## Machine Learning

## Math Essentials

## Areas of math essential to machine learning

- Machine learning is part of both statistics and computer science
- Probability
- Statistical inference
- Validation
- Estimates of error, confidence intervals
- Linear algebra
- Hugely useful for compact representation of linear transformations on data
- Dimensionality reduction techniques
- Optimization theory


## Why worry about the math?

- There are lots of easy-to-use machine learning packages out there.
- After this course, you will know how to apply several of the most general-purpose algorithms.


## HOWEVER

- To get really useful results, you need good mathematical intuitions about certain general machine learning principles, as well as the inner workings of the individual algorithms.


## Why worry about the math?

These intuitions will allow you to:

- Choose the right algorithm(s) for the problem
- Make good choices on parameter settings, validation strategies
- Recognize over- or underfitting
- Troubleshoot poor / ambiguous results
- Put appropriate bounds of confidence / uncertainty on results
- Do a better job of coding algorithms or incorporating them into more complex analysis pipelines


## Notation

- $a \in A \quad$ set membership: $a$ is member of set $A$
- $|B|$ cardinality: number of items in set $B$
- || v || norm: length of vector $v$
- $\Sigma$
- 1
- $\mathfrak{R}$
- $\mathfrak{R}^{n}$
summation
integral
the set of real numbers
real number space of dimension $n$

$$
\begin{aligned}
& \mathrm{n}=2: \text { plane or 2-space } \\
& \mathrm{n}=3: 3 \text {-(dimensional) space } \\
& \mathrm{n}>3: n \text {-space or hyperspace }
\end{aligned}
$$

## Notation

- $\mathbf{x}, \mathbf{y}, \mathbf{z}, \quad$ vector (bold, lower case)
$\mathbf{u}, \mathbf{v}$
- A, B, X matrix (bold, upper case)
- $y=f(x)$ function (map): assigns unique value in range of $y$ to each value in domain of $x$
- $d y / d x$ derivative of $y$ with respect to single variable $x$
- $y=f(\mathbf{x})$ function on multiple variables, i.e. a vector of variables; function in $n$-space
- $\partial y / \partial x_{i} \quad$ partial derivative of $y$ with respect to element $i$ of vector $\mathbf{x}$


## The concept of probability

## Intuition:

- In some process, several outcomes are possible. When the process is repeated a large number of times, each outcome occurs with a characteristic relative frequency, or probability. If a particular outcome happens more often than another outcome, we say it is more probable.


## The concept of probability

Arises in two contexts:

- In actual repeated experiments.
- Example: You record the color of 1000 cars driving by. 57 of them are green. You estimate the probability of a car being green as $57 / 1000=0.0057$.
- In idealized conceptions of a repeated process.
- Example: You consider the behavior of an unbiased six-sided die. The expected probability of rolling a 5 is $1 / 6=0.1667$.
- Example: You need a model for how people's heights are distributed. You choose a normal distribution (bell-shaped curve) to represent the expected relative probabilities.


## Probability spaces

A probability space is a random process or experiment with three components:

- $\Omega$, the set of possible outcomes $O$
- number of possible outcomes $=|\Omega|=N$
- $F$, the set of possible events $E$
- an event comprises 0 to $N$ outcomes
- number of possible events $=|F|=2^{N}$
- $P$, the probability distribution
- function mapping each outcome and event to real number between 0 and 1 (the probability of $O$ or $E$ )
- probability of an event is sum of probabilities of possible outcomes in event


## Axioms of probability

1. Non-negativity: for any event $E \in F, p(E) \geq 0$
2. All possible outcomes:

$$
p(\Omega)=1
$$

3. Additivity of disjoint events:
for all events $E, E^{\prime} \in F$ where $E \cap E^{\prime}=\varnothing$,

$$
p\left(E \cup E^{\prime}\right)=p(E)+p\left(E^{\prime}\right)
$$

## Types of probability spaces

## Define $|\Omega|=$ number of possible outcomes

- Discrete space $\quad|\Omega|$ is finite
- Analysis involves summations ( $\Sigma$ )
- Continuous space $|\Omega|$ is infinite
- Analysis involves integrals ( $\int$ )


