Gaussian and Linear Discriminant Analysis; Multiclass Classification

Professor Ameet Talwalkar
Outline

1. Administration
2. Review of last lecture
3. Generative versus discriminative
4. Multiclass classification
Announcements

- Homework 2: due on Wednesday
Outline

1. Administration

2. Review of last lecture
   - Logistic regression

3. Generative versus discriminative

4. Multiclass classification
Logistic classification

Setup for two classes

- Input: \( x \in \mathbb{R}^D \)
- Output: \( y \in \{0, 1\} \)
- Training data: \( D = \{(x_n, y_n), n = 1, 2, \ldots, N\} \)
- Model of conditional distribution

\[
p(y = 1|x; b, w) = \sigma[g(x)]
\]

where

\[
g(x) = b + \sum_d w_d x_d = b + w^T x
\]
Why the sigmoid function?

What does it look like?

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

where

\[a = b + \mathbf{w}^T \mathbf{x}\]

Properties

- Bounded between 0 and 1 (thus, interpretable as probability)
- Monotonically increasing (thus, usable to derive classification rules)
  - \(\sigma(a) > 0.5\), positive (classify as '1')
  - \(\sigma(a) < 0.5\), negative (classify as '0')
  - \(\sigma(a) = 0.5\), undecidable

Nice computational properties

Linear or nonlinear classifier?
Why the sigmoid function?

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- Nice computational properties Derivative is in a simple form
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Linear or nonlinear classifier?
\( \sigma(a) \) is nonlinear, however, the decision boundary is determined by

\[ \sigma(a) = 0.5 \Rightarrow a = 0 \Rightarrow g(x) = b + \mathbf{w}^T \mathbf{x} = 0 \]

which is a linear function in \( \mathbf{x} \).

We often call \( b \) the offset term.
Likelihood function

Probability of a single training sample \((x_n, y_n)\)

\[
p(y_n|x_n; b, w) = \begin{cases} 
\sigma(b + w^T x_n) & \text{if } y_n = 1 \\
1 - \sigma(b + w^T x_n) & \text{otherwise}
\end{cases}
\]
Likelihood function

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\]

Compact expression, exploring that \(y_n\) is either 1 or 0

\[
p(y_n|x_n; b; w) = \sigma(b + w^T x_n)^{y_n} [1 - \sigma(b + w^T x_n)]^{1-y_n}
\]
Maximum likelihood estimation

Cross-entropy error (negative log-likelihood)

\[ E(b, w) = - \sum_n \{ y_n \log \sigma(b + w^T x_n) + (1 - y_n) \log [1 - \sigma(b + w^T x_n)] \} \]

Numerical optimization

- Gradient descent: simple, scalable to large-scale problems
- Newton method: fast but not scalable
Numerical optimization

**Gradient descent**

- Choose a proper step size $\eta > 0$
- Iteratively update the parameters following the negative gradient to minimize the error function

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \sum_n \{ \sigma(w^T x_n) - y_n \} x_n$$
Numerical optimization

**Gradient descent**

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**Remarks**

- Gradient is direction of steepest ascent.
- The step size needs to be chosen carefully to ensure convergence.
- The step size can be adaptive (i.e. varying from iteration to iteration).
- Variant called *stochastic* gradient descent (later this quarter).
Intuition for Newton’s method

Approximate the true function with an easy-to-solve optimization problem

In particular, we can approximate the cross-entropy error function around $w^{(t)}$ by a quadratic function (its second order Taylor expansion), and then minimize this quadratic function.
Update Rules

Gradient descent

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \sum_n \left\{ \sigma(\mathbf{w}^T \mathbf{x}_n) - y_n \right\} \mathbf{x}_n$$

Newton method

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - H^{(t)}^{-1} \nabla \mathcal{E}(\mathbf{w}^{(t)})$$
Contrast gradient descent and Newton’s method

**Similar**

- Both are iterative procedures.

**Different**

- Newton’s method requires second-order derivatives (less scalable, but faster convergence)
- Newton’s method does not have the magic $\eta$ to be set
Outline

1 Administration

2 Review of last lecture

3 Generative versus discriminative
   - Contrast Naive Bayes and logistic regression
   - Gaussian and Linear Discriminant Analysis

4 Multiclass classification
Naive Bayes and logistic regression: two different modelling paradigms

Consider spam classification problem

- **First Strategy:**
  - Use training set to find a decision boundary in the feature space that separates spam and non-spam emails
  - Given a test point, predict its label based on which side of the boundary it is on.

