Probability Theory for Machine Learning

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Introduction to Machine Learning
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Introduction to Notation

Motivation

Uncertainty arises through:

- Noisy measurements
- Finite size of data sets
- Ambiguity
- Limited Model Complexity

Probability theory provides a consistent framework for the quantification and manipulation of uncertainty.

Sample Space

Sample space Ω is the set of all possible outcomes of an experiment.

Observations $\omega \in \Omega$ are points in the space also called sample outcomes, realizations, or elements.

Events $E \subset \Omega$ are subsets of the sample space.

Sample Space Coin Example

In this experiment we flip a coin twice:

Sample space All outcomes $\Omega = \{HH, HT, TH, TT\}$

Observation $\omega = HT$ valid sample since $\omega \in \Omega$

Event Both flips same $E = \{HH, TT\}$ valid event since $E \subset \Omega$

Probability

Probability

The probability of an event E, $P(E)$, satisfies three axioms:

1: $P(E) \geq 0$ for every E

2: $P(\Omega) = 1$

3: If $E_1, E_2, \ldots$ are disjoint then

$$P(\bigcup_{i=1}^{\infty} E_i) = \sum_{i=1}^{\infty} P(E_i)$$

Joint and Conditional Probabilities

Joint Probability of A and B is denoted $P(A, B)$

Conditional Probability of A given B is denoted $P(A|B)$.

- Assuming $P(B) > 0$, then $P(A|B) = P(A, B)/P(B)$
- Product Rule: $P(A, B) = P(A|B)P(B) = P(B|A)P(A)$

Conditional Example

60% of ML students pass the final and 45% of ML students pass both the final and the midterm.
What percent of students who passed the final also passed the midterm?

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Reword: What percent passed the midterm given they passed the final?

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\begin{aligned}
P(M|F) &= P(M, F)/P(F) \\
&= 0.45/0.60 \\
&= 0.75
\end{aligned}
$$

Independence

Events A and B are independent if $P(A, B) = P(A)P(B)$

Events A and B are conditionally independent given C if
$P(A, B|C) = P(B|A, C)P(A|C) = P(B|C)P(A|C)$

Marginalization and Law of Total Probability

Marginalization (Sum Rule)

$$P(X) = \sum_{Y} P(X, Y)$$

Law of Total Probability

$$P(X) = \sum_{Y} P(X|Y)P(Y)$$

Bayes' Rule

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

$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

$$\text{Posterior} = \frac{\text{Likelihood} * \text{Prior}}{\text{Evidence}}$$

$$Posterior \propto Likelihood \times Prior$$

Bayes' Example

Suppose you have tested positive for a disease. What is the probability you actually have the disease?

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Suppose you have tested positive for a disease. What is the probability you actually have the disease?
This depends on accuracy and sensitivity of test and prior probability of the disease:

$$P(T = 1|D = 1) = 0.95 \text{ (true positive)}$$
$$P(T = 1|D = 0) = 0.10 \text{ (false positive)}$$
$$P(D = 1) = 0.1 \text{ (prior)}$$

So $P(D = 1|T = 1) = ?$

Bayes' Example

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So $P(D = 1|T = 1) = ?$

Use Bayes' Rule:

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

$$P(D = 1|T = 1) = \frac{P(T = 1|D = 1)P(D = 1)}{P(T = 1)}$$

Bayes' Example

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$P(T = 1|D = 1) = 0.95$ (true positive)

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Use Bayes' Rule:

$$P(D = 1|T = 1) = \frac{P(T = 1|D = 1)P(D = 1)}{P(T = 1)}$$

$$P(D = 1|T = 1) = \frac{0.95 * 0.1}{P(T = 1)}$$

Bayes' Example

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$P(T = 1|D = 1) = 0.95$ (true positive)
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$P(D = 1) = 0.1$ (prior)

$$P(D = 1|T = 1) = \frac{0.95 * 0.1}{P(T = 1)} \qquad \text{(Bayes' Rule)}$$

By Law of Total Probability

$$\begin{aligned} P(T = 1) &= \sum_D P(T = 1|D)P(D) \\ &= P(T = 1|D = 1)P(D = 1) + P(T = 1|D = 0)P(D = 0) \\ &= 0.95 * 0.1 + 0.1 * 0.90 \\ &= 0.185 \end{aligned}$$

Bayes' Example

Suppose you have tested positive for a disease. What is the probability you actually have the disease?

