## Machine Learning CSE 6363 (Fall 2016)

## Lecture 3 Probability Distribution

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## Fitting Data with Linear Model (Regression)



- Force exerted by spring is proportional to square of length.
- Rod will settle at position that minimizes

$$
\sum_{i}^{N}\left(t_{i}-f\left(x_{i}\right)\right)^{2} \quad \text { where } \mathrm{N}=4
$$

- If $f$ is affine (linear + constant) function of $x$,

$$
f(x)=w_{o}+w_{1} x \quad \text { with parameters } \boldsymbol{w}=\left(w_{0}, w_{1}\right)
$$

- Which parameter values give best fit?

$$
\boldsymbol{w}_{\text {best }}=\underset{w}{\operatorname{argmin}} \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right)^{2}
$$

- Set derivative with respect to $w$ to zero and solve for $w$.


## Fitting Data with Linear Model

$$
\boldsymbol{w}_{\text {best }}=\operatorname{argmin} \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right)^{2}
$$

- Set derivative with respect to $w$ to zero and solve for $w$.

$$
\begin{aligned}
\frac{d \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right)^{2}}{d w_{0}}= & 2 \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right) \frac{\left(-d f\left(x_{i} ; \boldsymbol{w}\right)\right)}{d w_{0}}=0 \\
& -2 \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right)=0 \\
& \sum_{i}^{N} t_{i}-N w_{0}-w_{1} \sum_{i=1}^{N} x_{i}=0 \\
\frac{d \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right)^{2}}{d w_{1}}= & 2 \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right) \frac{\left(-d f\left(x_{i} ; \boldsymbol{w}\right)\right)}{d w_{1}}=0 \\
- & 2 \sum_{i}^{N}\left(t_{i}-f\left(x_{i} ; \boldsymbol{w}\right)\right) x_{i}=0 \\
& \sum_{i}^{N} t_{i}-w_{0} \sum_{i=1}^{N} x_{i}-w_{1} \sum_{i=1}^{N} x_{i}^{2}=0
\end{aligned}
$$

- Two simultaneous linear equations to solve for $w_{0}$ and $w_{1}$.


## Fitting Curves with Gaussian Conditional Distribution



- Now, to find $w$ that maximizes this likelihood, set derivative of log likelihood with respect to $w$ equal to zero and solve for $w$.
- Recall that before we

$$
\text { maximized }-\frac{1}{2 \sigma^{2}} \sum_{i}^{N}\left(t_{i}-\mu\right)^{2} \text { to get } \mu=\frac{1}{N} \sum_{i=1}^{N} t_{i}
$$

- Now we will
maximize $-\frac{1}{2 \sigma^{2}} \sum_{i}^{N}\left(t_{i}-y\left(x_{i}, \boldsymbol{w}\right)\right)^{2}$ or minimize $\frac{1}{2 \sigma^{2}} \sum_{i}^{N}\left(t_{i}-y\left(x_{i}, \boldsymbol{w}\right)\right)^{2}$ which is the usual (non-probabilistic) approach of fitting a function to minimize the squared error.


## Bayes Theorem




Probability of observed


Posterior probability of weight vector W given training data D


## Why we maximize sums of log probs

- We want to maximize the product of the probabilities of the outputs on the training cases
- Assume the output errors on different training cases, c, are independent.

$$
p(D \mid W)=\prod_{c} p\left(d_{c} \mid W\right)
$$

- Because the log function is monotonic, it does not change where the maxima are. So we can maximize sums of $\log$ probabilities

$$
\log p(D \mid W)=\sum_{c} \log p\left(d_{c} \mid W\right)
$$

## An even cheaper trick

- Suppose we completely ignore the prior over weight vectors
- This is equivalent to giving all possible weight vectors the same prior probability density.
- Then all we have to do is to maximize:

$$
\log p(D \mid W)=\sum_{c} \log p\left(D_{c} \mid W\right)
$$

- This is called maximum likelihood learning. It is very widely used for fitting models in statistics.


## Decision Theory <br> Probabilities and Bayes' Theorem

- Classify images as the correct digit.
- Given $p($ Image $=i \mid$ Digit $=d), p($ Image $=i)$, and $p($ Digit $=d)$.
- Calculate

$$
p(\text { Digit }=d \mid \text { Image }=i)=\frac{p(\text { Image }=i \mid \text { Digit }=d) p(\text { Digit }=d)}{p(\text { Image }=i)}
$$

- or, more generally

$$
p(\text { Class }=k \mid X=x)=\frac{p(X=x \mid \text { Class }=k) p(\text { Class }=k)}{p(X=x)}
$$

- or, more concisely

$$
p\left(C_{k} \mid x\right)=\frac{p\left(x \mid C_{k}\right) p\left(C_{k}\right)}{p(x)}
$$

- To classify $x$,

$$
\underset{C_{k}}{\operatorname{argmax}} p\left(C_{k} \mid x\right) \quad \text { for example }, \underset{C_{k}}{\operatorname{argmax}} p(\text { Digit }=d \mid \text { Image }=i)
$$

- We get to this by first defining measure of decision accuracy.