- **Second Strategy:**
  - Look at spam emails and build a model of what they look like.
  - Similarly, build a model of what non-spam emails look like.
  - To classify a new email, match it against both the spam and non-spam models to see which is the better fit.

First strategy is discriminative (e.g., logistic regression)
Second strategy is generative (e.g., naive bayes)
Naive Bayes and logistic regression: two different modelling paradigms

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Second strategy is generative (e.g., naive bayes)
Generative vs Discriminative

**Discriminative**

- Requires only specifying a model for the conditional distribution $p(y|x)$, and thus, maximizes the *conditional* likelihood
  $$\sum_n \log p(y_n|x_n).$$
- Models that try to learn mappings directly from feature space to the labels are also discriminative, e.g., perceptron, SVMs (covered later)
Generative vs Discriminative

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**Generative**
- Aims to model the joint probability $p(x, y)$ and thus maximize the *joint* likelihood $\sum_n \log p(x_n, y_n)$.
- The generative models we’ll cover do so by modeling $p(x|y)$ and $p(y)$
Generative vs Discriminative

**Discriminative**

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**Generative**

- Aims to model the joint probability $p(x, y)$ and thus maximize the *joint* likelihood $\sum_n \log p(x_n, y_n)$.
- The generative models we’ll cover do so by modeling $p(x|y)$ and $p(y)$
- Let’s look at two more examples: Gaussian (or Quadratic) Discriminative Analysis and Linear Discriminative Analysis
Determining sex based on measurements
Generative approach

Model joint distribution of \((x = (\text{height, weight}), \ y = \text{sex})\)

**our data**

<table>
<thead>
<tr>
<th>Sex</th>
<th>Height</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6′</td>
<td>175</td>
</tr>
<tr>
<td>0</td>
<td>5’2”</td>
<td>120</td>
</tr>
<tr>
<td>1</td>
<td>5’6”</td>
<td>140</td>
</tr>
<tr>
<td>1</td>
<td>6’2”</td>
<td>240</td>
</tr>
<tr>
<td>0</td>
<td>5.7”</td>
<td>130</td>
</tr>
</tbody>
</table>

Intuition: we will model how heights vary (according to a Gaussian) in each sub-population (male and female).
Model of the joint distribution (1D)

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

\[ = \begin{cases} 
  p_0 \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{(x-\mu_0)^2}{2\sigma_0^2}} & \text{if } y = 0 \\
  p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x-\mu_1)^2}{2\sigma_1^2}} & \text{if } y = 1 
\end{cases} \]

\[ p_0 + p_1 = 1 \] are prior probabilities, and \( p(x | y) \) is a class conditional distribution.
Model of the joint distribution (1D)

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

\[ = \begin{cases} 
  p_0 \frac{1}{\sqrt{2\pi\sigma_0}} e^{-\frac{(x-\mu_0)^2}{2\sigma_0^2}} & \text{if } y = 0 \\
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\end{cases} \]

\( p_0 + p_1 = 1 \) are prior probabilities, and \( p(x|y) \) is a class conditional distribution

What are the parameters to learn?
Parameter estimation

**Log Likelihood of training data** \( \mathcal{D} = \{(x_n, y_n)\}_{n=1}^N \) with \( y_n \in \{0, 1\} \)

\[
\log P(\mathcal{D}) = \sum_n \log p(x_n, y_n)
\]

\[
= \sum_{n:y_n=0} \log \left( p_0 \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{(x_n-\mu_0)^2}{2\sigma_0^2}} \right) \\
+ \sum_{n:y_n=1} \log \left( p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x_n-\mu_1)^2}{2\sigma_1^2}} \right)
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\log P(\mathcal{D}) = \sum_{n} \log p(x_n, y_n)
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**Max log likelihood** \((p_0^*, p_1^*, \mu_0^*, \mu_1^*, \sigma_0^*, \sigma_1^*) = \arg \max \log P(\mathcal{D})\)
Parameter estimation

