1 Probability Basics

- Probability space $(\Omega, \mathcal{A}, P)$ is a real-world process with random outcomes (i.e. an experiment). Ex. Flip two coins and see how many heads show up.
- Sample space $\Omega$: set of all possible outcomes of the experiment. Ex. $\{\text{hh, tt, ht, th}\}$
- Event space $\mathcal{A}$: the space of potential results (events). Ex. the power set of of $\Omega$.
- Probability $P$: With each event $A \in \mathcal{A}$, we associate a number $P(A)$ that measures the belief that the event will occur. Ex. $P\{\text{hh, tt}\} = 0.5$
- Target space $\mathcal{T}$: target quantities of interest. Ex. $\mathcal{T} = \{0, 1, 2\}$ possible heads.
- Random Variable $X : \Omega \to \mathcal{T}$ lets us convert probabilities on the sample space $\Omega$ to probabilities on targets $\mathcal{T}$ (i.e. $\mathcal{T} = \mathbb{R}$).
- If $S \subseteq \mathcal{T}$, then $P_X(S) = P(\{\omega \in \Omega : X(\omega) \in S\})$. $P_X$ is the distribution of random variable $X$.
- If $\mathcal{T}$ is finite, $X$ is a discrete random variable. If $\mathcal{T}$ is continuous, $X$ is a continuous random variable.

Aside: Data points $x_1, \ldots, x_N$ are observations of a random variable (i.e. each observation is the result of an experiment). Probability lets us reason over these random experiments as $n \to \infty$. This will be key for studying generalization.

- Probability mass function: For a discrete random variable and a a potential observation $x \in \mathcal{T}$, we can write $P_X(x) = P(X = x)$. We often take $X$ to be implicit and people just write $P(x)$.
- Joint probability: we can consider probabilities of multiple random variables, i.e. $P(X = x, Y = y) = P(X = x \cap Y = y)$, often abbreviated as $p(x, y)$.
- For example: for a dataset of examples with labels $(x_1, y_1), \ldots, (x_N, y_N)$ we can let $X$ be a random variable for examples $x_i$, and $Y$ be a random variable for the labels $y_i$. This lets us formalize the probability of observing an example and its label as $p(x_i, y_i)$.
- Marginal probability: the marginal of $X$ is $P(X = x)$, which is irrespective of the random variable $Y$, often lazily written as $p(x)$
- Conditional probability: the conditional probability of $Y$ given $X$ is $P(Y = y | X = x)$, often lazily written as $p(y|x)$
Aside: In ML we will want to be modeling predictions from your data, i.e. $p(y|x)$ where $x$ is the input to your model and $y$ is the prediction. We’ll now consider real valued continuous distributions, where $\mathcal{T} = \mathbb{R}^D$.

- Probability density function: A function $f : \mathbb{R}^D \rightarrow \mathbb{R}$ is a PDF if (1) $\forall x \in \mathbb{R}^D : f(x) \geq 0$ and (2) $\int_{\mathbb{R}^D} f(x) dx = 1$.
- This is like the probability mass function, where the integral is replaced by a sum.
- We can associate a PDF with a random variable $X$, in the 1D case, $P(a \leq X \leq b) = \int_a^b f(x) dx$ where $a, b, x \in \mathbb{R}$. In this case, $P$ is the distribution of $X$.
- The multi-dimensional PDF is similar:
  \[
P(a_1 \leq X_1 \leq b_1, \ldots, a_D \leq X_D \leq b_D) = \int_{a_1}^{b_1} \cdots \int_{a_D}^{b_D} f(x_1, \ldots, x_D) dx_D \cdots dx_1
  \]
  We will often abbreviate these to vectors $a, b, x \in \mathbb{R}^D$ as $\int_a^b f(x) dx$.
- $P(X = x)$ no longer makes sense here as it is equal to 0 (equivalent to taking the interval $[a, b]$ where $a = b = x$).
- Typically we use a one-sided interval: for a particular outcome $x \in \mathcal{T}$, we often refer to to $F_X(x) = P(X \leq x)$ as the cumulative density function (CDF).
- For a vector of random variables (i.e. the joint distribution), this can be explicitly written out as $P(X_1 \leq x_1, \ldots, X_D \leq x_d)$, but will typically also be abbreviated as $F_X(x) = P(X \leq x)$.

