# Learning as Inference

## DD2421

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# Check your understanding!

Before I took a COVID test, the doctor said 99% of the people in the area have COVID, and 90% of those with COVID are testing positive. A few days later the doctor called and said my test was positive, and that the probability I have COVID given this positive test is $p$% — I can't remember because I was in shock. Find the minimum value of $p$ such that I can compute the probability I got a positive test but don't have COVID, and then compute the maximum probability I don't have COVID given my positive test.

$P(+|\neg C)$ (1

(2

$P[D] = 0.99$
$P[+|D] = 0.90$

$P(\neg C \mid +)$

$$y_{max}(x) = \arg\max_{y \in Y} P_r(X = x | Y = y) \cdot P_r(Y = y)$$

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*Define:*

1. $+$ is "positive test"
2. $C$ is "have COVID"
3. $\neg C$ is "does not have COVID"

# Check your understanding!

Before I took a COVID test, the doctor said 99% of the people in the area have COVID, and 90% of those with COVID are testing positive.

*Translating:*

- $P[C] = 0.99$ (prior) $\rightarrow$ knowledge about $Y$ before any observation : $P(Y=y)$
- $P[+|C] = 0.9$ (likelihood) $\rightarrow$ probability of $X=x$ given $Y=y$ : $P(X=x|Y=y)$

# Check your understanding!

evidence

The doctor called and said my test was positive, and that the probability I have COVID given this positive test is $p$% — I can't remember because I was in shock.

*Translating:*

- OMG I have "+" (evidence) $\mathcal{X} = x$
- $P[C|+] = p$ (posterior) probability of $\mathcal{Y} = y$ after knowing $\mathcal{X} = x$ : $P(\mathcal{Y} = y | \mathcal{X} = x)$

# Check your understanding!

Find the minimum value of $p \equiv P[C|+]$ such that I can compute the probability I got a positive test but don't have COVID
*Translating:*

- I want to find $P[+|\neg C]$.
- I also know $P[C|+]$ is a probability, and so its value must be in a range restricted by the axioms of probability.

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- I also know $P[C|+]$ is a probability, and so its value must be in a range restricted by the axioms of probability.

Using Bayes':

$$P[+|\neg C] = \frac{P[\neg C|+]P[+]}{P[\neg C]} = \frac{(1 - P[C|+])P[+]}{1 - P[C]} = \frac{(1-p)P[+]}{1 - P[C]}$$

since $P[\neg C|+] = 1 - P[C|+]$, and $P[\neg C] = 1 - P[C]$ as there are only two possibilities. We need to find $P[+]$.

→ I am "+" → I also have C.
→ but don't have C.

## Check your understanding!

We know

$$P[+|C] = \frac{P[C|+]P[+]}{P[C]}$$

and so solving for $P[+]$

$$P[+] = \frac{P[+|C]P[C]}{P[C|+]} = \frac{P[+|C]P[C]}{p}$$

# Check your understanding!

We know:

$$P[+|\neg C] = \frac{(1-p)P[+]}{1-P[C]} \qquad (1)$$

and we have just found

$$P[+] = \frac{P[+|C]P[C]}{p} \qquad (2)$$

Substituting the latter into the former produces

$$\begin{aligned}
(1) \quad P[+|\neg C] &= \frac{(1-P[C|+])}{1-P[C]} \frac{P[+|C]P[C]}{P[C|+]} \quad (2) \\
&= \frac{P[C]}{1-P[C]} \frac{(1-\boxed{P[C|+]})}{P[C|+]} P[+|C] \quad = p. \\
&= \frac{P[C]}{1-P[C]} \frac{(1-p)}{p} P[+|C].
\end{aligned}$$

# Check your understanding!

Our crowning achievement:

$$\underline{P[+|\neg C]} = \frac{P[C]}{1-P[C]}\frac{(1-p)}{p}P[+|C].$$

The left hand side must obey the axioms of probability, which means $\underline{0 \leq P[+|\neg C] \leq 1}$. So

$$0 \leq \underbrace{\frac{P[C]}{1-P[C]}\frac{(1-p)}{p}P[+|C]}_{=P(+|\neg C)} \leq 1$$

$$0 \leq \frac{(1-p)}{p} \leq \frac{1-P[C]}{P[C]}\frac{1}{P[+|C]} \quad *$$

$$0 \leq \frac{(1-p)}{p} \leq \frac{1/100}{99/100}\frac{1}{9/10} \rightarrow 891/901 \leq p \leq 1$$

* $P[C] = 0.95$
$P[+|C] = 0.50$

## Check your understanding!

The minimum value of $p$ such that I can compute the probability I got a positive test but don't have COVID:

$$p \geq 891/901$$

The maximum probability I don't have COVID given my positive test is thus:

$$P[\neg C|+] = 1 - P[C|+] = 1 - p \leq 1 - 891/901 = 10/901.$$

# Outline

1. Introduction
   - Probabilistic Classification and Regression
   - Discriminative vs Generative Models
   - Parametric vs Non-parametric Inference
2. Maximum Likelihood (ML) Estimation
   - Regression
   - Classification
3. Special Cases
   - Naïve Bayes Classifier
   - Logistic Regression

# Outline

# Probabilistic Classification and Regression

- In both cases we compute the posterior

$$Pr(y \,|\, X = x) = \frac{Pr(x \,|\, Y = y) Pr(Y = y)}{Pr(X = x)}$$

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- Classification: $Y$ is discrete, finite
- Regression: $Y$ is continuous

Until now we assumed we knew:

- $Pr(Y = y) \equiv Pr(y) \leftarrow$ *Prior*
- $Pr(x \,|\, Y = y) \equiv Pr(x|y) \leftarrow$ *Likelihood*
- $Pr(X = x) \equiv Pr(x) \leftarrow$ *Evidence*

what if we don't,
but we can estimate them?

# Probabilistic Classification and Regression

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- $Pr(X = x) \equiv Pr(x) \leftarrow$ *Evidence*

How can we obtain these distributions from data?

