Probability Basics for Machine Learning

CSC411
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*Based on many others’ slides and resources from Wikipedia
Outline

• Motivation
• Notation, definitions, laws
• Exponential family distributions
  – E.g. Normal distribution
• Parameter estimation
• Conjugate prior
Why Represent Uncertainty?

• The world is full of uncertainty
  – “Is there a person in this image?”
  – “What will the weather be like today?”
  – “Will I like this movie?”

• We’re trying to build systems that understand and (possibly) interact with the real world

• We often can’t prove something is true, but we can still ask how likely different outcomes are or ask for the most likely explanation
Why Use Probability to Represent Uncertainty?

• Write down simple, reasonable criteria that you'd want from a system of uncertainty (common sense stuff), and you always get probability:
  – Probability theory is nothing but common sense reduced to calculation. — Pierre Laplace, 1812
• Cox Axioms (Cox 1946); See Bishop, Section 1.2.3
• We will restrict ourselves to a relatively informal discussion of probability theory.
Notation

• A **random variable X** represents outcomes or states of the world.

• We will write $p(x)$ to mean $\text{Probability}(X = x)$

• **Sample space**: the space of all possible outcomes (may be discrete, continuous, or mixed)

• $p(x)$ is the **probability mass (density) function**
  – Assigns a number to each point in sample space
  – Non-negative, sums (integrates) to 1
  – Intuitively: how often does $x$ occur, how much do we believe in $x$. 
Joint Probability Distribution

- \( \text{Prob}(X=x, Y=y) \)
  - “Probability of \( X=x \) and \( Y=y \)”
  - \( p(x, y) \)

Conditional Probability Distribution

- \( \text{Prob}(X=x \mid Y=y) \)
  - “Probability of \( X=x \) given \( Y=y \)”
  - \( p(x \mid y) = \frac{p(x,y)}{p(y)} \)
The Rules of Probability

• Sum Rule (marginalization/summing out):

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

\[ p(x_1) = \sum_{x_2} \sum_{x_3} \ldots \sum_{x_N} p(x_1, x_2, \ldots, x_N) \]

• Product/Chain Rule:

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

\[ p(x_1, \ldots, x_N) = p(x_1) p(x_2 \mid x_1) \ldots p(x_N \mid x_1, \ldots, x_{N-1}) \]
Bayes’ Rule

- One of the most important formulas in probability theory

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

- This gives us a way of “reversing” conditional probabilities
Independence

• Two random variables are said to be **independent** iff their joint distribution factors
\[ X \perp Y \iff p(x, y) = p(y \mid x)p(x) = p(x \mid y)p(y) = p(x)p(y) \]

• Two random variables are **conditionally independent** given a third if they are independent after conditioning on the third
\[ X \perp Y \mid Z \iff p(x, y \mid z) = p(y \mid x, z)p(x \mid z) = p(y \mid z)p(x \mid z) \quad \forall z \]
Continuous Random Variables

• Outcomes are real values. Probability density functions define distributions.
  – E.g.,

\[
P(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2} (x - \mu)^2 \right\}
\]

• Continuous joint distributions: replace sums with integrals, and everything holds
  – E.g., Marginalization and conditional probability

\[
P(x, z) = \int P(x, y, z) = \int P(x, z \mid y)P(y)
\]
Summarizing Probability Distributions

• It is often useful to give summaries of distributions without defining the whole distribution (E.g., mean and variance)

• Mean: \( E[x] = \langle x \rangle = \int_{x} x \cdot p(x) \, dx \)

• Variance: \( \text{var}(x) = \int_{x} (x - E[x])^2 \cdot p(x) \, dx \)
  \[ = E[x^2] - E[x]^2 \]

• Nth moment: \( \mu_n = \int_{x} (x - c)^n \cdot p(x) \, dx \)
Exponential Family