Aside: all probabilities, discrete or continuous, are positive and sum to one. But for continuous distributions, the PDF may be more than one at some points. See Example 6.3 in the textbook on the uniform distribution.

- There are really only two fundamental rules in probability for reasoning about distributions: the sum and the product rule.
- The sum rule is also known as the marginalization property (recall the marginal of $x$ is $p(x)$) and relates the joint distribution to the marginal distribution
- Sum rule (discrete):
  \[
p(x) = \sum_{y \in \mathcal{Y}} p(x, y)
  \]
- Sum rule (continuous):
  \[
p(x) = \int_{y \in \mathcal{Y}} p(x, y) dy
  \]
- Note that, as always, $x, y$ can be vectors
- Example: for a joint distribution $p(x) = p(x_1, \ldots, x_D)$, we can sum out all but one to get $p(x_i) = \int p(x) dx_{\setminus i}$
The product rule says that every joint distribution can be factorized into a product of a conditional and marginal.

Product rule (discrete and continuous):

\[ p(x, y) = p(y|x)p(x) \]

Ordering of \( x, y \) is arbitrary, and uses PDF/PMF for continuous/discrete distributions

Bayes theorem:

\[ p(x|y) = \frac{p(y|x)p(x)}{p(y)} \]

Consequence of the product rule

In ML terms, this relates the posterior with the likelihood, prior and evidence (Eq 6.23 from the textbook)

Prior \( p(x) \): subjective belief about target of interest \( x \) without observing anything

Likelihood \( p(y|x) \) relates the evidence \( y \) and the target of interest \( x \) (likelihood of \( x \) given \( y \))

Posterior \( p(x|y) \) is what we know about \( x \) after seeing the evidence \( y \) and is usually what we care about

Evidence \( p(y) \) keeps the distribution normalized, sometimes called the marginalized likelihood since \( p(y) = \int p(y|x)p(x)dx \). This can be hard to compute for vector valued \( x \).

Bayes theorem lets us “invert” a conditional. This can be useful when the target we care about \( x \) is not directly observable, other evidence \( y \) is observable. By choosing a prior \( p(x) \), we can reason about \( p(x|y) \) in terms of only the evidence \( y \) without explicitly observing \( x \).

Aside: A common application of this section of probability is to reason about the parameters of your hypothesis class and find the most likely set of parameters given the data (hence maximum likelihood). Recall that in ML, we try to select the “best” function from the hypothesis class \( f_\theta \in \mathcal{F} \) where \( \theta \) is a set of parameters that determines the exact function. Some hypothesis classes directly parameterize a probability.

Recall that in ML, we try to minimize the risk on a dataset:

\[ \min_\theta R_{\text{emp}}(f_\theta, X, Y) = \sum_{i=1}^{N} \ell(f(x_i), y_i) \]

where \( \theta \) is a set of parameters that determines a particular function from the hypothesis class, \( f_\theta \in \mathcal{F} \)

Often, in ML we define a function class that directly predicts \( f_\theta(x) = p(y|x; \theta) \)
For example, a simple linear model that predicts one of two classes is

\[ f(x) = p(1|x) = \sigma(\theta^T x) \]

where \( \sigma \) is the sigmoid function

\[ \sigma(x) = \frac{1}{1 + e^{-x}} \]

- The sigmoid function parameterizes a smooth function that transitions between \([0, 1]\)
- One common choice for loss function is called the negative log likelihood: \( \ell(f(x), y) = -\log p(y|x; \theta) \).
- Maximizing/minimizing the log of a function results in the same solution as maximizing/minimizing the original function
- This results in maximum likelihood estimation (MLE):

\[ \min_\theta R_{\text{emp}}(f_\theta, X, Y) = \max_\theta \sum_{i=1}^{N} \log p(y|x; \theta) \]

- Example: MLE for the linear model is

\[ \max_\theta \sum_{i=1}^{N} \log p(y|x; \theta) = \max_\theta \sum_{i=1}^{N} \log \sigma(\theta^T x_i) = \max_\theta \sum_{i=1}^{N} -\log(1 + e^{\theta^T x_i}) \]

- In ML we call this (MLE + linear model + binary classification) logistic regression. Note that even though this is called logistic regression, it is confusingly predicting a classification problem.