# Learning as Inference

Given:

- the training data $\mathcal{D} = \{(\mathbf{x}, y)_1, (\mathbf{x}, y)_2, \ldots, (\mathbf{x}, y)_N\}$
- a new observation $\mathbf{x}$ $\longrightarrow$ might very well be similar to $x \in \mathcal{D}$

Estimate the posterior probability of $y$:

$$Pr(y|\mathbf{x}, \mathcal{D})$$

# Discriminative vs Generative Models

directly relating a probability given some data

Discriminative modeling:

- This models $Pr(y|\mathbf{x}, \mathcal{D})$ directly
- examples: logistic regression

Generative modeling:

- This models $Pr(\mathbf{x}|y, \mathcal{D})$
- example: Naive Bayes

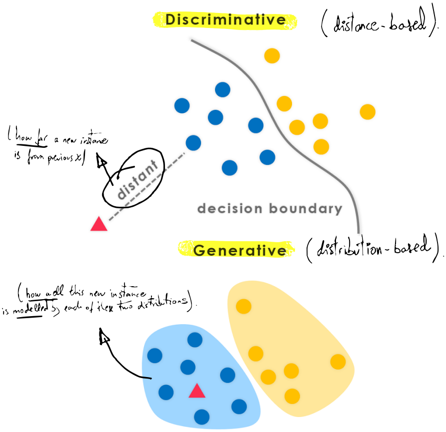


Figure from Nguyen *et al.* 2015.

# Parametric vs Non-parametric Inference

$$Pr(y|\mathbf{x}) = Pr(y|\mathbf{x}, \theta)$$

The distribution is characterized by parameters $\theta$.

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The distribution is characterized by parameters $\theta$.

**Parametric Inference**:

- Estimate $\theta$ using $\mathcal{D}$ → estimate params from observations
- Compute $Pr(y|\mathbf{x}, \hat{\theta})$ to make inference. → compute the posterior. (based on those params estimation).

*Learning* corresponds to estimating $\theta$

# Parametric vs Non-parametric Inference

$$Pr(y|\mathbf{x}) = Pr(y|\mathbf{x}, \theta)$$

The distribution is characterized by parameters $\theta$.

**Parametric Inference**:

- Estimate $\theta$ using $\mathcal{D}$
- Compute $Pr(y|\mathbf{x}, \hat{\theta})$ to make inference.

*Learning* corresponds to estimating $\theta$

**Non-Parametric Inference**:

- Estimate $\underline{Pr(\theta|\mathcal{D})} \longrightarrow$ (a distribution of theta $\theta$)
- Compute $\underline{Pr(y|\mathbf{x}, \mathcal{D})}$ from $Pr(y|\mathbf{x}, \theta, \mathcal{D})Pr(\theta|\mathcal{D})$ by marginalizing out $\theta$

The number of parameters can grow with the data!

(incorporates some uncertainty into our params' estimation.)

(construct a 'posterior' that involves marginalizing out the parameters)

## Three Approaches

Parametric inference:

- Maximum Likelihood (ML) Estimation (today)
- Maximum A Posteriori (MAP) Estimation (next time)

Non-parametric inference:

- Bayesian methods (a little today and the rest next time)

# Fundamental Assumption: i.i.d.

( $o_i$ won't tell anything about $o_j$ ). ( all have the same probability distribution ).

Observations are independent and identically distributed (i.i.d.):

$$\mathcal{D} = \{\mathbf{o}_1, \ldots, \mathbf{o}_N\}, \mathbf{o}_i = (\mathbf{x}, y)_i$$

The likelihood of the whole data set can be factorized:

$$Pr(\mathcal{D}) = Pr(\mathbf{o}_1, \ldots, \mathbf{o}_N) = \prod_{i=1}^{N} Pr(\mathbf{o}_i)$$

independent since depend not on $y$.

increasing # $o_i$ will make $pr(D)$ smaller.

Taking the log creates the *log-likelihood*:

$$\log Pr(\mathcal{D}) = \sum_{i=1}^{N} \log Pr(\mathbf{o}_i)$$

taking the "log" prevents it from being too small.

# Outline



GOAL : find the optimal way to fit a distribution to the data

# Maximum Likelihood (ML) Estimate

→ we do not know the following distributions:

$$\underbrace{Pr(\mathbf{x}|y) \equiv Pr(\mathbf{x}|y,\theta)}_{\text{generative model}} \quad \text{or} \quad \underbrace{Pr(y|\mathbf{x}) \equiv Pr(y|\mathbf{x},\theta)}_{\text{discriminative model}}$$

to describe a distribution — that best fits the data — (by adjusting the parameters $\theta$)

*Find the parameter values that make the data most likely.*

- *ML optimality* is defined as maximizing the likelihood of $\mathcal{D}$:

$$\theta_{\mathsf{ML}} = \arg\max_{\theta} P(\mathcal{D}|\theta) = \arg\max_{\theta} \underbrace{\log}_{\text{does not alter order}} P(\mathcal{D}|\theta)$$

$(\mu, \sigma)$

(monotonically larger function)

- We can then approximate distributions given the data:

$$Pr(\mathbf{x}|y,\mathcal{D}) \approx Pr(\mathbf{x}|y,\theta_{\mathsf{ML}}) \quad \text{or} \quad Pr(y|\mathbf{x},\mathcal{D}) \approx Pr(y|\mathbf{x},\theta_{\mathsf{ML}})$$

↳ allow an approximation of the previous distributions.

# Probabilistic Linear Regression

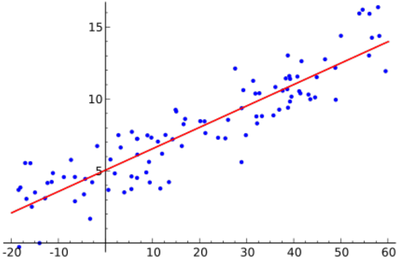
Model (deterministic):

$$y = \mathbf{w}^T \mathbf{x} + \epsilon$$

But now:

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

if model is good, eok will be normally distributed.