## Decision Theory <br> Decision Regions and Measures of Accuracy

- Decision regions

$$
\begin{aligned}
p(\text { mistake }) & =p\left(x \in R_{1}, \text { Digit }=2\right)+p\left(x \in R_{2}, \text { Digit }=1\right) \\
& =p\left(x \in R_{1}, C_{2}\right)+p\left(x \in R_{2}, C_{1}\right)
\end{aligned}
$$

- If $x$ is discrete $=\sum_{x \in R_{1}} p\left(x, C_{2}\right)+\sum_{x \in R_{2}} p\left(x, C_{1}\right)$
- If $x$ is continuous

$$
=\int_{R_{1}} p\left(x, C_{2}\right) d x+\int_{R_{2}} p\left(x, C_{1}\right) d x
$$

- Make assignment of $x$ to $R_{k}$ to minimize $p$ (mistake), or to maximize $p$ (correct)

$$
\begin{aligned}
p(\text { correct })= & p\left(x \in R_{1}, C_{1}\right)+p\left(x \in R_{2}, C_{2}\right) \\
=\sum_{k=1}^{K} p\left(x \in R_{k}, C_{k}\right) & =\sum_{k=1}^{K} \sum_{x \in R_{k}} p\left(x, C_{k}\right) \\
& =\sum_{k=1}^{K} \int_{R_{k}} p\left(x, C_{k}\right)
\end{aligned}
$$

## Decision Theory

## Decision Regions and Measures of Accuracy

- which, by Bayes' theorem $\sum_{k=1}^{K} \int_{R_{k}} p\left(x, C_{k}\right)=\sum_{k=1}^{K} \int_{R_{k}} p\left(C_{k} \mid x\right) p(x)$
- Maximize by constructing $R_{1^{\prime}} \ldots R_{k}$ as best you can.
- If separating by straight lines

- Each $x$ is assigned to an $R_{i}$.
- Since $p(x)$ is same for all $k$, regions resulting from maximizing $p$ (correct) same as regions resulting from maximizing $\sum_{k=1}^{K} \int_{R_{t}} p\left(C_{k} \mid x\right)$
- If $x$ is one-dimensional, and we model $p\left(C_{k} \mid x\right)$ as Gaussian, then

$$
k=2 \quad k=1
$$

- $p\left(C_{1} \mid x\right)$
- $p\left(C_{2} \mid x\right)$
?

$$
\text { Class 1, because } p\left(C_{1} \mid x\right)>p\left(C_{2} \mid x\right)
$$

## Example

- e.g., the optimal decision threshold is when $\hat{x}=x_{0}$



## Decision Theory

## Decision Regions and Measures of Accuracy

- So far we assumed each missclassification is equally bad, or each correct classification is equally good.
- But, predictions of whether or not a particular space shuttle launch given all known current conditions will result in damage from loose tiles are not equally risky.
- incorrect prediction of damage (no launch) is better than incorrect prediction of no damage (launch, damage)!
- Define a loss matrix $L_{k j} \quad$ Predicted

|  |  | damage | no damage |
| :--- | ---: | ---: | ---: |
|  | Truedamage <br>  <br> no damage | 0 | 10,000 |

- or, utility matrix

Predicted

| damage |  |  |
| :---: | :---: | :---: |
|  | 100 | -10000 |
| no damage | -10 | 100 |

## Decision Theory <br> Measures of Accuracy

- Given an $x$, we pick column but do not know true class. We will know probability of true class.
- If we classify $x$ as Class $j$ our loss will be $\sum_{k=1}^{K} L_{k j} p\left(x, C_{k}\right)$
- Call this expected value of loss, given $x$ classified as Class $j$.
- Given all $x$ 's and a classification scheme that partitions the $x$ space into regions $R_{1^{\prime}} \ldots R_{k^{\prime}}$ the overall expected loss is

$$
E[L]=\sum_{k=1}^{K} \sum_{j=1}^{K} \int_{R_{j}} L_{k j} p\left(x, C_{k}\right) d x
$$

- By Bayes' theorem, to minimize $E[L]$ we would assign $x$ to Class $j$ that minimizes

$$
\sum_{k=1}^{K} L_{k j} p\left(C_{k} \mid x\right)
$$

- Would classify current shuttle condition as "damage" much more often than "no damage" because of

| dition | Predicted damage no damage |  |
| :---: | :---: | :---: |
| damage | 0 | 10,000 |
| no damage | 10 | 0 |

## Decision Theory <br> Three ways of making classification decision

- Generative model
- Learn class-conditional probability (generative model) $p\left(x \mid C_{k}\right)$
- Use Bayes' Theorem to convert to $\quad p\left(C_{k} \mid x\right)$
- Use decision theory to minimize loss
- Discriminative model
- Learn posterior class probability (discriminative model) $p\left(C_{k} \mid x\right)$
- Use decision theory to minimize loss
- Discriminant function
- Learn discriminant function $f(x)$ that calculates a class directly. Probabilities not involved.
- Advantages and disadvantages of each, in Section 1.5.4.


