# CS-567 Machine Learning 

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- Uncertainty is a key concept in pattern recognition.
- Uncertainty arises due to
- Noise on measurements.
- Finite size of data sets.
- Uncertainty can be quantified via probability theory.


## Probability

- $P$ (event) is fraction of times event occurs out of total number of trials.
- $P=\lim _{N \rightarrow \infty} \frac{\# \text { successes }}{N}$.

$P(B=b)=0.6, P(B=r)=0.4 p($ apple $)=p(F=a)=$ ?
$p($ blue box given that apple was selected $)=p(B=b \mid F=a)=$ ?


## Terminology

- Joint $P(X, Y)$
- Marginal $P(X)$
- Conditional $P(X \mid Y)$




## Elementary rules of probability



Elementary rules of probability

- Sum rule: $p(X)=\sum_{Y} p(X, Y)$
- Product rule: $p(X, Y)=p(Y \mid X) p(X)$

These two simple rules form the basis of all the probabilistic machinery that will be used in this course.

- The sum and product rules can be combined to write

$$
p(X)=\sum_{Y} p(X \mid Y) p(Y)
$$

- A fancy name for this is Theorem of Total Probability.
- Since $p(X, Y)=p(Y, X)$, we can use the product rule to write another very simple rule

$$
p(Y \mid X)=\frac{p(X \mid Y) p(Y)}{p(X)}
$$

- Fancy name is Bayes' Theorem.
- Plays a central role in machine learning.


## Terminology

- If you don't know which fruit was selected, and I ask you which box was selected, what will your answer be?
- The box with greater probability of being selected.
- Blue box because $P(B=b)=0.6$.
- This probability is called the prior probability.
- Prior because the data has not been observed yet.


## Terminology

- Which box was chosen given that the selected fruit was orange?
- The box with greater $p(B \mid F=0)$ (via Bayes' theorem).
- Red box
- This is called the posterior probability.
- Posterior because the data has been observed.


## Independence

- If joint $p(X=x, Y=y)$ equals the product of marginals $p(X=x) p(Y=y)$ for all values $x$ and $y$, then random variables $X$ and $Y$ are independent.
- Independence $\leftrightarrow p(X, Y)$ factors into $p(X) p(Y)$.
- Using the product rule, for independent $X$ and $Y$, $p(Y \mid X)=p(Y)$.
- Intuitively, if $Y$ is independent of $X$, then knowing $X$ does not change the chances of $Y$.
- Example: if fraction of apples and oranges is same in both boxes, then knowing which box was selected does not change the chance of selecting an apple.


## Probability density

- So far, our set of events was discrete.
- Probability can also be defined for continuous variables via

$$
\operatorname{Prob}(x \in(a, b))=\int_{a}^{b} p(x) d x
$$

- Probability density function $p(x)$
- is always non-negative, and
- integrates to 1.
- Caution: Probability density is not the same as probability. Density can be greater than 1.


## Probability density

- Sum rule: $p(x)=\int p(x, y) d y$.
- Product rule: $p(x, y)=p(y \mid x) p(x)$
- Probability density can also be defined for a multivariate random variable $\mathbf{x}=\left(x_{1}, \ldots, x_{D}\right)$.

$$
\begin{aligned}
p(\mathrm{x}) & \geq 0 \\
\int_{\mathrm{x}} p(\mathrm{x}) d \mathrm{x} & =\int_{x_{D}} \ldots \int_{x_{1}} p\left(x_{1}, \ldots, x_{D}\right) d x_{1} \ldots d x_{D}=1
\end{aligned}
$$

## Expectation

- Expectation is a weighted average of a function.
- Weights are given by $p(x)$.

$$
\begin{array}{rr}
\mathbb{E}[f]=\sum_{x} p(x) f(x) & \longleftarrow \text { For discrete } x \\
\mathbb{E}[f]=\int_{x} p(x) f(x) d x & \longleftarrow \text { For continuous } x
\end{array}
$$

- When data is finite, expectation $\approx$ ordinary average. Approximation becomes exact as $N \rightarrow \infty$ (Law of large numbers).