Therefore:

$$\begin{aligned} Y|X \;\; &\sim \;\; \mathcal{N}(\mu_Y(\mathbf{x}), \sigma_Y^2(\mathbf{x})) \\ &= \mathcal{N}(\mathbf{w}^T\mathbf{x}, \sigma^2) \end{aligned}$$

find a "y" for that distribution of "x"

Learning: find $\mathbf{w}$ that maximizes $Pr(y|\mathbf{x}, \mathbf{w}, \sigma^2)$

Maximize the posterior directly $\implies$ discriminative method

# MLE for Probabilistic Linear Regression

$$\underline{\log Pr(y|\mathbf{x}, \mathbf{w}, \sigma^2)} = \log \prod_i Pr(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2) \longrightarrow \text{(multiple them since "iid")}.$$

$$= \sum_i \log Pr(y_i|\mathbf{x}_i, \mathbf{w}, \sigma^2) \longrightarrow$$

costly to apply "Chain Rule" upon multiplications.

$$= \sum_i \log \left[ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2}} \right]$$

: Normal distribution equation

$$= \sum_i \left[ -\frac{1}{2} \log(2\pi\sigma^2) - \frac{(y_i - \mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2} \right]$$

(only w-dependent term).

→ (maximizing the probability of making this observation)

$\Rightarrow$ maximize this (w) = minimize "$y_i - w^T \cdot x_i$" term.

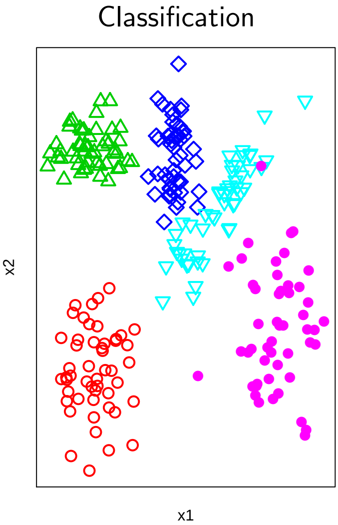
# MLE for Probabilistic Linear Regression

$$
\begin{aligned}
\log Pr(y|\mathbf{x},\mathbf{w},\sigma^2) &= \log \prod_i Pr(y_i|\mathbf{x}_i,\mathbf{w},\sigma^2) \\
&= \sum_i \log Pr(y_i|\mathbf{x}_i,\mathbf{w},\sigma^2) \\
&= \sum_i \log \left[\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-\mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2}}\right] \\
&= \sum_i \left[-\frac{1}{2}\log(2\pi\sigma^2) - \frac{(y_i-\mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2}\right]
\end{aligned}
$$

$$
\arg\max_{\mathbf{w}} Pr(y|x,\mathbf{w},\sigma^2) = \arg\min_{\mathbf{w}} \sum_i (y_i - \mathbf{w}^T\mathbf{x}_i)^2
$$

NEAT-O! Choosing parameters that maximize $Pr(y|x,\mathbf{w},\sigma^2) \equiv$ minimizing mean square error! (in this case)

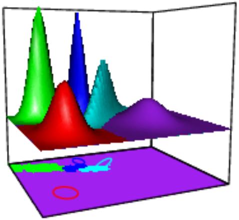
# MLE for Classification



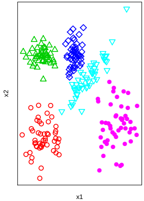

features: $\mathbf{x} \in \mathbb{R}^d$

class: $y \in \{y_1, \ldots, y_K\}$

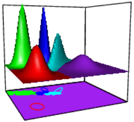
$$k_{\text{MAP}} = \arg\max_k Pr(y_k|\mathbf{x})$$
$$= \arg\max_k Pr(\mathbf{x}|y_k)Pr(y_k)$$



# Assumption: Class Independence




$\longrightarrow$



samples from class $i$ do not influence estimate for class $j$, $i \neq j$

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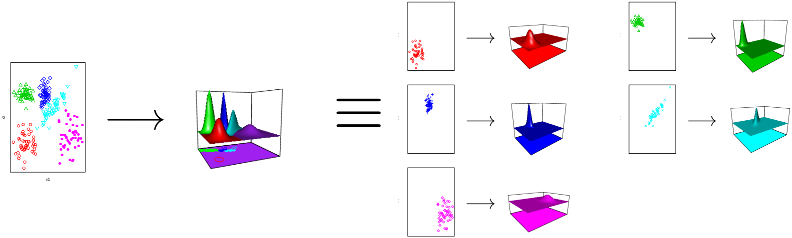

- distribution of $\mathbf{x}$ for class $y_k$ is the likelihood $Pr(\mathbf{x}|\theta_k)$
- in the following, we drop the class index $k$ and write $Pr(\mathbf{x}|\theta)$
- also we call $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ the set of data point belonging to a single class $y_k$

# ML estimation of Gaussian mean

$$X \sim \mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right], \text{ with } \underbrace{\theta = \{\mu,\sigma^2\}}_{\text{(our parameters)}}$$

Log-likelihood of data (i.i.d. samples):

$$\log Pr(\mathcal{D}|\theta) = \sum_{n=1}^{N} \log \mathcal{N}(x_n|\mu,\sigma^2)$$

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$$\log Pr(\mathcal{D}|\theta) = \sum_{n=1}^{N} \log \mathcal{N}(x_n|\mu, \sigma^2) = -N \log\left(\sqrt{2\pi\sigma^2}\right) - \sum_{n=1}^{N} \frac{(x_n-\mu)^2}{2\sigma^2}$$

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$$0 = \frac{d \log Pr(\mathcal{D}|\theta)}{d\mu}$$

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$$\mu_{\text{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

# ML estimation of Gaussian parameters

$$\mu_{\mathsf{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

max. likelihood of $\mu$

$$\sigma^2_{\mathsf{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu_{\mathsf{ML}})^2$$

(variance)

# ML estimation of Gaussian parameters

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$$\sigma^2_{\mathsf{ML}} = \frac{1}{N}\sum_{n=1}^{N} (x_n - \mu_{\mathsf{ML}})^2$$

- This is the same result as minimizing the sum of square errors!
- but now out assumptions are explicit (i.e., how the data is distributed)
- This estimate of the variance is *biased*, i.e., $\mathbb{E}[\sigma^2_{\mathsf{ML}}] - \sigma^2 \neq 0$. The unbiased ML estimate is

$$\sigma'^2_{\mathsf{ML}} = \frac{1}{N-1}\sum_{n=1}^{N} (x_n - \mu_{\mathsf{ML}})^2$$

(unbiased)

# MLE with Discrete Variables

Will I go and play orienteering given the forecast?

$$x \in \{\text{sunny}, \text{overcast}, \text{rainy}\}$$
$$y \in \{\text{yes}, \text{no}\}$$

$$X \sim ?$$
$$Y \sim ?$$
$$X|Y \sim ?$$
$$Y|X \sim ?$$

how should these variables be distributed?