## Example of discrete probability space

Single roll of a six-sided die

- 6 possible outcomes: $O=1,2,3,4,5$, or 6
$-2^{6}=64$ possible events
- example: $E=(O \in\{1,3,5\})$, i.e. outcome is odd
- If die is fair, then probabilities of outcomes are equal

$$
\begin{aligned}
& p(1)=p(2)=p(3)= \\
& p(4)=p(5)=p(6)=1 / 6
\end{aligned}
$$

- example: probability of event $E=($ outcome is odd $)$ is

$$
p(1)+p(3)+p(5)=1 / 2
$$

## Example of discrete probability space

Three consecutive flips of a coin

- 8 possible outcomes: $\mathrm{O}=\mathrm{HHH}, \mathrm{HHT}, \mathrm{HTH}, \mathrm{HTT}$, THH, THT, TTH, TTT
$-2^{8}=256$ possible events
- example: $E=(O \in\{H H T, H T H, T H H\})$, i.e. exactly two flips are heads
- example: $E=(O \in\{$ THT, TTT $\}$ ), i.e. the first and third flips are tails
- If coin is fair, then probabilities of outcomes are equal $p(\mathrm{HHH})=p(\mathrm{HHT})=p(\mathrm{HTH})=p(\mathrm{HTT})=$ $p(\mathrm{THH})=p(\mathrm{THT})=p(\mathrm{TTH})=p($ TTT $)=1 / 8$
- example: probability of event $E=$ ( exactly two heads ) is

$$
p(\mathrm{HHT})+p(\mathrm{HTH})+p(\mathrm{THH})=3 / 8
$$

## Example of continuous probability space

Height of a randomly chosen American male

- Infinite number of possible outcomes: O has some single value in range 2 feet to 8 feet
- Infinite number of possible events
- example: $E=(O \mid O<5.5$ feet $)$, i.e. individual chosen is less than 5.5 feet tall
- Probabilities of outcomes are not equal, and are described by a continuous function, $p(\mathrm{O})$



## Example of continuous probability space

Height of a randomly chosen American male

- Probabilities of outcomes $O$ are not equal, and are described by a continuous function, $p(O)$
$-p(O)$ is a relative, not an absolute probability
$-p(O)$ for any particular $O$ is zero
$-\int p(O)$ from $O=-\infty$ to $\infty$ (i.e. area under curve) is 1
- example: $p\left(0=5 \prime 8^{\prime \prime}\right)>p\left(0=62^{\prime \prime}\right)$
- example: $p\left(O<5^{\prime} 6^{\prime \prime}\right)=\left(\int p(O)\right.$ from $O=-\infty$ to $\left.5^{\prime \prime} 6^{\prime \prime}\right) \approx 0.25$



## Probability distributions

- Discrete:
example:
sum of two fair dice
probability mass function (pmf)

probability density function (pdf)



## Random variables

- A random variable $X$ is a function that associates a number $x$ with each outcome $O$ of a process
- Common notation: $X(O)=x$, or just $X=x$
- Basically a way to redefine (usually simplify) a probability space to a new probability space
- X must obey axioms of probability (over the possible values of $x$ )
- $X$ can be discrete or continuous
- Example: $X=$ number of heads in three flips of a coin
- Possible values of $X$ are $0,1,2,3$
$-p(X=0)=p(X=3)=1 / 8 \quad p(X=1)=p(X=2)=3 / 8$
- Size of space (number of "outcomes") reduced from 8 to 4
- Example: $X=$ average height of five randomly chosen American men
- Size of space unchanged ( $X$ can range from 2 feet to 8 feet), but pdf of $X$ different than for single man


## Multivariate probability distributions

- Scenario
- Several random processes occur (doesn't matter whether in parallel or in sequence)
- Want to know probabilities for each possible combination of outcomes
- Can describe as joint probability of several random variables
- Example: two processes whose outcomes are represented by random variables $X$ and $Y$. Probability that process $X$ has outcome $x$ and process $Y$ has outcome $y$ is denoted as:

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

## Example of multivariate distribution



## Multivariate probability distributions

- Marginal probability
- Probability distribution of a single variable in a joint distribution
- Example: two random variables $X$ and $Y$ :

$$
p(X=x)=\sum_{b=a l l} \text { values of } Y p(X=x, Y=b)
$$

- Conditional probability
- Probability distribution of one variable given that another variable takes a certain value
- Example: two random variables $X$ and $Y$ :

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

## Example of marginal probability

marginal probability: $p(X=$ minivan $)=0.0741+0.1111+0.1481=0.3333$


## Example of conditional probability



## Continuous multivariate distribution

- Same concepts of joint, marginal, and conditional probabilities apply (except use integrals)
- Example: three-component Gaussian mixture in two dimensions



## Expected value

## Given:

- A discrete random variable $X$, with possible values $x=x_{1}, x_{2}, \ldots x_{n}$
- Probabilities $p\left(X=x_{i}\right)$ that $X$ takes on the various values of $x_{i}$
- A function $y_{i}=f\left(x_{i}\right)$ defined on $X$

The expected value of $f$ is the probability-weighted "average" value of $f\left(x_{i}\right)$ :

$$
\mathrm{E}(f)=\sum_{i} p\left(x_{i}\right) \cdot f\left(x_{i}\right)
$$

## Example of expected value

- Process: game where one card is drawn from the deck
- If face card, dealer pays you \$10
- If not a face card, you pay dealer \$4
- Random variable $X=\{$ face card, not face card $\}$
$-p($ face card $)=3 / 13$
$-p($ not face card $)=10 / 13$
- Function $f(X)$ is payout to you
$-f($ face card $)=10$
$-f($ not face card $)=-4$
- Expected value of payout is:

$$
E(f)=\sum_{i} p\left(x_{i}\right) \cdot f\left(x_{i}\right)=3 / 13 \cdot 10+10 / 13 \cdot-4=-0.77
$$

## Expected value in continuous spaces

$$
E(f)=\int_{x=a \rightarrow b} p(x) \cdot f(x)
$$



## Common forms of expected value (1)

- Mean $(\mu)$
$f\left(x_{i}\right)=x_{i} \Rightarrow \quad \mu=\mathrm{E}(f)=\sum_{i} p\left(x_{i}\right) \cdot x_{i}$
- Average value of $X=x_{i}$, taking into account probability of the various $x_{i}$
- Most common measure of "center" of a distribution
- Compare to formula for mean of an actual sample

$$
\mu=\frac{1}{N} \sum_{i=1}^{n} x_{i}
$$

## Common forms of expected value (2)

- Variance ( $\sigma^{2}$ )
$f\left(x_{i}\right)=\left(x_{i}-\mu\right) \Rightarrow \sigma^{2}=\sum_{i} p\left(x_{i}\right) \cdot\left(x_{i}-\mu\right)^{2}$
- Average value of squared deviation of $X=x_{i}$ from mean $\mu$, taking into account probability of the various $x_{i}$
- Most common measure of "spread" of a distribution
- $\sigma$ is the standard deviation
- Compare to formula for variance of an actual sample

$$
\sigma^{2}=\frac{1}{N-1} \sum_{i=1}^{n}\left(x_{i}-\mu\right)^{2}
$$

## Common forms of expected value (3)

- Covariance

$$
\begin{aligned}
& f\left(x_{i}\right)=\left(x_{i}-\mu_{x}\right), g\left(y_{i}\right)=\left(y_{i}-\mu_{y}\right) \Rightarrow \\
& \quad \operatorname{cov}(x, y)=\sum_{i} p\left(x_{i}, y_{i}\right) \cdot\left(x_{i}-\mu_{x}\right) \cdot\left(y_{i}-\mu_{y}\right)
\end{aligned}
$$

- Measures tendency for $x$ and $y$ to deviate from their means in same (or opposite) directions at same time