$P(T = 1|D = 1) = 0.95$ (true positive)

$P(T = 1|D = 0) = 0.10$ (false positive)

$P(D = 1) = 0.1$ (prior)

$P(T = 1) = 0.185$ (from Law of Total Probability)

$$
\begin{aligned}
P(D = 1|T = 1) &= \frac{0.95 * 0.1}{P(T = 1)} \\
&= \frac{0.95 * 0.1}{0.185} \\
&= 0.51
\end{aligned}
$$

Probability you have the disease given you tested positive is 51%

Random Variables and Statistics

Random Variable

How do we connect sample spaces and events to data?

A random variable is a mapping which assigns a real number $X(\omega)$ to each observed outcome $\omega \in \Omega$

For example, let's flip a coin 10 times. $X(\omega)$ counts the number of Heads we observe in our sequence. If $\omega = HHTHTHHTHT$ then $X(\omega) = 6$.

I.I.D.

Random variables are said to be independent and identically distributed (i.i.d.) if they are sampled from the same probability distribution and are mutually independent.
This is a common assumption for observations. For example, coin flips are assumed to be iid.

Discrete and Continuous Random Variables

Discrete Random Variables

- Takes countably many values, e.g., number of heads
- Distribution defined by probability mass function (PMF)
- Marginalization: $p(x) = \sum_y p(x, y)$

Continuous Random Variables

- Takes uncountably many values, e.g., time to complete task
- Distribution defined by probability density function (PDF)
- Marginalization: $p(x) = \int_y p(x, y) dy$

Probability Distribution Statistics

Mean: First Moment, μ

$$E[x] = \sum_{i=1}^{\infty} x_i p(x_i) \qquad \text{(univariate discrete r.v.)}$$

$$E[x] = \int_{-\infty}^{\infty} x p(x) dx \qquad \text{(univariate continuous r.v.)}$$

Variance: Second Moment, σ^2

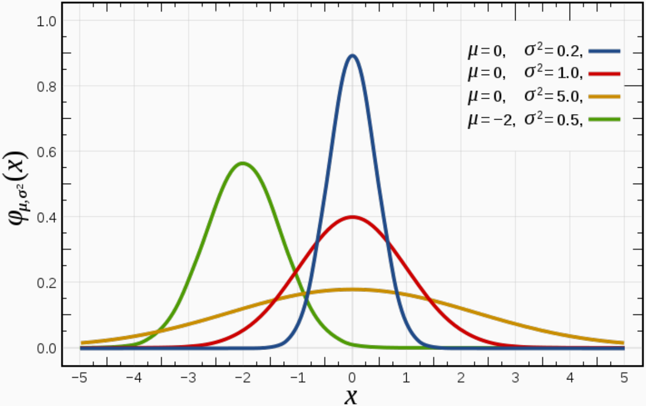
$$\begin{aligned} Var[x] &= \int_{-\infty}^{\infty} (x - \mu)^2 p(x) dx \\ &= E[(x - \mu)^2] \\ &= E[x^2] - E[x]^2 \end{aligned}$$

Gaussian Distribution

Univariate Gaussian Distribution

Also known as the Normal Distribution, $\mathcal{N}(\mu, \sigma^2)$

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\}$$



Multivariate Gaussian Distribution

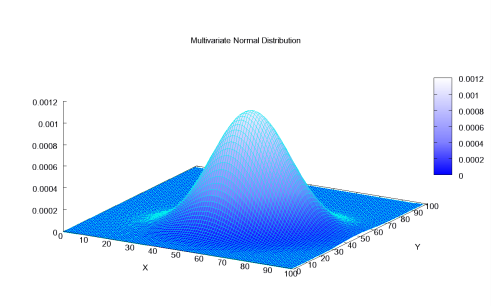
Multidimensional generalization of the Gaussian.

$\mathbf{x}$ is a D-dimensional vector

μ is a D-dimensional mean vector

Σ is a $D \times D$ covariance matrix with determinant $|\Sigma|$

$$\mathcal{N}(\mathbf{x}|\mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\}$$



Covariance Matrix

Recall that $\mathbf{x}$ and μ are D-dimensional vectors

Covariance matrix Σ is a matrix whose (i, j) entry is the covariance

$$
\begin{aligned}
\Sigma_{ij} &= Cov(\mathbf{x}_i, \mathbf{x}_j) \\
&= E[(\mathbf{x}_i - \mu_i)(\mathbf{x}_j - \mu_j)] \\
&= E[(\mathbf{x}_i \mathbf{x}_j)] - \mu_i \mu_j
\end{aligned}
$$

so notice that the diagonal entries are the variance of each elements.