Log Likelihood of training data \( D = \{ (x_n, y_n) \}_{n=1}^N \) with \( y_n \in \{0, 1\} \)

\[
\log P(D) = \sum_n \log p(x_n, y_n)
\]

\[
= \sum_{n: y_n=0} \log \left( p_0 \frac{1}{\sqrt{2\pi}\sigma_0} e^{-\frac{(x_n-\mu_0)^2}{2\sigma_0^2}} \right) \\
+ \sum_{n: y_n=1} \log \left( p_1 \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{(x_n-\mu_1)^2}{2\sigma_1^2}} \right)
\]

Max log likelihood \( (p_0^*, p_1^*, \mu_0^*, \mu_1^*, \sigma_0^*, \sigma_1^*) = \arg \max \log P(D) \)

Max likelihood \( (D = 2) \) \( (p_0^*, p_1^*, \mu_0^*, \mu_1^*, \Sigma_0^*, \Sigma_1^*) = \arg \max \log P(D) \)
Parameter estimation

**Log Likelihood of training data** $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N}$ with $y_n \in \{0, 1\}$

$$\log P(\mathcal{D}) = \sum_n \log p(x_n, y_n)$$

$$= \sum_{n: y_n=0} \log \left( p_0 \frac{1}{\sqrt{2\pi} \sigma_0} e^{-\frac{(x_n-\mu_0)^2}{2\sigma_0^2}} \right)$$

$$+ \sum_{n: y_n=1} \log \left( p_1 \frac{1}{\sqrt{2\pi} \sigma_1} e^{-\frac{(x_n-\mu_1)^2}{2\sigma_1^2}} \right)$$

**Max log likelihood** $(p_0^*, p_1^*, \mu_0^*, \mu_1^*, \sigma_0^*, \sigma_1^*) = \arg \max \log P(\mathcal{D})$

**Max likelihood** $(\mathcal{D} = 2)$ $(p_0^*, p_1^*, \mu_0^*, \mu_1^*, \Sigma_0^*, \Sigma_1^*) = \arg \max \log P(\mathcal{D})$

- For Naive Bayes we assume $\Sigma_i^*$ is diagonal
Decision boundary

As before, the Bayes optimal one under the assumed joint distribution depends on

\[ p(y = 1|x) \geq p(y = 0|x) \]

which is equivalent to

\[ p(x|y = 1)p(y = 1) \geq p(x|y = 0)p(y = 0) \]
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Namely,

\[ -\frac{(x - \mu_1)^2}{2\sigma_1^2} - \log \sqrt{2\pi\sigma_1} + \log p_1 \geq -\frac{(x - \mu_0)^2}{2\sigma_0^2} - \log \sqrt{2\pi\sigma_0} + \log p_0 \]
Decision boundary

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\[ -\frac{(x - \mu_1)^2}{2\sigma_1^2} - \log \sqrt{2\pi}\sigma_1 + \log p_1 \geq -\frac{(x - \mu_0)^2}{2\sigma_0^2} - \log \sqrt{2\pi}\sigma_0 + \log p_0 \]

\[ \Rightarrow ax^2 + bx + c \geq 0 \quad \leftarrow \text{the decision boundary not linear!} \]
Example of nonlinear decision boundary

*Note*: the boundary is characterized by a quadratic function, giving rise to the shape of a parabolic curve.
A special case: what if we assume the two Gaussians have the same variance?

\[-\frac{(x - \mu_1)^2}{2\sigma_1^2} - \log \sqrt{2\pi \sigma_1} + \log p_1 \geq -\frac{(x - \mu_0)^2}{2\sigma_0^2} - \log \sqrt{2\pi \sigma_0} + \log p_0\]

with \( \sigma_0 = \sigma_1 \)
A special case: what if we assume the two Gaussians have the same variance?

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with \(\sigma_0 = \sigma_1\)

We get a linear decision boundary: \(bx + c \geq 0\)
A special case: what if we assume the two Gaussians have the same variance?

\[-\frac{(x - \mu_1)^2}{2\sigma_1^2} - \log \sqrt{2\pi \sigma_1} + \log p_1 \geq -\frac{(x - \mu_0)^2}{2\sigma_0^2} - \log \sqrt{2\pi \sigma_0} + \log p_0\]

with $\sigma_0 = \sigma_1$

We get a linear decision boundary: $bx + c \geq 0$

*Note*: equal variances across two different categories could be a very strong assumption.