Training data

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
| 2 | sunny | no | 9 | sunny | yes |
| 3 | overcast | yes | 10 | rainy | yes |
| 4 | rainy | yes | 11 | sunny | yes |
| 5 | rainy | yes | 12 | overcast | yes |
| 6 | rainy | no | 13 | overcast | yes |
| 7 | overcast | yes | 14 | rainy | no |

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$$y \in \{\text{yes}, \text{no}\}$$

$$X \sim \text{Cat}(\lambda_1, \lambda_2, \lambda_3)$$
$$Y \sim ?$$
categorical
$$X|Y \sim ?$$
$$Y|X \sim ?$$

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$$X \sim \text{Cat}(\lambda_1, \lambda_2, \lambda_3)$$
$$Y \sim \text{Bernoulli}(\lambda) \quad \text{yes/no}$$
$$X|Y \sim ?$$
$$Y|X \sim ?$$

Training data

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# MLE with Discrete Variables

Will I go and play orienteering given the forecast?

$$
\begin{aligned}
x &\in \{\text{sunny}, \text{overcast}, \text{rainy}\} \\
y &\in \{\text{yes}, \text{no}\}
\end{aligned}
$$

$$
\begin{aligned}
X &\sim \text{Cat}(\lambda_1, \lambda_2, \lambda_3) \\
Y &\sim \text{Bernoulli}(\lambda) \\
X|Y &\sim \text{Cat}(\lambda_1', \lambda_2', \lambda_3') \\
Y|X &\sim \text{Bernoulli}(\lambda')
\end{aligned}
$$

* (Y does not change X counts).
α (tick "..." means they are parametrized)

Training data

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# MLE: Bernoulli

$$Pr(y) = \begin{cases} \lambda & \text{if } y = \text{yes} \\ 1-\lambda & \text{if } y = \text{no} \end{cases}$$

1. compute (log) likelihood of the data $P(\mathcal{D}|\lambda)$
2. find $\lambda_{\text{ML}}$ that optimizes $P(\mathcal{D}|\lambda)$

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
| 2 | sunny | no | 9 | sunny | yes |
| 3 | overcast | yes | 10 | rainy | yes |
| 4 | rainy | yes | 11 | sunny | yes |
| 5 | rainy | yes | 12 | overcast | yes |
| 6 | rainy | no | 13 | overcast | yes |
| 7 | overcast | yes | 14 | rainy | no |

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Likelihood of the data
($n$=number of yes in $\mathcal{D}$, $N$=number of examples):

$$\begin{aligned} Pr(\mathcal{D}|\lambda) &= \prod_n Pr(y_n|\lambda) = \prod_{n \text{ s.t. } y=\text{yes}} \lambda \prod_{n \text{ s.t. } y=\text{no}} (1-\lambda) \\ &= \lambda^n (1-\lambda)^{N-n} \end{aligned}$$

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&= \lambda^n (1-\lambda)^{N-n} \\
\log Pr(\mathcal{D}|\lambda) &= n \log \lambda + (N-n) \log(1-\lambda) \\
\frac{d}{d\lambda} \log Pr(\mathcal{D}|\lambda) &= \frac{n - N\lambda}{\lambda(1-\lambda)} = 0 \iff \lambda_{\text{ML}} = \frac{n}{N}
\end{aligned}$$

# MLE Example: Discrete Variables

Will I go and play orienteering given the forecast?

$$x \in \{\text{sunny}, \text{overcast}, \text{rainy}\}$$
$$y \in \{\text{yes}, \text{no}\}$$

Training data

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
| 2 | sunny | no | 9 | sunny | yes |
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| 4 | rainy | yes | 11 | sunny | yes |
| 5 | rainy | yes | 12 | overcast | yes |
| 6 | rainy | no | 13 | overcast | yes |
| 7 | overcast | yes | 14 | rainy | no |

$$Y \sim \text{Bernoulli}(\lambda)$$
$$\lambda_{\text{ML}} = \frac{9}{14}$$

(y: 9   n: 5)

# MLE: Categorical

Similar derivation:

$$\lambda_{k,\text{ML}} = \frac{n_k}{N}$$

where $n_k$ is the number of examples of the $k$th category

$$X \sim \text{Cat}(\lambda_{\text{sunny}}, \lambda_{\text{overcast}}, \lambda_{\text{rainy}})$$

$$\lambda_{\text{ML}} = \left\{ \frac{5}{14}, \frac{4}{14}, \frac{5}{14} \right\}$$

Training data

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
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# MLE: Categorical

Similar derivation:

$$\lambda_{k,\mathsf{ML}} = \frac{n_k}{N}$$

where $n_k$ is the number of examples of the $k$th category

$$\begin{aligned} X &\sim \mathsf{Cat}(\lambda_{\mathsf{sunny}}, \lambda_{\mathsf{overcast}}, \lambda_{\mathsf{rainy}}) \\ \lambda_{\mathsf{ML}} &= \left\{ \frac{5}{14}, \frac{4}{14}, \frac{5}{14} \right\} \\ \underline{X|Y} &\sim \mathsf{Cat}(\lambda'_1, \ldots, \lambda'_k) \end{aligned}$$

how can Y change things?