- Compare to formula for covariance of actual samples

$$
\operatorname{cov}(x, y)=\frac{1}{N-1} \sum_{i=1}^{n}\left(x_{i}-\mu_{x}\right)\left(y_{i}-\mu_{y}\right)
$$

## Correlation

- Pearson's correlation coefficient is covariance normalized by the standard deviations of the two variables

$$
\operatorname{corr}(x, y)=\frac{\operatorname{cov}(x, y)}{\sigma_{x} \sigma_{y}}
$$

- Always lies in range -1 to 1
- Only reflects linear dependence between variables
Linear dependence
with noise


## Complement rule

Given: event $A$, which can occur or not

$$
p(\operatorname{not} A)=1-p(A)
$$


areas represent relative probabilities

## Product rule

Given: events $A$ and $B$, which can co-occur (or not)

$$
p(A, B)=p(A \mid B) \cdot p(B)
$$

(same expression given previously to define conditional probability)


## Example of product rule

- Probability that a man has white hair (event $A$ ) and is over 65 (event $B$ )
$-p(B)=0.18$
$-p(A \mid B)=0.78$
$-p(A, B)=p(A \mid B) \cdot p(B)=$ $0.78 \cdot 0.18=$
0.14


## Rule of total probability

Given: events $A$ and $B$, which can co-occur (or not)

$$
p(A)=p(A, B)+p(A, \operatorname{not} B)
$$

(same expression given previously to define marginal probability)


## I ndependence

Given: events $A$ and $B$, which can co-occur (or not)

$$
p(A \mid B)=p(A) \quad \text { or } \quad p(A, B)=p(A) \cdot p(B)
$$


areas represent relative probabilities

## Examples of independence / dependence

- Independence:
- Outcomes on multiple rolls of a die
- Outcomes on multiple flips of a coin
- Height of two unrelated individuals
- Probability of getting a king on successive draws from a deck, if card from each draw is replaced
- Dependence:
- Height of two related individuals
- Duration of successive eruptions of Old Faithful
- Probability of getting a king on successive draws from a deck, if card from each draw is not replaced


## Example of independence vs. dependence

- Independence: All manufacturers have identical product mix. $p(X=x \mid Y=y)=p(X=x)$.
- Dependence: American manufacturers love SUVs, Europeans manufacturers don't.



## Bayes rule

A way to find conditional probabilities for one variable when conditional probabilities for another variable are known.

$$
\begin{gathered}
p(B \mid A)=p(A \mid B) \cdot p(B) / p(A) \\
\text { where } p(A)=p(A, B)+p(A, \operatorname{not} B)
\end{gathered}
$$



## Bayes rule



## Example of Bayes rule

- Marie is getting married tomorrow at an outdoor ceremony in the desert. In recent years, it has rained only 5 days each year. Unfortunately, the weatherman is forecasting rain for tomorrow. When it actually rains, the weatherman has forecast rain $90 \%$ of the time. When it doesn't rain, he has forecast rain $10 \%$ of the time. What is the probability it will rain on the day of Marie's wedding?
- Event $A$ : The weatherman has forecast rain.
- Event $B$ : It rains.
- We know:
- $p(B)=5 / 365=0.0137$ [ It rains 5 days out of the year.]
$-p(\operatorname{not} B)=360 / 365=0.9863$
- $p(A \mid B)=0.9$ [When it rains, the weatherman has forecast rain $90 \%$ of the time.]
- $p(A \mid \operatorname{not} B)=0.1 \quad$ [When it does not rain, the weatherman has forecast rain $10 \%$ of the time.]