In this example, MLE/negative log likelihood defines the objective, while linear binary classifier defines the model. This is just one possible example—many different machine learning models simply vary the the type of model. However, we can also vary the objective. A common choice is to use Bayes rule and is called maximum a posterior estimation (MAP).

- An alternative type of risk to minimize is the Bayes risk:

\[ \min_\theta R_{\text{Bayes}}(f_\theta, X, Y) = \min_\theta -\log p(\theta|X, Y) = \max_\theta \log p(\theta|X, Y) \]

- This is in contrast to the empirical risk:

\[ \min_\theta R_{\text{emp}}(f_\theta, X, Y) = \max_\theta \log p(Y|X, \theta) \]

- To calculate the Bayes risk, we simply apply Bayes rule to get something similar to the empirical risk:

\[ p(\theta|X, Y) = \frac{p(Y|X; \theta)p(\theta|X)}{p(Y|X)} \]

- Minimizing the Bayes risk is known as maximum a posterior estimation (MAP):

\[ \max_\theta \log p(Y|X; \theta) + \log p(\theta|X) - \log p(Y|X) \propto \max_\theta \log p(Y|X; \theta) + \log p(\theta) \]
• This differs from MLE only via the prior term \( \log p(\theta) \)
• The posterior in MAP in this case is \( p(\theta|X,Y) \), hence maximum a posterior
• Whereas the MLE maximizes the likelihood, \( p(Y|X,\theta) \)

Aside: Up to this point, we’ve used random variables to represent examples from a given distribution, such as \((X_1,Y_1),\ldots,(X_N,Y_N)\) to represent \(N\) datapoints with \(N\) labels. However, we typically want to summarize these sets of random variables with a single quantity. This is called a statistic, which is a deterministic function of random variables. These statistics describe how random variables behave.

• Two common statistics: mean and variance
  • Expected value of a function \( g : \mathbb{R} \to \mathbb{R} \) of random variables is the average over many random draws. For continuous distributions this is:
    \[
    \mathbb{E}_X[g(x)] = \int_X g(x)p(x)dx
    \]
  For discrete distributions, this is:
    \[
    \mathbb{E}_X[g(x)] = \sum_x g(x)p(x)dx
    \]
  • Sometimes, this is written as \( \mathbb{E}_X[g(x)] = \mathbb{E}_{x \sim X}[g(x)] = \mathbb{E}[g(x)] \)
  • If \( X \) is a random variable with probability \( p \), then we can also write this as \( \mathbb{E}_X[g(x)] = E_p(g(x)) \) or \( E_p[g(x)] \) or \( E_{x \sim p}[g(x)] \)
  • A conditional expectation is the same, using a conditional probability distribution:
    \[
    \mathbb{E}_X[g(x)|y] = \int_X g(x)p(x|y)dx
    \]
  • An expectation of a vector of random variables is the vector of expectations of each random variable:
    \[
    \mathbb{E}_X[g(x)] = \begin{bmatrix} \mathbb{E}_{X_1}[g(x_1)] \\ \vdots \\ \mathbb{E}_{X_N}[g(x_N)] \end{bmatrix}
    \]
  • The mean statistic is the special case where \( g(x) = x \), for example \( \mathbb{E}[x] = \int_X xp(x)dx \)
  • Often we use the symbol \( \mathbb{E}[x] = \mu \)
  • Intuitively, the mean is the “average” value. We will use averages when summing many random variables together from the same distribution.
  • The expected value is a linear operator. This means that if \( f(x) = ag(x) + bh(x) \), then
    \[
    \mathbb{E}[f(x)] = a\mathbb{E}[g(x)] + b\mathbb{E}[h(x)]
    \]
• Covariance is the expected product of deviations of two random variables from their means.

\[
\text{Cov}_{X,Y}[x,y] = \mathbb{E}_{X,Y}[(x - \mathbb{E}[x])(y - \mathbb{E}[y])]
\]

• Covariance measures how dependent two random variables are. If it is high, they more dependent

\[
\text{Cov}_{X,Y}[x,y] = \mathbb{E}_{X,Y}[xy] - \mathbb{E}[x]\mathbb{E}[y]
\]