Training data

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
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Similar derivation:

$$\lambda_{k,\text{ML}} = \frac{n_k}{N}$$

where $n_k$ is the number of examples of the $k$th category

$$\begin{aligned}
X &\sim \text{Cat}(\lambda_{\text{sunny}}, \lambda_{\text{overcast}}, \lambda_{\text{rainy}}) \\
\lambda_{\text{ML}} &= \left\{\frac{5}{14}, \frac{4}{14}, \frac{5}{14}\right\} \\
X|Y &\sim \text{Cat}(\lambda'_1, \ldots, \lambda'_k) \\
\lambda'_{\text{ML}}(\text{yes}) &= \left\{\frac{2}{9}, \frac{4}{9}, \frac{3}{9}\right\} \\
\lambda'_{\text{ML}}(\text{no}) &= \left\{\frac{3}{5}, 0, \frac{2}{5}\right\}
\end{aligned}$$

Training data

| $n$ example | $x_n$ outlook | $y_n$ play | $n$ example | $x_n$ outlook | $y_n$ play |
|---|---|---|---|---|---|
| 1 | sunny | no | 8 | sunny | no |
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# But . . . will I play orienteering given a rainy outlook?

$$\begin{aligned} Pr(y = \text{yes}|\text{outlook=rainy}) &= \frac{Pr(\text{outlook=rainy}|y = \text{yes})Pr(y = \text{yes})}{Pr(\text{outlook=rainy})} \\ &= \frac{\frac{3}{9}\frac{9}{14}}{\frac{5}{14}} = \frac{3}{5} \end{aligned}$$

# But . . . will I play orienteering given a rainy outlook?

$$Pr(y = \text{yes}|\text{outlook=rainy}) = \frac{Pr(\text{outlook=rainy}|y = \text{yes})Pr(y = \text{yes})}{Pr(\text{outlook=rainy})} = \frac{\frac{3}{9}\frac{9}{14}}{\frac{5}{14}} = \frac{3}{5}$$

$$Pr(y = \text{no}|\text{outlook=rainy}) = \frac{Pr(\text{outlook=rainy}|y = \text{no})Pr(y = \text{no})}{Pr(\text{outlook=rainy})} = \frac{\frac{2}{5}\frac{5}{14}}{\frac{5}{14}} = \frac{2}{5}$$

→ or: $(1 - 3/5)$.

Then

find y st (y is max) given a condition

$$y_{\text{MAP}} = \arg\max_y Pr(y|\text{outlook=rainy}) = \text{yes} \; (\overbrace{3/5}^{y = \text{yes}} > \overbrace{2/5}^{y = \text{no}})$$

→ "y = yes" maximizes Pr(y | rainy).

! "y = yes" is the most likely y given that x = rainy. !

# But . . . will I play orienteering given a rainy outlook?

$$Pr(y = \text{yes}|\text{outlook=rainy}) = \frac{Pr(\text{outlook=rainy}|y = \text{yes})Pr(y = \text{yes})}{Pr(\text{outlook=rainy})}$$

$$= \frac{\frac{3}{9}\frac{9}{14}}{\frac{5}{14}} = \frac{3}{5}$$

$$Pr(y = \text{no}|\text{outlook=rainy}) = \frac{Pr(\text{outlook=rainy}|y = \text{no})Pr(y = \text{no})}{Pr(\text{outlook=rainy})}$$

$$= \frac{\frac{2}{5}\frac{5}{14}}{\frac{5}{14}} = \frac{2}{5}$$

Then

looking at the discriminative model

$$y_{\text{MAP}} = \arg\max_y Pr(y|\text{outlook=rainy}) = \underline{\text{yes}}\ (3/5 > 2/5)$$

find y s.t. y makes (an event most likely)

$$y_{\text{ML}} = \arg\max_y Pr(\text{outlook=rainy}|y) = \underline{\text{no}}\ (2/5 > 3/9)$$

looking at the generative model

¡ ( y = no maximizes the likelihood of outlook = rainy ) !

( " y = no " maximizes "rainy" ) !

# Source of confusion

Maximum a Posteriori (MAP) and Maximum Likelihood (ML) classification are *different*:

find a "y" that maximizes the likelihood of... :

we are always finding a "y" that maximizes (1) an output "y" given a condition or (2) an event (data) "x"

$$(1)\quad y_{\text{MAP}} = \arg\max_y P(y|x, \theta_{\text{ML}}) \rightarrow \text{find } y \text{ that is most likely for that given } x$$

$$(2)\quad y_{\text{ML}} = \arg\max_y P(x|y, \theta_{\text{ML}}) \rightarrow \text{find "}y\text{" that make "}x\text{" most likely}$$

even with parameters $\theta$ estimated with the ML *optimality criterion*:

$$\theta_{\text{ML}} = \underbrace{\arg\max_\theta P(D|y, \theta)}_{\text{params that best fit our data (observations)}} = \arg\max_\theta \underbrace{\prod_n}_{\text{loop}} P(x_n|y_n, \theta)$$

$\equiv$ for all observations

NB: ML *parameter* estimation is not ML regression/classification.

# Outline

# Problem: Curse of Dimensionality

| $n$ | $\mathbf{x}_n$ | | | | $y_n$ |
|---|---|---|---|---|---|
| example | outlook | temperature | humidity | windy | play |
| 1 | sunny | hot | high | false | no |
| 2 | sunny | hot | high | true | no |
| 3 | overcast | hot | high | false | yes |
| 4 | rainy | mild | high | false | yes |
| 5 | rainy | cool | normal | false | yes |
| 6 | rainy | cool | normal | true | no |
| 7 | overcast | cool | normal | true | yes |
| 8 | sunny | mild | high | false | no |
| 9 | sunny | cool | normal | false | yes |
| 10 | rainy | mild | normal | false | yes |
| 11 | sunny | mild | normal | true | yes |
| 12 | overcast | mild | high | true | yes |
| 13 | overcast | hot | normal | false | yes |
| 14 | rainy | mild | high | true | no |

difficult to model $Pr(\text{outlook}, \text{temperature}, \text{humidity}, \text{windy}|\text{play})$

# Problem: Curse of Dimensionality

- Volume of feature space exponential in number of features.
- More features $\implies$ potential for better description of the objects but ...
- ... $\implies$ need more and more data to model $Pr(x, y)$ well

# Problem: Curse of Dimensionality

- Volume of feature space exponential in number of features.
- More features $\implies$ potential for better description of the objects but ...
- ... $\implies$ need more and more data to model $Pr(x, y)$ well

Approximation: **Naïve Bayes classifier**

- All features (dimensions) regarded as conditionally independent.
- Instead of modelling one $D$-dimensional distribution: $Pr$(outlook, temperature, humidity, windy|play) model $D$ one-dimensional distributions: $Pr$(outlook|play), $Pr$(temperature|play), $Pr$(humidity|play), $Pr$(windy|play)