• Family of probability distributions
• Many of the standard distributions belong to this family
  – Bernoulli, binomial/multinomial, Poisson, Normal (Gaussian), beta/Dirichlet,…
• Share many important properties
  – e.g. They have a conjugate prior (we’ll get to that later. Important for Bayesian statistics)
• First – let’s see some examples
Definition

• The exponential family of distributions over $x$, given parameter $\eta$ (eta) is the set of distributions of the form

$$p(x \mid \eta) = h(x) g(\eta) \exp\{\eta^T u(x)\}$$

• $x$-scalar/vector, discrete/continuous
• $\eta$ – ‘natural parameters’
• $u(x)$ – some function of $x$ (sufficient statistic)
• $g(\eta)$ - normalizer

$$g(\eta) \int h(x) \exp\{\eta^T u(x)\} dx = 1$$
Example 1: Bernoulli

- Binary random variable -  \( X \in \{0,1\} \)
- \( p(\text{heads}) = \mu \)
- Coin toss

\[
p(x \mid \mu) = \mu^x (1 - \mu)^{1-x}
\]
Example 1: Bernoulli

\[ p(x \mid \eta) = h(x) g(\eta) \exp \{ \eta^T u(x) \} \]

\[
p(x \mid \mu) = \mu^x (1 - \mu)^{1-x}
= \exp \{ x \ln \mu + (1 - x) \ln(1 - \mu) \}
= (1 - \mu) \exp \{ \ln \left( \frac{\mu}{1 - u} \right) x \}
\]

\[
p(x \mid \eta) = \sigma(-\eta) \exp(\eta x)
\]

\[
h(x) = 1
u(x) = x
\eta = \ln \left( \frac{\mu}{1 - \mu} \right) \Rightarrow \mu = \sigma(\eta) = \frac{1}{1 + e^{-\eta}}
g(\eta) = \sigma(-\eta)\]
Example 2: Multinomial

- \( p(\text{value } k) = \mu_k \) \( \mu_k \in [0,1], \sum_{k=1}^{M} \mu_k = 1 \)
- For a single observation – die toss
  - Sometimes called Categorical
- For multiple observations
  - integer counts on \( N \) trials
  - \( \text{Prob}(1 \text{ came out 3 times, 2 came out once,...,6 came out 7 times if I tossed a die 20 times}) \)

\[
P(x_1, \ldots, x_M \mid \mu) = \frac{N!}{\prod_{k} x_k!} \prod_{k=1}^{M} \mu_k^{x_k}
\]
Example 2: Multinomial (1 observation)

\[ p(x \mid \eta) = h(x)g(\eta) \exp\{\eta^T u(x)\} \]

\[ P(x_1, \ldots, x_M \mid \mu) = \prod_{k=1}^{M} \mu_k^{x_k} \]

\[ = \exp\left\{ \sum_{k=1}^{M} x_k \ln \mu_k \right\} \]

\[ p(x \mid \eta) = \exp(\eta^T x) \]

\[ h(x) = 1 \]
\[ u(x) = x \]

Parameters are not independent due to constraint of summing to 1, there’s a slightly more involved notation to address that, see Bishop 2.4
Example 3: Normal (Gaussian) Distribution

- Gaussian (Normal)

\[
p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{ -\frac{1}{2\sigma^2} (x - \mu)^2 \right\}
\]
Example 3: Normal (Gaussian) Distribution

\[ p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2} (x - \mu)^2 \right\} \]

- \( \mu \) is the mean
- \( \sigma^2 \) is the variance
- Can verify these by computing integrals. E.g.,

\[
\int_{x \to -\infty}^{x \to \infty} x \cdot \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{-\frac{1}{2\sigma^2} (x - \mu)^2 \right\} \, dx = \mu
\]
Example 3: Normal (Gaussian) Distribution

- Multivariate Gaussian

\[
P(x | \mu, \Sigma) = \left|2\pi \Sigma\right|^{-1/2} \exp\left\{ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right\}
\]
Example 3: Normal (Gaussian) Distribution