• The covariance of a variable with itself is the variance \(\text{Var}_X[x] = \mathbb{V}[x] = \text{Cov}_{X,X}[x,x]\)

• Often we use the symbol \(\mathbb{V}[x] = \Sigma\)

• For a single random variable, the square root of the variance is the standard deviation, \(\sigma(x) = \sqrt{\text{Var}_X[x]}\)

• Using the second form of the covariance, we can generalize this to vectors \(x, y \in \mathbb{R}^D \times \mathbb{R}^E\) as

\[
\text{Cov}_{X,Y}[x,y] = \mathbb{E}_{X,Y}[xy^T] - \mathbb{E}[x]\mathbb{E}[y]^T \in \mathbb{R}^{D \times E}
\]

and the variance is

\[
\mathbb{V}[x] = \text{Cov}[x,x]
\]

, also called the covariance matrix (measures spread)

• Correlation is a normalized form of covariance between two random variables (i.e. the covariance is divided by the variance of the two random variables and measures how closely two variables change together):

\[
\text{corr}[x,y] = \frac{\text{Cov}[x,y]}{\sqrt{\mathbb{V}[x]\mathbb{V}[y]}}
\]

• Variance can be done in three ways:

  1. \(\mathbb{V}[x] = \mathbb{E}[(x - \mu)^2]\) measures spread of a random variable
  2. \(\mathbb{V}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2\) is the “raw score formula” that can be done in one pass but is numerically unstable
  3. \(\frac{1}{N} \sum_{ij} (x_i - x_j)^2 = 2 \left[ \frac{1}{N} \sum_i x_i^2 - \left( \frac{1}{N} \sum_i x_i \right)^2 \right]\) is the sum of pairwise differences

• \(\mathbb{E}[x + y] = \mathbb{E}[x] + \mathbb{E}[y]\)

• \(\mathbb{E}[x - y] = \mathbb{E}[x] - \mathbb{E}[y]\)

• \(\mathbb{V}[x + y] = \mathbb{V}[x] + \mathbb{V}[y] + \text{Cov}[x,y] + \text{Cov}[y,x]\)

• \(\mathbb{V}[x - y] = \mathbb{V}[x] + \mathbb{V}[y] - \text{Cov}[x,y] - \text{Cov}[y,x]\)

• If \(y = Ax + b\) where \(x, y\) are random variables, then

\[
\mathbb{E}[y] = \mathbb{E}[Ax + b] = A\mathbb{E}[x] + b = A\mu + b
\]

and

\[
\mathbb{V}[y] = \mathbb{V}[Ax + b] = \mathbb{V}[Ax] = A\mathbb{V}[x]A^T = A\Sigma A^T
\]

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Aside: In practice, we don’t typically have the true distributions of \( X, Y \) but instead have a finite number of observations of the random variables \((x_1, y_1), \ldots, (x_N, y_N)\). Therefore, we will often estimate the an expected value with these samples by replacing the expected value with a summation:

\[
\mathbb{E}[g(x)] \approx \frac{1}{N} \sum_{i=1}^{N} g(x_i)
\]

Therefore, the empirical mean and empirical covariance are simply

\[
\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i
\]

and

\[
\Sigma = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T
\]

- Independence: Two random variable \( X, Y \) are statistically independent if and only if \( p(x, y) = p(x)p(y) \)
- This implies the following:
  1. \( p(y|x) = p(y) \)
  2. \( p(x|y) = p(x) \)
  3. \( \forall x + y = V[x] + V[y] \)
  4. \( \text{Cov}[x, y] = 0 \)
- The converse is not true, i.e. if \( \mathbb{E}[x] = 0 \) and \( \mathbb{E}[x^3] = 0 \) and let \( y = x^2 \), then \( \text{Cov}[x, y] = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y] = \mathbb{E}[x^3] = 0 \) (they are dependent but not correlated)
- A standard assumption in ML is that random variables are independent and identically distributed (i.i.d.), typically for the random variables representing the observations in the dataset \((X_1, \ldots, X_N)\)
- This means that each random variable has the same distribution \( p \), and that each random variable is independent from each other
- We used this earlier when defining the empirical risk: \( p(Y|X; \theta) = \prod_{i=1}^{N} p(y_i|x_i; \theta) \)
- Conditional independence: \( X, Y \) are conditionally independent given \( Z \) if and only if \( p(x, y|z) = p(x|z)p(y|z) \) for all \( z \in \mathcal{Z} \)
- Alternatively, \( p(x|y, z = p(x|z). \) This can be seen by using the product rule on the LHS and comparing it to the definition of conditional independence.