# Naïve Bayes Classifier

- $\mathbf{x}$ is a vector $(x_1, \ldots, x_D)$ of attribute or feature values.
- Let $\mathcal{Y} = \{1, 2, \ldots, K\}$ be the set of possible classes.
- MAP classification is

Bayes

$$y_{\text{MAP}} = \arg\max_{y \in \mathcal{Y}} Pr(y \mid x_1, \ldots, x_D) = \arg\max_{y \in \mathcal{Y}} \frac{Pr(x_1, \ldots, x_D \mid y)\, Pr(y)}{Pr(x_1, \ldots, x_D)}$$
$$= \arg\max_{y \in \mathcal{Y}} Pr(x_1, \ldots, x_D \mid y)\, Pr(y)$$

not y-dependent

# Naïve Bayes Classifier

- $\mathbf{x}$ is a vector $(x_1, \ldots, x_D)$ of attribute or feature values.
- Let $\mathcal{Y} = \{1, 2, \ldots, K\}$ be the set of possible classes.
- MAP classification is

$$\begin{aligned} y_{\text{MAP}} &= \arg\max_{y \in \mathcal{Y}} Pr(y \,|\, x_1, \ldots, x_D) = \arg\max_{y \in \mathcal{Y}} \frac{Pr(x_1, \ldots, x_D \,|\, y)\, Pr(y)}{Pr(x_1, \ldots, x_D)} \\ &= \arg\max_{y \in \mathcal{Y}} Pr(x_1, \ldots, x_D \,|\, y)\, Pr(y) \end{aligned}$$

- Naïve Bayes assumption:
$Pr(x_1, \ldots, x_D \,|\, y) = \prod_{d=1}^{D} Pr(x_d \,|\, y)$

→ since all features are presumably independent.

# Naïve Bayes Classifier

- $\mathbf{x}$ is a vector $(x_1, \ldots, x_D)$ of attribute or feature values.
- Let $\mathcal{Y} = \{1, 2, \ldots, K\}$ be the set of possible classes.
- MAP classification is

$$\begin{aligned} y_{\mathsf{MAP}} &= \arg\max_{y \in \mathcal{Y}} Pr(y \mid x_1, \ldots, x_D) = \arg\max_{y \in \mathcal{Y}} \frac{Pr(x_1, \ldots, x_D \mid y)\, Pr(y)}{Pr(x_1, \ldots, x_D)} \\ &= \arg\max_{y \in \mathcal{Y}} Pr(x_1, \ldots, x_D \mid y)\, Pr(y) \end{aligned}$$

- Naïve Bayes assumption:
  $Pr(x_1, \ldots, x_D \mid y) = \prod_{d=1}^{D} Pr(x_d \mid y)$
- MAP classification with Naïve Bayes:

$$y_{\mathsf{MAP}} = \arg\max_{y \in \mathcal{Y}} Pr(y) \prod_{d=1}^{D} Pr(x_d \mid y)$$

# Naïve Bayes Classifier

$$y_{\text{MAP}} = \arg\max_{y \in \mathcal{Y}} Pr(y) \prod_{d=1}^{D} Pr(x_d \,|\, y)$$

Naïve Bayes is one of the most common learning methods.
When to use:

- Moderate or large training set available.
- Feature dimensions are conditionally independent given class (or at least reasonably independent, still works with a little dependence).

Successful applications:

- Medical diagnoses (symptoms independent)
- Classification of text documents (words independent)

# Example: Play Orienteering?

Question: Will I go and play orienteering given the forecast?

My measurements:

- **outlook** $\in$ {sunny, overcast, rainy},
- **temperature** $\in$ {hot, mild, cool},

categorical variables.

- **humidity** $\in$ {high, normal},
- **windy** $\in$ {false, true}.

Bernoulli

Possible decisions: $y \in$ {yes, no}

# Example: Play Orienteering?

What I did in the past:

| $n$ | $\mathbf{x}_n$ | | | | $y_n$ |
|---|---|---|---|---|---|
| example | outlook | temperature | humidity | windy | play |
| 1 | sunny | hot | high | false | no |
| 2 | sunny | hot | high | true | no |
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| 14 | rainy | mild | high | true | no |

# xample: Play Orienteering?

## Counts of when I played orienteering (did not play)

| Outlook | | | Temperature | | | Humidity | | Windy | |
|---|---|---|---|---|---|---|---|---|---|
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| 2 (3) | 4 (0) | 3 (2) | 2 (2) | 4 (2) | 3 (1) | 3 (4) | 6 (1) | 6 (2) | 3 (3) |
| Y N | Y N | Y N | | | | | | | |

(played). (did not play).

# xample: Play Orienteering?

## Counts of when I played orienteering (did not play)

| Outlook | | | Temperature | | | Humidity | | Windy | |
|---|---|---|---|---|---|---|---|---|---|
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| 2 (3) | 4 (0) | 3 (2) | 2 (2) | 4 (2) | 3 (1) | 3 (4) | 6 (1) | 6 (2) | 3 (3) |

## Prior of whether I played orienteering or not

Counts:

| Play | |
|---|---|
| yes | no |
| 9 | 5 |

Prior Probabilities:

| Play | |
|---|---|
| yes | no |
| $\frac{9}{14}$ | $\frac{5}{14}$ |

# xample: Play Orienteering?

## Counts of when I played orienteering (did not play)

| Outlook | | | Temperature | | | Humidity | | Windy | |
|---|---|---|---|---|---|---|---|---|---|
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| 2 (3) | 4 (0) | 3 (2) | 2 (2) | 4 (2) | 3 (1) | 3 (4) | 6 (1) | 6 (2) | 3 (3) |

## Prior of whether I played orienteering or not

Counts:

| Play | |
|---|---|
| yes | no |
| 9 | 5 |

Prior Probabilities:

| Play | |
|---|---|
| yes | no |
| $\frac{9}{14}$ | $\frac{5}{14}$ |

## Likelihood of attribute when orienteering played $Pr(x_i \,|\, \text{y=yes})(Pr(x_i \,|\, \text{y=no}))$

| Outlook | | | Temperature | | | Humidity | | Windy | |
|---|---|---|---|---|---|---|---|---|---|
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| $\frac{2}{9}$ $(\frac{3}{5})$ | $\frac{4}{9}$ $(\frac{0}{5})$ | $\frac{3}{9}$ $(\frac{2}{5})$ | $\frac{2}{9}$ $(\frac{2}{5})$ | $\frac{4}{9}$ $(\frac{2}{5})$ | $\frac{3}{9}$ $(\frac{1}{5})$ | $\frac{3}{9}$ $(\frac{4}{5})$ | $\frac{6}{9}$ $(\frac{1}{5})$ | $\frac{6}{9}$ $(\frac{2}{5})$ | $\frac{3}{9}$ $(\frac{3}{5})$ |

# Example: Play Orienteering?

Inference: Use the learnt model to classify a new instance.