- Multivariate Gaussian

\[
p(x \mid \mu, \Sigma) = \left| 2\pi \Sigma \right|^{-1/2} \exp\left\{ -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right\}
\]

- \(x\) is now a vector
- \(\mu\) is the **mean vector**
- \(\Sigma\) is the **covariance matrix**
Important Properties of Gaussians

• All marginals of a Gaussian are again Gaussian
• Any conditional of a Gaussian is Gaussian
• The product of two Gaussians is again Gaussian
• Even the sum of two independent Gaussian RVs is a Gaussian.
Exponential Family Representation

\[ p(x \mid \eta) = h(x)g(\eta)\exp\{\eta^T u(x)\} \]

\[ p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}}\exp\left\{-\frac{1}{2\sigma^2}(x - \mu)^2\right\} \]

\[ = \frac{1}{\sqrt{2\pi\sigma}}\exp\left\{-\frac{1}{2\sigma^2}x^2 + \frac{\mu}{\sigma^2}x + \frac{-1}{2\sigma^2}\mu^2\right\} = \]

\[ = (2\pi)^{-\frac{1}{2}}(-2\eta_2)^{-\frac{1}{2}}\exp\left(\frac{-\eta_1^2}{4\eta_2}\right)\exp\left\{\frac{\mu}{\sigma^2} \begin{bmatrix} \frac{-1}{2\sigma^2} \\ \eta^T \\ u(x) \end{bmatrix} \begin{bmatrix} x \\ x^2 \end{bmatrix}\right\} \]

\[ \begin{align*}
&h(x) &\quad &g(\eta) &\quad &\begin{bmatrix} \frac{-1}{2\sigma^2} \\ \eta^T \\ u(x) \end{bmatrix} \begin{bmatrix} x \\ x^2 \end{bmatrix}
\end{align*} \]
Example: Maximum Likelihood For a 1D Gaussian

• Suppose we are given a data set of samples of a Gaussian random variable $X$, $D=\{x^1,\ldots, x^N\}$ and told that the variance of the data is $\sigma^2$

What is our best guess of $\mu$?

*Need to assume data is independent and identically distributed (i.i.d.)
Example: Maximum Likelihood For a 1D Gaussian

What is our best guess of $\mu$?

- We can write down the **likelihood function**:

$$ p(d \mid \mu) = \prod_{i=1}^{N} p(x^i \mid \mu, \sigma) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma}} \exp\left\{ -\frac{1}{2\sigma^2} (x^i - \mu)^2 \right\} $$

- We want to choose the $\mu$ that maximizes this expression
  - Take log, then basic calculus: differentiate w.r.t. $\mu$, set derivative to 0, solve for $\mu$ to get **sample mean**

$$ \mu_{ML} = \frac{1}{N} \sum_{i=1}^{N} x_i $$
Example: Maximum Likelihood For a 1D Gaussian

Maximum Likelihood
ML estimation of model parameters for Exponential Family

\[ p(D \mid \eta) = p(x_1, \ldots, x_N) = \left( \prod_n h(x_n) \right) g(\eta)^N \exp\{\eta^T \sum_n u(x_n)\} \]

\[ \partial \frac{p(D \mid \eta)}{\partial \eta} = \ldots, \text{set to } 0, \text{ solve for } \nabla g(\eta) \]

\[ -\nabla \ln g(\eta_{ML}) = \frac{1}{N} \sum_{n=1}^N u(x_n) \]

• Can in principle be solved to get estimate for eta.
• The solution for the ML estimator depends on the data only through sum over \( u \), which is therefore called \textbf{sufficient statistic}
• What we need to store in order to estimate parameters.
Bayesian Probabilities

\[ p(\theta \mid d) = \frac{p(d \mid \theta)p(\theta)}{p(d)} \]

- \( p(d \mid \theta) \) is the **likelihood function**
- \( p(\theta) \) is the **prior probability** of (or our **prior belief** over) \( \theta \)
  - our beliefs over what models are likely or not before seeing any data
- \( p(d) = \int p(d \mid \theta)P(\theta)d\theta \) is the **normalization constant** or **partition function**
- \( p(\theta \mid d) \) is the **posterior distribution**
  - Readjustment of our prior beliefs in the face of data
Example: Bayesian Inference For a 1D Gaussian