## Information Theory

- Useful to have measure $h(x)$ of how much information is provided by an event, $x$. We would like it to reflect how "surprising" the event is, so it should be related monotonically to probability $p(x)$.
- If two events $x$ and $y$ are unrelated, total information gained should be sum of each


## Information Content of A Random Variable

- Random variable X
- Outcome of a random experiment
- Discrete R.V. takes on values from a finite set of possible outcomes PMF: $\mathrm{P}(\mathrm{X}=\mathrm{y})=\mathrm{Px}(\mathrm{y})$
- How much information is contained in the event $\mathrm{X}=\mathrm{y}$ ?
- Will the sun rise today?
- Revealing the outcome of this experiment provides no information
- Will the Maverick win the NBA championship?
- Since this is unlikely, revealing yes provides more information than revealing no
- Events that are less likely contain more information than likely events


## Entropy

The entropy of a random variable $X$ with a probability mass function $p(x)$ is defined by

$$
H(X)=-\sum_{x} p(x) \log _{2} p(x) .
$$

The entropy is measured in bits and is a measure of the average uncertainty in the random variable. It is the number of bits on the average required to describe the random variable.

We write $\log x:=\log _{2} x$ in the sequel.

## Example: Variable with Uniform Distribution

Consider a random variable with uniform distribution over $32\left(=2^{5}\right)$ outcomes. Obviously, 5 -bit strings suffice to identify an outcome. The entropy is

$$
H(X)=-\sum_{i=1}^{32} p(i) \log p(i)=-\sum_{i=1}^{32} \frac{1}{32} \log \frac{1}{32}=\log 32=5 \mathrm{bits},
$$

which agrees with the number of bits needed to describe $X$.

## Example: Variable with Nonuniform

As the win probabilities are not uniform, it makes sense to use shorter descriptions for the more probably horses, and longer descriptions for the less probable ones. For example, the following strings can be used to represent the eight horses:

$$
0,10,110,1110,111100,111101,111110,111111 .
$$

The average description length is then 2 bits (=entropy).
$\triangleright$ The entropy gives a lower bound for the average description length.

## Example: Variable with Nonuniform

Assume that the probabilities of winning for eight horses taking part in a horse race are $\left\{\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}\right\}$. The entropy of this distribution (that is, of the horse race) is then
$H(X)=-\frac{1}{2} \log \frac{1}{2}-\frac{1}{4} \log \frac{1}{4}-\frac{1}{8} \log \frac{1}{8}-\frac{1}{16} \log \frac{1}{16}-4 \frac{1}{64} \log \frac{1}{64}=2$ bits.

To send a message indicating the winner of the race, one can send the index of the winning horse $(000, \ldots, 111)$; this requires 3 bits for any of the horses. But there is another (better) description.

## Joint and Conditional Entropy

Entropy

$$
\begin{gathered}
H(X)=-E[\log P(X)] \\
H(X, Y)=-E_{X, Y}[\log P(X, Y)]
\end{gathered}
$$

this is really just entropy with a shift of perspective, in which the pair $X, Y$ is the new random variable. Because $P(X, Y)=P(X) P(Y \mid X)$

$$
\begin{aligned}
H(X, Y) & \left.=-E_{X, Y}[\log P(X) P(Y \mid X))\right] \\
& =-E_{X, Y}[\log (P(X)+\log (P(Y \mid X)] \\
& =H(X)-E_{X, Y}[\log (P(Y \mid X)]
\end{aligned}
$$

so we dignify the last term with the name conditional entropy and the notation $H(Y \mid X)$.

## Mutual Information

We just derived a chain rule for entropy:

$$
H(X, Y)=H(X)+H(Y \mid X)=H(Y)+H(X \mid Y)
$$

from which it follows that

$$
H(X)-H(X \mid Y)=H(Y)-H(Y \mid X)
$$

and we call this quantity $I(X ; Y)$. If $Y$ is informative about $X$ then $H(X \mid Y)<H(X)$. In the limit $Y$ determines $X$ and $H(X \mid Y)=0$.

$$
\begin{aligned}
I(X ; Y) & =H(X)-H(X \mid Y) \\
& =H(X)-(H(X, Y)-H(Y)) \\
& =H(X)+H(Y)-H(X, Y) \\
& =-E_{x}[\log P(x)]-E_{y}[\log (P(y))]+E_{x, y}[\log P(x, y)] \\
& =E\left[\log \frac{P(x, y)}{P(x) P(y)}\right]
\end{aligned}
$$