For example, from the plot, it does seem that the male population has slightly bigger variance (i.e., bigger ellipse) than the female population. So the assumption might not be applicable.
Mini-summary

**Gaussian discriminant analysis**
- A generative approach, assuming the data modeled by
  \[ p(x, y) = p(y)p(x|y) \]
  where \( p(x|y) \) is a Gaussian distribution.
- Parameters (of Gaussian distributions) estimated by max likelihood
- Decision boundary
Mini-summary

Gaussian discriminant analysis

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

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  - In general, nonlinear functions of \( x \) (quadratic discriminant analysis)
  - Linear under various assumptions about Gaussian covariance matrices
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Gaussian discriminant analysis

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- Decision boundary
  - In general, nonlinear functions of \( x \) (quadratic discriminant analysis)
  - Linear under various assumptions about Gaussian covariance matrices
    - Single arbitrary matrix (linear discriminant analysis)
    - Multiple diagonal matrices (Gaussian Naive Bayes (GNB))
    - Single diagonal matrix (GNB in HW2 Problem 1)
So what is the discriminative counterpart?

**Intuition**

The decision boundary in Gaussian discriminant analysis is

\[ ax^2 + bx + c = 0 \]

Let us model the conditional distribution analogously

\[ p(y|x) = \sigma[ax^2 + bx + c] = \frac{1}{1 + e^{-(ax^2+bx+c)}} \]

Or, even simpler, going after the decision boundary of linear discriminant analysis

\[ p(y|x) = \sigma[bx + c] \]

Both look very similar to logistic regression — i.e. we focus on writing down the *conditional* probability, *not* the joint probability.
Does this change how we estimate the parameters?

**First change: a smaller number of parameters to estimate**

Models only parameterized by $a$, $b$ and $c$. There are no prior probabilities $(p_0, p_1)$ or Gaussian distribution parameters $(\mu_0, \mu_1, \sigma_0 \text{ and } \sigma_1)$. 
Does this change how we estimate the parameters?

First change: a smaller number of parameters to estimate

Models only parameterized by $a, b$ and $c$. There are no prior probabilities $(p_0, p_1)$ or Gaussian distribution parameters $(\mu_0, \mu_1, \sigma_0$ and $\sigma_1)$.

Second change: maximize the conditional likelihood $p(y|x)$

\[
(a^*, b^*, c^*) = \text{arg min} - \sum_n \{y_n \log \sigma(ax_n^2 + bx_n + c) \tag{1}
+ (1 - y_n) \log[1 - \sigma(ax_n^2 + bx_n + c)]\} \tag{2}
\]

No closed form solutions!
How easy for our Gaussian discriminant analysis?

Example

\[ p_1 = \frac{\text{# of training samples in class 1}}{\text{# of training samples}} \]  \hspace{1cm} (3)

\[ \mu_1 = \frac{\sum_{n:y_n=1} x_n}{\text{# of training samples in class 1}} \]  \hspace{1cm} (4)

\[ \sigma_1^2 = \frac{\sum_{n:y_n=1} (x_n - \mu_1)^2}{\text{# of training samples in class 1}} \]  \hspace{1cm} (5)

**Note:** see textbook for detailed derivation (including generalization to higher dimensions and multiple classes)
Generative versus discriminative: which one to use?

There is no fixed rule

- Selecting which type of method to use is dataset/task specific
- It depends on how well your modeling assumption fits the data

For instance, as we show in HW2, when data follows a specific variant of the Gaussian Naive Bayes assumption, $p(y|x)$ necessarily follows a logistic function. However, the converse is not true.