## Example of Bayes rule, cont'd.

- We want to know $p(B \mid A)$, the probability it will rain on the day of Marie's wedding, given a forecast for rain by the weatherman. The answer can be determined from Bayes rule:

1. $p(B \mid A)=p(A \mid B) \cdot p(B) / p(A)$
2. $p(A)=p(A \mid B) \cdot p(B)+p(A \mid \operatorname{not} B) \cdot p(\operatorname{not} B)=$ $(0.9)(0.014)+(0.1)(0.986)=0.111$
3. $p(B \mid A)=(0.9)(0.0137) / 0.111=0.111$

- The result seems unintuitive but is correct. Even when the weatherman predicts rain, it only rains only about $11 \%$ of the time. Despite the weatherman's gloomy prediction, it is unlikely Marie will get rained on at her wedding.


## Probabilities: when to add, when to multiply

- ADD: When you want to allow for occurrence of any of several possible outcomes of a single process. Comparable to logical OR.
- MULTIPLY: When you want to allow for simultaneous occurrence of particular outcomes from more than one process. Comparable to logical AND.
- But only if the processes are independent.


## Linear algebra applications

1) Operations on or between vectors and matrices
2) Coordinate transformations
3) Dimensionality reduction
4) Linear regression
5) Solution of linear systems of equations
6) Many others

Applications 1) - 4) are directly relevant to this course. Today we'll start with 1).

## Why vectors and matrices?

- Most common form of data organization for machine learning is a 2D array, where
- rows represent samples (records, items, datapoints)
- columns represent attributes (features, variables)
- Natural to think of each sample as a vector of attributes, and whole array as a matrix

matrix


## Vectors

- Definition: an $n$-tuple of values (usually real numbers).
- $n$ referred to as the dimension of the vector
- $n$ can be any positive integer, from 1 to infinity
- Can be written in column form or row form
- Column form is conventional
- Vector elements referenced by subscript

$$
\mathbf{x}=\left(\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right) \quad \begin{array}{lll}
\mathbf{x}^{\mathrm{T}}=\left(\begin{array}{lll}
x_{1} & \cdots & x_{n}
\end{array}\right) \\
{ }^{\mathrm{T}} \text { means "transpose" }
\end{array}
$$

## Vectors

- Can think of a vector as:
- a point in space or
- a directed line segment with a magnitude and direction




## Vector arithmetic

- Addition of two vectors
- add corresponding elements

$$
\mathbf{z}=\mathbf{x}+\mathbf{y}=\left(\begin{array}{lll}
x_{1}+y_{1} & \cdots & x_{n}+y_{n}
\end{array}\right)^{\mathrm{T}}
$$

- result is a vector

- Scalar multiplication of a vector
- multiply each element by scalar

$$
\mathbf{y}=a \mathbf{x}=\left(\begin{array}{lll}
a x_{1} & \cdots & a x_{n}
\end{array}\right)^{\mathrm{T}}
$$

- result is a vector



## Vector arithmetic

- Dot product of two vectors
- multiply corresponding elements, then add products

$$
a=\mathbf{x} \cdot \mathbf{y}=\sum_{i=1}^{n} x_{i} y_{i}
$$

- result is a scalar
- Dot product alternative form

$$
a=\mathbf{x} \cdot \mathbf{y}=\|\mathbf{x}\|\|\mathbf{y}\| \cos (\theta)
$$



## Matrices

- Definition: an $m \times n$ two-dimensional array of values (usually real numbers).
- $m$ rows
- $n$ columns
- Matrix referenced by two-element subscript
- first element in subscript is row
- second element in subscript is column

$$
\mathbf{A}=\left(\begin{array}{ccc}
a_{11} & \cdots & a_{1 n} \\
\vdots & \ddots & \vdots \\
a_{m 1} & \cdots & a_{m n}
\end{array}\right)
$$

- example: $\mathbf{A}_{24}$ or $a_{24}$ is element in second row, fourth column of $\mathbf{A}$


## Matrices

- A vector can be regarded as special case of a matrix, where one of matrix dimensions $=1$.
- Matrix transpose (denoted ${ }^{\mathrm{T}}$ )
- swap columns and rows
- row 1 becomes column 1, etc.
$-m \times n$ matrix becomes $n \times m$ matrix
- example:

$$
\mathbf{A}=\left(\begin{array}{lllll}
2 & 7 & -1 & 0 & 3 \\
4 & 6 & -3 & 1 & 8
\end{array}\right)
$$

$$
\mathbf{A}^{\mathrm{T}}=\left(\begin{array}{cc}
2 & 4 \\
7 & 6 \\
-1 & -3 \\
0 & 1 \\
3 & 8
\end{array}\right)
$$