New instance:

$$\mathbf{x} = \underbrace{(\text{sunny, cool, high, true})}_{\text{variables to consider}}$$

Apply Naïve Bayes Classifier:

$$y_{\text{MAP}} = \arg \max_{y \,\in\, \{\text{yes, no}\}} Pr(y) \prod_{i=1}^{4} Pr(x_i \,|\, y)$$

$$\overbrace{P(\text{yes})}^{\text{prior.}}\ \overbrace{P(\text{sunny} \,|\, \text{yes})\ P(\text{cool} \,|\, \text{yes})\ P(\text{high} \,|\, \text{yes})\ P(\text{true} \,|\, \text{yes})}^{\text{likelihood of independent events.}} = \frac{9}{14} \times \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} = .005$$

$$P(\text{no})\ P(\text{sunny} \,|\, \text{no})\ P(\text{cool} \,|\, \text{no})\ P(\text{high} \,|\, \text{no})\ P(\text{true} \,|\, \text{no}) = \frac{5}{14} \times \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5} = .021$$

# Example: Play Orienteering?

Inference: Use the learnt model to classify a new instance.

New instance:

$$\mathbf{x} = (\text{sunny, cool, high, true})$$

Apply Naïve Bayes Classifier:

$$y_{\text{MAP}} = \arg \max_{y \in \{\text{yes, no}\}} Pr(y) \prod_{i=1}^{4} Pr(x_i \,|\, y)$$

$$P(\text{yes})\, P(\text{sunny} \,|\, \text{yes})\, P(\text{cool} \,|\, \text{yes})\, P(\text{high} \,|\, \text{yes})\, P(\text{true} \,|\, \text{yes}) = \frac{9}{14} \times \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} = .005$$

$$P(\text{no})\, P(\text{sunny} \,|\, \text{no})\, P(\text{cool} \,|\, \text{no})\, P(\text{high} \,|\, \text{no})\, P(\text{true} \,|\, \text{no}) = \frac{5}{14} \times \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5} = .021$$

more likely!

$$\Longrightarrow \quad y_{\text{MAP}} = \text{no}$$

# Naïve Bayes: Independence Violation

- Conditional independence assumption:

$$Pr(x_1, x_2, \ldots, x_D \,|\, y) = \prod_{d=1}^{D} Pr(x_d \,|\, y)$$

  often violated – but it works surprisingly well anyway!

- Since dependencies ignored, naïve Bayes posteriors often unrealistically close to 0 or 1.
  *Different attributes say the same thing to a higher degree than we expect as they are correlated in reality.*

# Naïve Bayes: Estimating Probabilities

- **Problem:** What if none of the training instances with target value $y$ have attribute $x_i$? Then

$$Pr(x_i \mid y) = 0 \implies Pr(y) \prod_{i=1}^{D} Pr(x_i \mid y) = 0$$

for some x, y always has the same value (Y/N), and never takes the other (0).

(probability is zero and multiplication collapses)

# Naïve Bayes: Estimating Probabilities

- **Problem:** What if none of the training instances with target value $y$ have attribute $x_i$? Then

$$Pr(x_i \,|\, y) = 0 \quad \Longrightarrow \quad Pr(y)\prod_{i=1}^{D} Pr(x_i \,|\, y) = 0$$

- **Simple solution:** add pseudocounts to all counts so that no count is zero

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$$Pr(x_i \,|\, y) = 0 \quad \Longrightarrow \quad Pr(y) \prod_{i=1}^{D} Pr(x_i \,|\, y) = 0$$

- **Simple solution:** add pseudocounts to all counts so that no count is zero
- This is a form of regularization or smoothing

# Logistic Regression

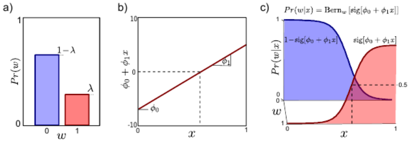



Figure from Prince (Ch. 9)

- Binary classification problem: $y \in \{0, 1\}$ treated as a regression problem: $\mathbf{x} \to \lambda$ (Bernoulli param.)

$$\begin{aligned} Y|\mathbf{X} &\sim \text{Bernoulli}(\lambda(\mathbf{x})) \\ Pr(y|\mathbf{x}) &= \lambda(\mathbf{x})^y (1 - \lambda(\mathbf{x}))^{(1-y)} \\ \lambda(\mathbf{x}) &= \text{sigmoid}(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}}} \end{aligned}$$

satisfies axioms of probability

# Logistic Regression

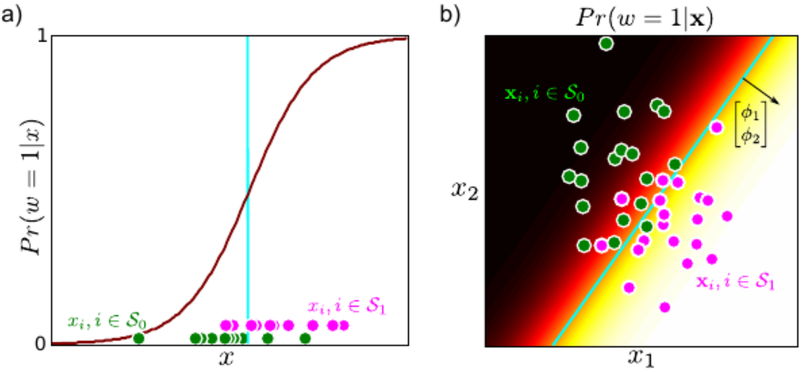
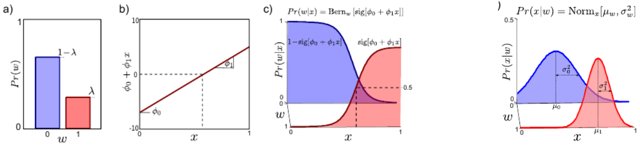



Figure from Prince (Ch. 9)

# Logistic Regression vs Gaussian Classifier




Figures from Prince (Ch. 9)

Different learning: (likelihood).