- Gaussian Naive Bayes makes a stronger assumption than logistic regression
- When data follows this assumption, Gaussian Naive Bayes will likely yield a model that better fits the data
- But logistic regression is more robust and less sensitive to incorrect modeling assumption
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4. Multiclass classification
   - Use binary classifiers as building blocks
   - Multinomial logistic regression
Setup

**Predict multiple classes/outcomes:** $C_1, C_2, \ldots, C_K$

- Weather prediction: sunny, cloudy, raining, etc
- Optical character recognition: 10 digits + 26 characters (lower and upper cases) + special characters, etc

**Studied methods**

- Nearest neighbor classifier
- Naive Bayes
- Gaussian discriminant analysis
- Logistic regression
Logistic regression for predicting multiple classes? Easy

The approach of “one versus the rest”

- For each class $C_k$, change the problem into binary classification
  1. Relabel training data with label $C_k$, into POSITIVE (or ‘1’)
  2. Relabel all the rest data into NEGATIVE (or ‘0’)
Logistic regression for predicting multiple classes? Easy

**The approach of “one versus the rest”**

- For each class $C_k$, change the problem into binary classification
  1. Relabel training data with label $C_k$, into **POSITIVE** (or ‘1’)
  2. Relabel all the rest data into **NEGATIVE** (or ‘0’)

This step is often called 1-of-$K$ encoding. That is, only one is nonzero and everything else is zero.

Example: for class $C_2$, data go through the following change

$$(x_1, C_1) \rightarrow (x_1, 0), (x_2, C_3) \rightarrow (x_2, 0), \ldots, (x_n, C_2) \rightarrow (x_n, 1), \ldots,$$
Logistic regression for predicting multiple classes? Easy

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- Train \( K \) binary classifiers using logistic regression to differentiate the two classes
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\]

- Train \( K \) binary classifiers using logistic regression to differentiate the two classes
- When predicting on \( x \), combine the outputs of all binary classifiers
  1. What if all the classifiers say **negative**?
  2. What if multiple classifiers say **positive**?
Yet, another easy approach

The approach of “one versus one”

- For each pair of classes $C_k$ and $C_{k'}$, change the problem into binary classification
  1. Relabel training data with label $C_k$, into positive (or ‘1’)
  2. Relabel training data with label $C_{k'}$, into negative (or ‘0’)
  3. Disregard all other data

Ex: for class $C_1$ and $C_2$, $(x_1, C_1), (x_2, C_3), (x_3, C_2), \ldots \rightarrow (x_1, 1), (x_3, 0), \ldots$
Yet, another easy approach

**The approach of “one versus one”**

- For each *pair* of classes $C_k$ and $C_{k'}$, change the problem into binary classification
  1. Relabel training data with label $C_k$, into **positive** (or ‘1’)
  2. Relabel training data with label $C_{k'}$, into **negative** (or ‘0’)
  3. **Disregard** all other data

Ex: for class $C_1$ and $C_2$,

$$(x_1, C_1), (x_2, C_3), (x_3, C_2), \ldots \rightarrow (x_1, 1), (x_3, 0), \ldots$$
Yet, another easy approach

The approach of “one versus one”

- For each pair of classes $C_k$ and $C_k'$, change the problem into binary classification
  1. Relabel training data with label $C_k$, into POSITIVE (or ‘1’)
  2. Relabel training data with label $C_k'$, into NEGATIVE (or ‘0’)
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- Train $K(K - 1)/2$ binary classifiers using logistic regression to differentiate the two classes
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- Train $K(K - 1)/2$ binary classifiers using logistic regression to differentiate the two classes
- When predicting on $x$, combine the outputs of all binary classifiers
  There are $K(K - 1)/2$ votes!
Contrast these two approaches

Pros of each approach

One versus the rest: only needs to train $K$ classifiers.
▶ Makes a big difference if you have a lot of classes to go through.

One versus one: only needs to train a smaller subset of data (only those labeled with those two classes would be involved).
▶ Makes a big difference if you have a lot of data to go through.

Bad about both of them: Combining classifiers' outputs seem to be a bit tricky.

Any other good methods?
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*Combining classifiers’ outputs seem to be a bit tricky.*

Any other good methods?
Multinomial logistic regression

Intuition: from the decision rule of our naive Bayes classifier

\[ y^* = \arg \max_k p(y = C_k | x) = \arg \max_k \log p(x | y = C_k)p(y = C_k) \]
\[ = \arg \max_k \log \pi_k + \sum_i z_i \log \theta_{ki} = \arg \max_k \mathbf{w}_k^T \mathbf{x} \]
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\[ = \arg \max_k \log \pi_k + \sum_i z_i \log \theta_{ki} = \arg \max_k w_k^T x \]

Essentially, we are comparing

\[ w_1^T x, w_2^T x, \ldots, w_K^T x \]

with one for each category.
So, can we define the following conditional model?

\[ p(y = C_k | x) = \sigma[w^T_k x] \]

This would not work because:

\[ \sum_k p(y = C_k | x) = \sum_k \sigma[w^T_k x] \neq 1 \]

as each summand can be any number (independently) between 0 and 1.