## Matrix arithmetic

- Addition of two matrices

$$
\begin{gathered}
\mathbf{C}=\mathbf{A}+\mathbf{B}= \\
\left(\begin{array}{ccc}
a_{11}+b_{11} & \cdots & a_{1 n}+b_{1 n} \\
\vdots & \ddots & \vdots \\
a_{m 1}+b_{m 1} & \cdots & a_{m n}+b_{m n}
\end{array}\right)
\end{gathered}
$$

- matrices must be same size
- add corresponding elements:

$$
c_{i j}=a_{i j}+b_{i j}
$$

- result is a matrix of same size
- Scalar multiplication of a matrix

$$
\begin{gathered}
\mathbf{B}=d \cdot \mathbf{A}= \\
\left(\begin{array}{ccc}
d \cdot a_{11} & \cdots & d \cdot a_{1 n} \\
\vdots & \ddots & \vdots \\
d \cdot a_{m 1} & \cdots & d \cdot a_{m n}
\end{array}\right)
\end{gathered}
$$

- multiply each element by scalar:

$$
b_{i j}=d \cdot a_{i j}
$$

- result is a matrix of same size


## Matrix arithmetic

- Matrix-matrix multiplication
- vector-matrix multiplication just a special case


## TO THE BOARD!!

- Multiplication is associative

$$
A \cdot(B \cdot C)=(A \cdot B) \cdot C
$$

- Multiplication is not commutative

$$
\mathbf{A} \cdot \mathbf{B} \neq \mathbf{B} \cdot \mathbf{A} \quad \text { (generally) }
$$

- Transposition rule:

$$
(\mathbf{A} \cdot \mathbf{B})^{\top}=\mathbf{B}^{\top} \cdot \mathbf{A}^{\top}
$$

## Matrix arithmetic

- RULE: In any chain of matrix multiplications, the column dimension of one matrix in the chain must match the row dimension of the following matrix in the chain.
- Examples

$$
\text { A } 3 \times 5 \quad \text { B } 5 \times 5 \quad \text { C } 3 \times 1
$$

Right:

$$
\mathbf{A} \cdot \mathbf{B} \cdot \mathbf{A}^{\top} \quad \mathbf{C}^{\top} \cdot \mathbf{A} \cdot \mathbf{B} \quad \mathbf{A}^{\top} \cdot \mathbf{A} \cdot \mathbf{B} \quad \mathbf{C} \cdot \mathbf{C}^{\top} \cdot \mathbf{A}
$$

Wrong:
A.B • A
C.A.B
A. $\mathbf{A}^{\top} \cdot \mathbf{B}$
$\mathbf{C l}^{\top} \cdot \mathbf{C} \cdot \mathbf{A}$

## Vector projection

- Orthogonal projection of $\mathbf{y}$ onto $\mathbf{x}$
- Can take place in any space of dimensionality $\geq 2$
- Unit vector in direction of $\mathbf{x}$ is
x / \| x \|
- Length of projection of $y$ in direction of $\mathbf{x}$ is

$$
\|\mathbf{y}\| \cdot \cos (\theta)
$$

- Orthogonal projection of
 $y$ onto $x$ is the vector

$$
\begin{aligned}
& \operatorname{proj}_{\mathbf{x}}(\mathbf{y})=\mathbf{x} \cdot\|\mathbf{y}\| \cdot \cos (\theta) /\|\mathbf{x}\|= \\
& {\left[(\mathbf{x} \cdot \mathbf{y}) /\|\mathbf{x}\|^{2}\right] \mathbf{x} \text { (using dot product alternate form) }}
\end{aligned}
$$

## Optimization theory topics

- Maximum likelihood
- Expectation maximization
- Gradient descent