Aside: In the previous linear example, recall that we wrote the empirical risk as a sum of losses over \( N \) examples:

\[
\min_{\theta} R_{\text{emp}}(f_\theta, X, Y) = \sum_{i=1}^{N} -\log p(y_i|x_i; \theta)
\]
where the loss was the negative log likelihood. Where did this loss come from? We actually cheated a little bit: this is only true if we assume that the random variables are i.i.d. Without any assumptions, our starting point is to actually maximize the joint likelihood of the entire dataset under the model parameterized by \( \theta \) (maximum likelihood):

\[
\max_{\theta} p(Y|X; \theta)
\]

However, modeling an entire dataset jointly is complicated! To simplify this, we assume that the vectors of \((x_i, y_i)\) are independent and identically distributed. Independence allows us to consider the product over \(N\) random variables:

\[
\max_{\theta} \prod_{i=1}^{N} p_i(y_i|x_i; \theta)
\]

and then identical allows us to use a single model to represent all data points:

\[
\max_{\theta} \prod_{i=1}^{N} p(y_i|x_i; \theta)
\]

Lastly, we take a log for numerical stability since the solution to the maximum is the same:

\[
\max_{\theta} \sum_{i=1}^{N} \log p(y_i|x_i; \theta)
\]

Flipping to minimizing the negative objective gets us the minimum likelihood formulation:

\[
\min_{\theta} \sum_{i=1}^{N} -\log p(y_i|x_i; \theta)
\]

2 Distributions

- (Multivariate) Gaussian/Normal distribution is one of the most commonly used distributions in ML
- It represents having most samples clustered around the mean with the ability to have outliers
- Univariate Gaussian - \( p(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left( -\frac{(x-\mu)^2}{2\sigma^2} \right) \) for \( x \in \mathbb{R} \)
- Multivariate Gaussian - \( p(x|\mu, \Sigma) = (2\pi)^{-\frac{D}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left( -\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu) \right) \) for \( x \in \mathbb{R}^D \)
- We write \( p(x) = \mathcal{N}(x|\mu, \Sigma) \), \( p(x) = \mathcal{N}(\mu, \Sigma) \), \( p \sim \mathcal{N}(x|\mu, \Sigma) \) or \( X \sim \mathcal{N}(\mu, \Sigma) \)
- \( \mathcal{N}(0, I) \) is the standard normal distribution where \( I \) is the identity matrix
- Joint distribution of MVN. Suppose we represent a MVN as the concatenation of two vectors of MVN:

\[
p(x, y) = \mathcal{N}\left( \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix} \right)
\]

where \( \Sigma_{xy} = \text{Cov}[x, y] \) and \( \Sigma_{xx}, \Sigma_{yy} \) are the marginal variances of \( x \) and \( y \)
• Then the marginals \( p(x) = \int p(x,y) dy = \mathcal{N}(\mu_x, \sigma_{xx}) \) and \( p_y = \int p(x,y) dx = \mathcal{N}(\mu_y, \sigma_{yy}) \) are Gaussian

• And the conditional distribution \( p(x|y) \) is also Gaussian

\[
p(x|y) = \mathcal{N}(\mu_{x|y}, \Sigma_{x|y})
\]

where

\[
\mu_{x|y} = \mu_x + \Sigma_{xy} \Sigma_{yy}^{-1} (y - \mu_y)
\]

and

\[
\Sigma_{x|y} = \Sigma_{xx} - \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{yx}
\]

Aside: Applications of the conditional Gaussian distribution are classic algorithms such as the Kalman filter (which does nothing but compute Gaussian conditions from joints) and Gaussian processes (assume that observations from a function are jointly Gaussian to get a Gaussian posterior over functions).