But we are close!

We can learn the K linear models jointly to ensure this property holds!
First try

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We can learn the \( K \) linear models jointly to ensure this property holds!
**Definition of multinomial logistic regression**

**Model**

For each class $C_k$, we have a parameter vector $w_k$ and model the posterior probability as

$$p(C_k|x) = \frac{e^{w_k^T x}}{\sum_{k'} e^{w_{k'}^T x}}$$

← This is called *softmax* function.
Definition of multinomial logistic regression

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$$p(C_k | \mathbf{x}) = \frac{e^{w_k^T \mathbf{x}}}{\sum_{k'} e^{w_{k'}^T \mathbf{x}}}$$

$\leftarrow$ This is called softmax function

Decision boundary: assign $\mathbf{x}$ with the label that is the maximum of posterior

$$\arg \max_k P(C_k | \mathbf{x}) \rightarrow \arg \max_k w_k^T \mathbf{x}$$
How does the softmax function behave?

**Suppose we have**

\[ w_1^T x = 100, \ w_2^T x = 50, \ w_3^T x = -20 \]
How does the softmax function behave?

Suppose we have

\[ \mathbf{w}_1^T \mathbf{x} = 100, \mathbf{w}_2^T \mathbf{x} = 50, \mathbf{w}_3^T \mathbf{x} = -20 \]

We would pick the winning class label 1.

**Softmax translates these scores into well-formed conditional probabilities**

\[ p(y = 1|\mathbf{x}) = \frac{e^{100}}{e^{100} + e^{50} + e^{-20}} < 1 \]

- preserves relative ordering of scores
- maps scores to values between 0 and 1 that also sum to 1
Sanity check

**Multinomial model reduce to binary logistic regression** when $K = 2$

\[
p(C_1|x) = \frac{e^{w_1^T x}}{e^{w_1^T x} + e^{w_2^T x}} = \frac{1}{1 + e^{-(w_1 - w_2)^T x}}
\]

**Multinomial thus generalizes the (binary) logistic regression to deal with multiple classes.**
Parameter estimation

**Discriminative approach:** maximize conditional likelihood

\[
\log P(D) = \sum_n \log P(y_n|x_n)
\]
Parameter estimation

**Discriminative approach:** maximize conditional likelihood

\[
\log P(D) = \sum_n \log P(y_n|x_n)
\]

We will change \(y_n\) to \(y_n = [y_{n1} \ y_{n2} \ \cdots \ y_{nK}]^T\), a \(K\)-dimensional vector using 1-of-\(K\) encoding.

\[
y_{nk} = \begin{cases} 
1 & \text{if } y_n = k \\
0 & \text{otherwise}
\end{cases}
\]

Ex: if \(y_n = 2\), then, \(y_n = [0 \ 1 \ 0 \ 0 \ \cdots \ 0]^T\).
Parameter estimation

**Discriminative approach:** maximize conditional likelihood

\[
\log P(D) = \sum_n \log P(y_n | x_n)
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y_{nk} = \begin{cases} 
1 & \text{if } y_n = k \\
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\end{cases}
\]

Ex: if \(y_n = 2\), then, \(\mathbf{y}_n = [0 \ 1 \ 0 \ 0 \ \cdots \ 0]^T\).

\[
\Rightarrow \sum_n \log P(y_n | x_n) = \sum_n \log \prod_{k=1}^{K} P(C_k | x_n)^{y_{nk}} = \sum_n \sum_k y_{nk} \log P(C_k | x_n)
\]
Cross-entropy error function

**Definition**: negative log likelihood

$$
\mathcal{E}(w_1, w_2, \ldots, w_K) = - \sum_n \sum_k y_{nk} \log P(C_k | x_n)
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Cross-entropy error function

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\[ \mathcal{E}(w_1, w_2, \ldots, w_K) = - \sum_n \sum_k y_{nk} \log P(C_k | x_n) \]

**Properties**
- Convex, therefore unique global optimum
- Optimization requires numerical procedures, analogous to those used for binary logistic regression