- Gaussians: generative model, optimize $Pr(\mathbf{x}|y_0)$ and $Pr(\mathbf{x}|y_1)$
- Logistic Regression: discriminative model, optimize $Pr(y_1|\mathbf{x})$

(posterior).

# Logistic Regression: MLE

Learning: maximize $Pr(y|\mathbf{x})$ (discriminative method)

$$
\begin{aligned}
Pr(y|\mathbf{x},\mathbf{w}) &= \prod_{i=1}^{N} \lambda(\mathbf{x}_i)^{y_i}(1-\lambda(\mathbf{x}_i))^{(1-y_i)} \\
\log Pr(y|\mathbf{x},\mathbf{w}) &= \sum_{i=1}^{N} [y_i \log \lambda(\mathbf{x}_i) + (1-y_i)\log(1-\lambda(\mathbf{x}_i))] \\
&= \sum_{i=1}^{N} \left[y_i \log \mathrm{sig}(\mathbf{w}^T\mathbf{x}_i) + (1-y_i)\log\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x}_i)\right)\right]
\end{aligned}
$$

(Bernoulli, binary example).

# Logistic Regression: MLE

Learning: maximize $Pr(y|\mathbf{x})$ (discriminative method)

$$\begin{aligned}
Pr(y|\mathbf{x},\mathbf{w}) &= \prod_{i=1}^{N} \lambda(\mathbf{x}_i)^{y_i}(1-\lambda(\mathbf{x}_i))^{(1-y_i)} \\
\log Pr(y|\mathbf{x},\mathbf{w}) &= \sum_{i=1}^{N} [y_i \log \lambda(\mathbf{x}_i) + (1-y_i)\log(1-\lambda(\mathbf{x}_i))] \\
&= \sum_{i=1}^{N} \left[y_i \log \mathrm{sig}(\mathbf{w}^T\mathbf{x}_i) + (1-y_i)\log\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x}_i)\right)\right]
\end{aligned}$$

Optimize by setting: no close form solution! Use gradient descent

$$\frac{d}{d\mathbf{w}} \log Pr(y|\mathbf{x},\mathbf{w}) = \sum_{i=1}^{N} \left(y_i - \mathrm{sig}(\mathbf{w}^T\mathbf{x}_i)\right)\mathbf{x}_i = 0$$

(global minimum garanteed).
because of using "sigmoid" function.

# Hints: derivatives of sigmoid

$$\mathsf{sig}(\mathbf{w}^T\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^T\mathbf{x}}}$$

$$\frac{d}{d\mathbf{w}}\,\mathrm{sig}(\mathbf{w}^T\mathbf{x}) = \mathrm{sig}(\mathbf{w}^T\mathbf{x})\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right)\mathbf{x}$$

$$\frac{d}{d\mathbf{w}}\log\left(\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right) = \frac{\mathrm{sig}(\mathbf{w}^T\mathbf{x})\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right)}{\mathrm{sig}(\mathbf{w}^T\mathbf{x})}\mathbf{x} = \left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right)\mathbf{x}$$

$$\frac{d}{d\mathbf{w}}\log\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right) = \frac{-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\left(1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})\right)}{1-\mathrm{sig}(\mathbf{w}^T\mathbf{x})}\mathbf{x} = -\mathrm{sig}(\mathbf{w}^T\mathbf{x})\ \mathbf{x}$$

# Logistic Regression vs Conditional Gaussian

**Number of parameters ($D$ dimensions, 2 classes):**

Gaussian distributions (equal priors)

| | |
|---|---|
| $2 \times D$ | (mean vectors) |
| $D(D+1)/2$ | (shared covariance) |
| $D(D+5)/2$ | (total, quadratic in $D$) |

Logistic Regression

$D$ (weights)

(less parameters)

**Training:**

Gaussian distributions

- closed form solution
- generative model

Logistic Regression

- gradient descent
- discriminative model

# Summary

1. Introduction
   - Probabilistic Classification and Regression
   - Discriminative vs Generative Models
   - Parametric vs Non-parametric Inference
2. Maximum Likelihood (ML) Estimation
   - Regression
   - Classification
3. Special Cases
   - Naïve Bayes Classifier
   - Logistic Regression

# Check your understanding!

Consider a dataset $\mathcal{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}$ of $N$ independent and identically distributed observations where each $\mathbf{x}_n$ is a $p$-dimensional real vector. Assume the random variable $Y_n$ is distributed Laplacian with a mean $\boldsymbol{\beta}^T\mathbf{x}_n$ and known scale parameter $b > 0$. In other words, $Y_n|\mathbf{x}_n, \boldsymbol{\beta} \sim \mathcal{L}(\boldsymbol{\beta}^T\mathbf{x}_n, b)$. Define the a priori distribution of the parameters $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)$ *multivariate* Gaussian with parameters mean $\mathbf{0}$ and variance $\sigma^2\mathbf{I}$.

# Check your understanding!

1. Derive the maximum likelihood (ML) estimate of $\boldsymbol{\beta}$.
2. Which of the following statements is not true? (There may be more than one.)
   1. As $b$ increases and $N$ remains constant, the ML estimate of $\boldsymbol{\beta}$ becomes poorer.
   2. As $N$ increases and $b$ remains constant, the ML estimate of $\boldsymbol{\beta}$ becomes poorer.
   3. As $b$ decreases and $N$ remains constant, the ML estimate of $\boldsymbol{\beta}$ becomes poorer.
   4. As $N$ decreases and $b$ remains constant, the ML estimate of $\boldsymbol{\beta}$ becomes poorer.