The covariant matrix has the property that it is symmetric and positive-semidefinite (this is useful for whitening).

Whitening Transform

Whitening is a linear transform that converts a d-dimensional random vector $\mathbf{x} = (x_1, \ldots, x_d)^T$
with mean $\mu = E[\mathbf{x}] = (\mu_1, \ldots, \mu_d)^T$ and
positive definite $d \times d$ covariance matrix $Cov(\mathbf{x}) = \Sigma$
into a new random d-dimensional vector

$$\mathbf{z} = (z_1, \ldots, z_d)^T = W\mathbf{x}$$

with "white" covariance matrix, $Cov(\mathbf{z}) = \mathbf{I}$
The $d \times d$ covariance matrix W is called the whitening matrix.
Mahalanobis or ZCA whitening matrix: $W_{ZCA} = \Sigma^{-\frac{1}{2}}$

Inferring Parameters

Inferring Parameters

We have data X and we assume it is sampled from some distribution.
How do we figure out the parameters that 'best' fit that distribution?
Maximum Likelihood Estimation (MLE)

$$\hat{\theta}_{MLE} = \underset{\theta}{\operatorname{argmax}} P(X|\theta)$$

Maximum a Posteriori (MAP)

$$\hat{\theta}_{MAP} = \underset{\theta}{\operatorname{argmax}} P(\theta|X)$$

MLE for Univariate Gaussian Distribution

We are trying to infer the parameters for a Univariate Gaussian Distribution, mean (μ) and variance (σ^2).

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \text{exp}\{-\frac{1}{2\sigma^2}(x-\mu)^2\}$$

The likelihood that our observations $x_1, \ldots, x_N$ were generated by a univariate Gaussian with parameters μ and σ^2 is

$$\text{Likelihood} = p(x_1 \ldots x_N|\mu, \sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \text{exp}\{-\frac{1}{2\sigma^2}(x_i-\mu)^2\}$$

MLE for Univariate Gaussian Distribution

For MLE we want to maximize this likelihood, which is difficult because it is represented by a product of terms

$$\text{Likelihood} = p(x_1 \ldots x_N|\mu, \sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \text{exp}\{-\frac{1}{2\sigma^2}(x_i - \mu)^2\}$$

So we take the log of the likelihood so the product becomes a sum

$$\begin{aligned} \text{Log Likelihood} &= \log p(x_1 \ldots x_N|\mu, \sigma^2) \\ &= \sum_{i=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}} \text{exp}\{-\frac{1}{2\sigma^2}(x_i - \mu)^2\} \end{aligned}$$

Since log is monotonically increasing $\max L(\theta) = \max \log L(\theta)$

MLE for Univariate Gaussian Distribution

The log Likelihood simplifies to

$$\mathcal{L}(\mu, \sigma) = \sum_{i=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp\{-\frac{1}{2\sigma^2}(x_i - \mu)^2\}$$
$$= -\frac{1}{2} N \log(2\pi\sigma^2) - \sum_{i=1}^{N} \frac{(x_i - \mu)^2}{2\sigma^2}$$

Which we want to maximize. How?

MLE for Univariate Gaussian Distribution

To maximize we take the derivatives, set equal to 0, and solve:

$$\mathcal{L}(\mu, \sigma) = -\frac{1}{2} N \log(2\pi\sigma^2) - \sum_{i=1}^{N} \frac{(x_i - \mu)^2}{2\sigma^2}$$

Derivative w.r.t. μ, set equal to 0, and solve for $\hat{\mu}$

$$\frac{\partial \mathcal{L}(\mu, \sigma)}{\partial \mu} = 0 \implies \hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Therefore the $\hat{\mu}$ that maximizes the likelihood is the average of the data points.

Derivative w.r.t. σ^2, set equal to 0, and solve for $\hat{\sigma}^2$

$$\frac{\partial \mathcal{L}(\mu, \sigma)}{\partial \sigma^2} = 0 \implies \hat{\sigma}^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \hat{\mu})^2$$