• Products of Gaussians is Gaussian:

\[
\mathcal{N}(x|a, A)\mathcal{N}(x|b, B) = c' \mathcal{N}(x|c, C)
\]

where

\[
C = (A^{-1} + B^{-1})^{-1}
\]

\[
c = C(A^{-1}a + B^{-1}b)
\]

\[
c' = (2\pi)^{-D/2}|A + B|^{-1/2} \exp \left( -\frac{1}{2} (a - b)^T (A + B)^{-1} (a - b) \right) = \mathcal{N}(a|b, A + B)
\]

• Note that in the definition of \( c' \), it is convenient to write it as the density of another Normal distribution even though \( c' \) is not random

• Sums of Gaussians is Gaussian:

\[
p(x + y) = \mathcal{N}(\mu_x + \mu_y, \Sigma_x + \Sigma_y)
\]

• Same for a weighted sum:

\[
p(ax + by) = \mathcal{N}(a\mu_x + b\mu_y, a^2\Sigma_x + b^2\Sigma_y)
\]

• This is related to but different from the sum of the densities: if \( p(x) = \alpha p_1(x) + (1 - \alpha) p_2(x) \) where \( p_1, p_2 \) are Gaussian. In this case, \( p \) is not Gaussian. The mean is similar, i.e. \( \mathbb{E}[x] = \alpha \mu_1 + (1 - \alpha) \mu_2 \), but the variance is different (Theorem 6.12):

\[
\mathbb{V}[x] = \alpha \sigma_1^2 + (1 - \alpha) \sigma_2^2 + [(\alpha \mu_1^2 + (1 - \alpha) \mu_2^2] - [\alpha \mu_1 + (1 - \alpha) \mu_2]^2)
\]

• This is an example of the law of total variance, i.e.

\[
\mathbb{V}[x] = \mathbb{E}[\mathbb{V}[x|y]] + \mathbb{V}[\mathbb{E}[x|y]]
\]
Linear transform of a Gaussian is Gaussian. If \( x \sim \mathcal{N}(\mu, \Sigma) \), and \( y = Ax \) is Gaussian where

\[
\mathbb{E}[y] = \mathbb{E}[Ax] = A\mathbb{E}[x] = A\mu
\]

and

\[
\mathbb{V}[y] = \mathbb{V}[Ax] = A\mathbb{V}[x]A^T = A\Sigma A^T
\]

so \( p(y) = \mathcal{N}(A\mu, A\Sigma A^T) \)

Aside: The Gaussian is a distribution that has a lot of very nice properties. Many operations of Gaussians also return Gaussians. However, there are many things in this world are not Gaussian (i.e. even the simple mixture of Gaussians is not Gaussian). There is a generalization of Gaussians called the exponential family that has similarly nice properties but allows for a more expressive set of distributions.

- Bernoulli distribution: for a random variable \( X \) with target state \( x \in \{0, 1\} \), Ber(\( \mu \)) is defined as

\[
p(x; \mu) = \mu^x(1-\mu)^{1-x}
\]

where \( \mathbb{E}[x] = \sum_x xp(x) = \mu \) and \( \mathbb{V}[x] = \sum_x (x-\mu)^2 p(x) = (1-\mu)^2 \mu + \mu^2(1-\mu) = \mu(1-\mu) \)

- Bernoulli simulates flipping a coin with probability \( \mu \) of being heads.

- This trick of using exponents for Boolean variables is often used in ML

- Binomial distribution: for a random variable \( X \) with target states \( 1, \ldots, N \), Bin(\( N, \mu \)) is defined as

\[
p(m; N, \mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}
\]

where \( \mathbb{E}[m] = N\mu \) and \( \mathbb{V}[m] = N\mu(1-\mu) \)

- Binomial simulates flipping a coin with probability \( \mu \) \( N \) times and counting the number of heads

- Beta distribution: for a random variable \( \mu \) with target states \( [0, 1] \), Beta(\( \alpha, \beta \)) for \( \alpha, \beta > 0 \) is defined as

\[
p(\mu; \alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \mu^{\alpha-1}(1-\mu)^{\beta-1}
\]

where \( \mathbb{E}[\mu] = \frac{\alpha}{\alpha+\beta} \) and \( \mathbb{V}[\mu] = \frac{\alpha \beta}{(\alpha+\beta)^2(\alpha+\beta+1)} \).

