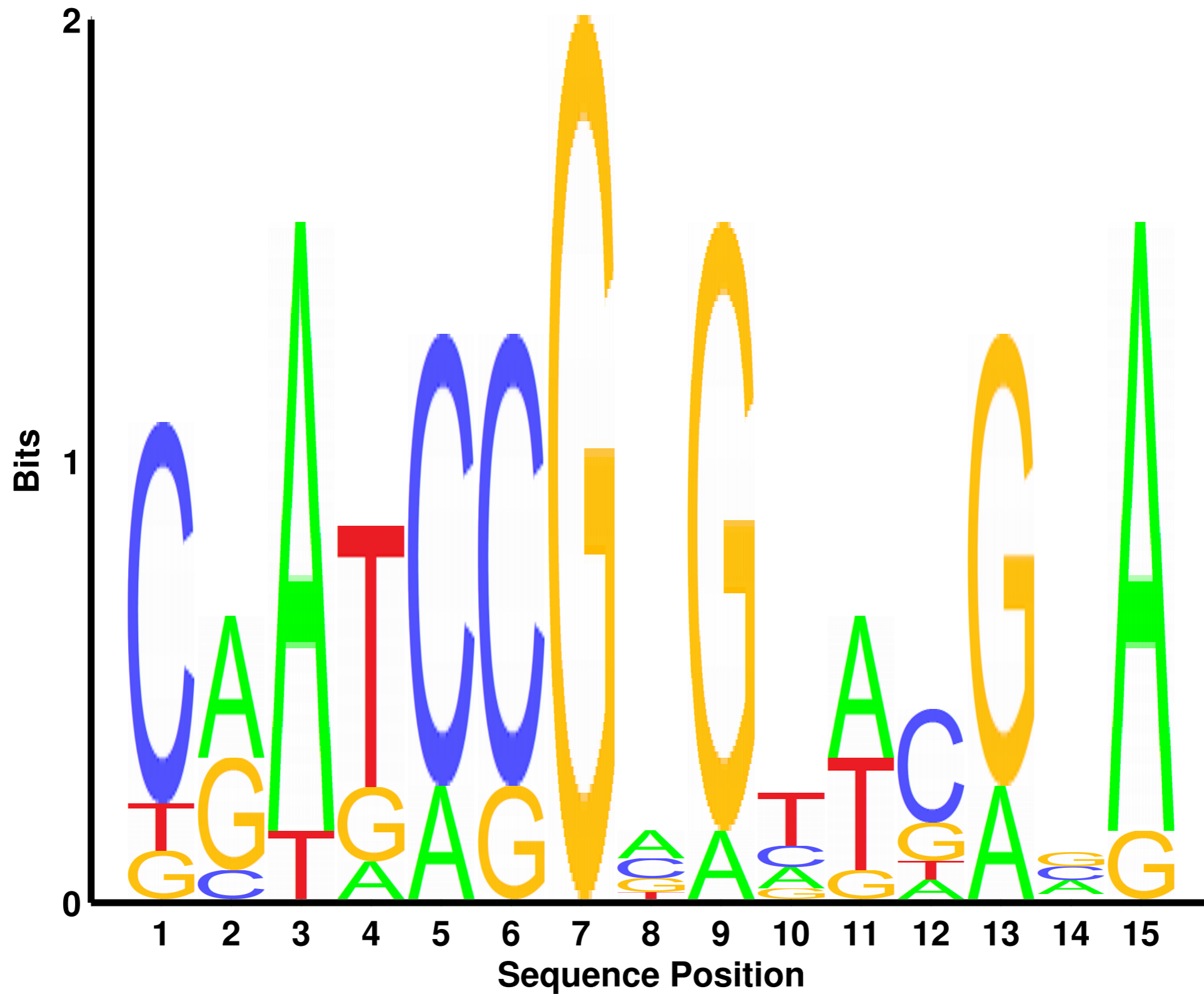
- **Multinomial Distribution:** Roll a single (possibly biased) die n times, and report the number n_k of each possible outcome

$$\text{Mu}(x | n, \theta) = \binom{n}{n_1 \dots n_K} \prod_{k=1}^K \theta_k^{n_k} \quad n_k = \sum_{i=1}^n x_{ik}$$

Aligned DNA Sequences

```
c g a t a c g g g g t c g a a  
c a a t c c g a g a t c g c a  
c a a t c c g t g t t g g g a  
c a a t c g g c a t g c g g g  
c g a g c c g c g t a c g a a  
c a t a c g g a g c a c g a a  
t a a t c c g g g c a t g t a  
c g a g c c g a g t a c a g a  
c c a t c c g c g t a a g c a  
g g a t a c g a g a t g a c a
```

Multinomial Model of DNA



Next Lecture:
Maximum Likelihood Estimation
(MLE)