## Expectation

- Expectation of a function of several variables

$$
\mathbb{E}_{x}[f(x, y)]=\sum_{x} p(x) f(x, y)
$$

(function of $y$ )

- Conditional expectation

$$
\mathbb{E}_{x}[f \mid y]=\sum_{x} p(x \mid y) f(x)
$$

## Variance

Measures variability of a random variable around its mean.

$$
\begin{aligned}
\operatorname{var}[f] & =\mathbb{E}\left[(f(x)-\mathbb{E}[f(x)])^{2}\right] \\
& =\mathbb{E}\left[\left(f(x)^{2}\right]-\mathbb{E}\left[f\left(x^{2}\right)\right]\right.
\end{aligned}
$$

## Covariance

## Univariate

- For 2 univariate random variables, covariance expresses how much $x$ and $y$ vary together.

$$
\begin{aligned}
\operatorname{cov}[x, y] & =\mathbb{E}_{x, y}[\{x-\mathbb{E}[x]\}\{y-\mathbb{E}[y]\}] \\
& =\mathbb{E}_{x, y}[x y]-\mathbb{E}[x] \mathbb{E}[y]
\end{aligned}
$$

- For independent random variables $x$ and $y, \operatorname{cov}[x, y]=0$.


## Covariance

- For multivariate random variables $\mathrm{x} \in \mathbb{R}^{D}$ and $\mathrm{y} \in \mathbb{R}^{K}$, $\operatorname{cov}[\mathrm{x}, \mathrm{y}]$ is a $D \times K$ matrix.
- Expresses how each element of $\mathbf{x}$ varies with each element of $\mathbf{y}$.

$$
\begin{align*}
\operatorname{cov}[\mathbf{x}, \mathbf{y}] & =\mathbb{E}_{\mathbf{x}, \mathbf{y}}\left[\{\mathbf{x}-\mathbb{E}[\mathbf{x}]\}\{\mathbf{y}-\mathbb{E}[\mathbf{y}]\}^{T}\right] \\
& =\mathbb{E}_{\mathbf{x}, \mathbf{y}}\left[\mathbf{x \mathbf { y } ^ { T } ] - \mathbb { E } [ \mathbf { x } ] \mathbb { E } [ \mathbf { y } ] ^ { T }}\right. \\
& =\left[\begin{array}{cccc}
\operatorname{cov}\left[x_{1}, y_{1}\right] & \operatorname{cov}\left[x_{1}, y_{2}\right] & \cdots & \operatorname{cov}\left[x_{1}, y_{K}\right] \\
\operatorname{cov}\left[x_{2}, y_{1}\right] & \operatorname{cov}\left[x_{2}, y_{2}\right] & \cdots & \operatorname{cov}\left[x_{2}, y_{K}\right] \\
\vdots & \vdots & \ddots & \vdots \\
\operatorname{cov}\left[x_{D}, y_{1}\right] & \operatorname{cov}\left[x_{D}, y_{2}\right] & \cdots & \operatorname{cov}\left[x_{D}, y_{K}\right]
\end{array}\right] \tag{1}
\end{align*}
$$

## Covariance

- Covariance of multivariate $x$ with itself can be written as $\operatorname{cov}[\mathrm{x}] \equiv \operatorname{cov}[\mathrm{x}, \mathrm{x}]$.
- $\operatorname{cov}[\mathrm{x}]$ expresses how each element of x varies with every other element.

$$
\operatorname{cov}[\mathrm{x}]=\left[\begin{array}{cccc}
\operatorname{var}\left[x_{1}\right] & \operatorname{cov}\left[x_{1}, x_{2}\right] & \cdots & \operatorname{cov}\left[x_{1}, x_{D}\right]  \tag{2}\\
\operatorname{cov}\left[x_{2}, x_{1}\right] & \operatorname{var}\left[x_{2}\right] & \cdots & \operatorname{cov}\left[x_{2}, x_{D}\right] \\
\vdots & \vdots & \ddots & \vdots \\
\operatorname{cov}\left[x_{D}, x_{1}\right] & \operatorname{cov}\left[x_{D}, x_{2}\right] & \cdots & \operatorname{var}\left[x_{D}\right]
\end{array}\right]
$$

## Bayesian View of Probability

- So far we have considered probability as the frequency of random, repeatable events.
- What if the events are not repeatable?
- Was the moon once a planet?
- Did the dinosaurs become extinct because of a meteor?
- Will the ice on the North Pole melt by the year 2100?
- For non-repeatable, yet uncertain events, we have the Bayesian view of probability.


## Bayesian View of Probability

$$
p(\mathbf{w} \mid \mathcal{D})=\frac{p(\mathcal{D} \mid \mathbf{w}) p(\mathbf{w})}{p(\mathcal{D})}
$$

- Measures the uncertainty in model w after observing the data D.
- This uncertainty is measured via conditional $p(\mathcal{D} \mid \mathbf{w})$ and prior $p(\mathbf{w})$.
- Treated as a function of $\mathbf{w}$, the conditional probability $p(\mathcal{D} \mid \mathbf{w})$ is also called the likelihood function.
- Expresses how likely the observed data is for any given model w.