- \( \Gamma(t) \) is the Gamma function defined as

\[
\Gamma(t) = \int_0^\infty n!ty^{t-1}\exp(-x)dx
\]

where \( \Gamma(t+1) = t\Gamma(t) \).

- The Gamma function serves to normalize the Beta distribution.

- Beta models a continuous distribution on the interval \([0, 1]\) often used to simulate the probability of a binary event (i.e. the parameter of the Bernoulli distribution).
• \( \alpha = \beta = 1 \) is the Uniform distribution
• \( \alpha, \beta < 1 \) is bimodal with spikes at 0 and 1
• \( \alpha, \beta > 1 \) is unimodal. If \( \alpha = \beta \) then it is symmetric and centered with mean/mode at 0.5.

**Aside:** We can define a whole slew of additional distributions. However there is a group of distributions that has a nice property like the Gaussian distribution, where combining two different distributions results in another known distribution. Remember that for the posterior, we have:

\[
p(\theta | X, Y) \propto p(Y | \theta, X)p(\theta)
\]

If we say, model the likelihood as a Binomial and the prior as a Beta, it turns out that the posterior is a Beta distribution! This relation is known as conjugacy and shows up in the exponential family. Because the form of the posterior is nice and simple, ML algorithms like to use conjugate priors.

• Example 6.11 (Beta-Binomial Conjugacy)
• Suppose \( x \sim \text{Bin}(N, \mu) \) (likelihood). Then consider a Beta prior on \( \mu \sim \text{Beta}(\alpha, \beta) \). Then

\[
p(\mu | x, N, \alpha, \beta) \propto p(x | N, \mu)p(\mu | \alpha, \beta) \propto \mu^{x}(1 - \mu)^{N-x}\mu^{\alpha-1}(1 - \mu)^{\beta-1} = \mu^{x+\alpha-1}(1 - \mu)^{N-x+\beta-1} \propto \text{Beta}(x+\alpha, N-x+\beta)
\]

• Similarly, Beta is also a conjugate prior for Bernoulli (Example 6.12). See Table 6.2 for more example of conjugate priors for common likelihoods.

**Aside:** We can generalize these “nice” distributions to a larger family known as the exponential family. Exponential families interact nicely with the log operator (i.e. when calculating log probabilities) and have small tails (i.e. good for concentration around the mean). We’ll abstract our
distributions from parametric distributions with fixed parameters (i.e. \( N(0, 1) \)) to parametric with learned parameters (i.e. \( N(\mu, \sigma^2) \) where \( \mu, \sigma \) are estimated from the data with MLE) to families of distributions that capture multiple parametric forms (the exponential family).

- **Sufficient statistic (Theorem 6.14, Fisher-Neyman):** Let \( X \sim p(x|\theta) \). Then, \( \phi(x) \) is a sufficient statistic for \( \theta \) if and only if \( p(x|\theta) \) can be written as
  \[
p(x|\theta) = h(x)g_\theta(\phi(x))
  \]
  where \( h(x) \) is independent of \( \theta \) and \( g_\theta \) captures all dependencies on \( \theta \) via \( \phi(x) \).

- **Exponential family is characterized by**
  \[
p(x|\theta) = h(x)\exp(\theta^T \phi(x) - A(\theta)) \propto \exp(\theta^T \phi(x))
  \]
  This is just a particular expression of \( g_\theta \) for sufficient statistics.

- To see the last proportional equivalence, move \( h(x) \) into the dot product by adding \( \log h(x) \) to the sufficient statistics and add \( \theta_0 = 1 \) to the parameters, and \( A(\theta) \) is just a normalizing constant, i.e.
  \[
  A(\theta) = \log \int e^{\theta^T \phi(x)} dx
  \]

- Gaussian, Bernoulli are exponential families and have nice log probabilities. Example 6.13 (univariate Gaussian) and 6.14 (Bernoulli).

- **Key property:** every member of the exponential family has a conjugate prior (Brown, 1986):
  \[
p(\theta|\gamma) = h_c(\theta)\exp \left( \left\langle \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}, \begin{bmatrix} \theta \\ -A(\theta) \end{bmatrix} \right\rangle - A_c(\gamma) \right)
  \]
  With this property, we can derive the conjugate prior without knowing it in advance for distributions in the exponential family.