• Suppose we have a prior belief that the mean of some random variable $X$ is $\mu_0$ and the variance of our belief is $\sigma_0^2$

• We are then given a data set of samples of $X$, $d=\{x^1, \ldots, x^N\}$ and somehow know that the variance of the data is $\sigma^2$

What is the posterior distribution over (our belief about the value of) $\mu$?
Example: Bayesian Inference For a 1D Gaussian
Example: Bayesian Inference For a 1D Gaussian
Example: Bayesian Inference For a 1D Gaussian

- Remember from earlier: \( p(\mu \mid d) = \frac{p(d \mid \mu)p(\mu)}{p(d)} \)

- \( p(d \mid \mu) \) is the likelihood function

\[
p(d \mid \mu) = \prod_{i=1}^{N} P(x^i \mid \mu, \sigma) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2\sigma^2}(x^i - \mu)^2\right\}
\]

- \( p(\mu) \) is the prior probability of (or our prior belief over) \( \mu \)

\[
p(\mu \mid \mu_0, \sigma_0) = \frac{1}{\sqrt{2\pi\sigma_0}} \exp\left\{-\frac{1}{2\sigma_0^2}(\mu - \mu_0)^2\right\}
\]
Example: Bayesian Inference For a 1D Gaussian

\( p(\mu \mid D) \propto p(D \mid \mu) p(\mu) \)

\[ p(\mu \mid D) = \text{Normal}(\mu \mid \mu_N, \sigma_N) \]

where

\[
\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \mu_{ML}
\]

\[
\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}
\]
Example: Bayesian Inference For a 1D Gaussian
Example: Bayesian Inference For a 1D Gaussian

Prior belief

Maximum Likelihood
Example: Bayesian Inference For a 1D Gaussian

Prior belief

Maximum Likelihood

Posterior Distribution
DID THE SUN JUST EXPLODE?
(IT'S NIGHT, SO WE'RE NOT SURE.)

THIS NEUTRINO DETECTOR MEASURES WHETHER THE SUN HAS GONE NOVA.

THEN, IT ROLLS TWO DICE. IF THEY BOTH COME UP SIX, IT LIES TO US. OTHERWISE, IT TELLS THE TRUTH.

LET'S TRY.
DETECTOR! HAS THE SUN GONE NOVA?

ROLL

YES.

FREQUENTIST STATISTICIAN:

THE PROBABILITY OF THIS RESULT HAPPENING BY CHANCE IS \( \frac{1}{36} = 0.027 \).

SINCE \( p < 0.05 \), I CONCLUDE THAT THE SUN HAS EXPLODED.

BAYESIAN STATISTICIAN:

BET YOU $50 IT HASN'T.
Conjugate Priors

• Notice in the Gaussian parameter estimation example that the functional form of the posterior was that of the prior (Gaussian)

• Priors that lead to that form are called ‘conjugate priors’

• For any member of the exponential family there exists a conjugate prior that can be written like

\[
p(\eta \mid \chi, \nu) = f(\chi, \nu)g(\eta)^\nu \exp\{\nu \eta^T \chi\}
\]

• Multiply by likelihood to obtain posterior (up to normalization) of the form

\[
p(\eta \mid D, \chi, \nu) \propto g(\eta)^{\nu+N} \exp\{\eta^T (\sum_{n=1}^{N} u(x_n) + \nu \chi)\}
\]

• Notice the addition to the sufficient statistic

• \(\nu\) is the effective number of pseudo-observations.
Conjugate Priors - Examples

• Beta for Bernoulli/binomial
• Dirichlet for categorical/multinomial
• Normal for mean of Normal
• And many more...
  – Conjugate Prior Table:
    • http://en.wikipedia.org/wiki/Conjugate_prior