18-661 Introduction to Machine Learning

Multi-class Classification

Spring 2023

ECE – Carnegie Mellon University

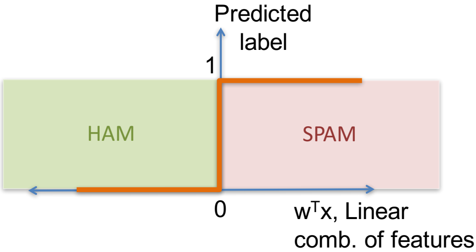
Outline

1. Review of Logistic Regression
2. Non-linear Decision Boundaries
3. Multi-class Classification
   - Multi-class Naïve Bayes
   - Multi-class Logistic Regression
4. Evaluating Classification Methods

Review of Logistic Regression

Visualizing a Linear Classifier

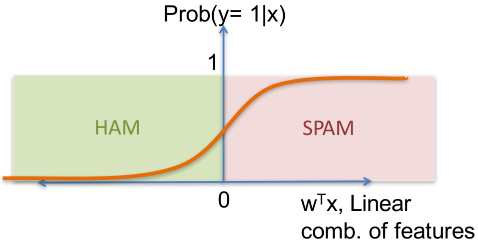
- x_1 = # of times 'lottery' appears in an email
- x_2 = # of times 'meet' appears in an email
- Define feature vector $\mathbf{x} = [1, x_1, x_2]$
- Learn the decision boundary $w_0 + w_1 x_1 + w_2 x_2 = 0$ such that
  - If $\mathbf{w}^\top \mathbf{x} \geq 0$ declare $y = 1$ (spam)
  - If $\mathbf{w}^\top \mathbf{x} < 0$ declare $y = 0$ (ham)



$y = 1$ for spam, $y = 0$ for ham

Intuition: Logistic Regression

- Suppose we want to output the probability of an email being spam/ham instead of just 0 or 1
- This gives information about the confidence in the decision
- Use a function $\sigma(\mathbf{w}^\top \mathbf{x})$ that maps $\mathbf{w}^\top \mathbf{x}$ to a value between 0 and 1



Probability that predicted label is 1 (spam)

Key Problem: Finding optimal weights $\mathbf{w}$ that accurately predict this probability for a new email

Formal Setup: Binary Logistic Classification

- Input/features: $\boldsymbol{x} = [1, x_1, x_2, \dots x_D] \in \mathbb{R}^{D+1}$
- Output: $y \in \{0, 1\}$
- Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \dots, N\}$
- Model:

$$p(y = 1|\boldsymbol{x}; \boldsymbol{w}) = \sigma[g(\boldsymbol{x})]$$

where

$$g(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = \boldsymbol{w}^\top \boldsymbol{x}$$

and $\sigma[\cdot]$ stands for the sigmoid function

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

How to Optimize w?

- Probability of a single training sample $(\boldsymbol{x}_n, y_n)$

$$P(y_n|\boldsymbol{x}_n; \boldsymbol{w}) = \begin{cases} \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) & \text{if} \quad y_n = 1 \\ 1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) & \text{otherwise} \end{cases}$$

- Compact expression, exploiting that y_n is either 1 or 0

$$P(y_n|\boldsymbol{x}_n; \boldsymbol{w}) = \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)^{y_n}[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]^{1-y_n}$$

- Minimize the negative log-likelihood of the whole training data $\mathcal{D}$, i.e., the cross-entropy error function

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

Cross-Entropy as a Loss Function

Supervised learning

We aim to build a function $h(\boldsymbol{x})$ to predict the true value y associated with $\boldsymbol{x}$. If we make a mistake, we incur a loss

$$\ell(h(\boldsymbol{x}), y)$$

Cross-entropy is also a sum over all data samples:

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

where $h(\boldsymbol{x}) = \sigma\left(\boldsymbol{w}^T \boldsymbol{x}\right)$.

What is the loss function?

$$\ell(h(\boldsymbol{x}_n), y) = -\{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

Gradient Descent for Logistic Regression

- We want to minimize the cross-entropy error function:

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

- Simple fact: derivatives of $\sigma(a)$ have a nice form:

$$\frac{d}{d\,a}\sigma(a) = \sigma(a)[1 - \sigma(a)]$$

- Gradient of cross-entropy loss is then

$$\frac{\partial \mathcal{E}(\boldsymbol{w})}{\partial \boldsymbol{w}} = \sum_n \underbrace{\left\{\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) - y_n\right\}}_{:=e_n} \boldsymbol{x}_n$$

- $e_n = \left\{\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) - y_n\right\}$ is called the *error* for the nth training sample.

Gradient descent for logistic regression

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

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

Stochastic gradient descent for logistic regression

- Choose a proper step size $\eta > 0$
- Draw a sample n uniformly at random
- Iteratively update the parameters following the negative gradient to minimize the error function

$$\boldsymbol{w}^{(t+1)} \leftarrow \boldsymbol{w}^{(t)} - \eta \left\{ \sigma\big(\boldsymbol{w}^{(t)\top} \boldsymbol{x}_n\big) - y_n \right\} \boldsymbol{x}_n$$

Naïve Bayes vs. Logistic Regression

Both classification models are linear functions of features

Joint vs. conditional distribution
Naive Bayes models the joint distribution: $P(X, Y) = P(Y)P(X|Y)$

Logistic regression models the conditional distribution: $P(Y|X)$

Correlated vs. independent features
Naive Bayes assumes independence of features and multiple occurences

Logistic Regression implicitly captures correlations when training weights

Generative vs. Discriminative
NB is a generative model, LR is a discriminative model

Logistic Regression vs. Linear Regression

	Logistic regression	**Linear regression**
Training data	$(\boldsymbol{x}_n, y_n), y_n \in \{0, 1\}$	$(\boldsymbol{x}_n, y_n), y_n \in \mathbb{R}$
Loss function	cross-entropy	RSS
Interpretation of $y_n \mid \boldsymbol{x}_n, \boldsymbol{w}$	$\sim \mathrm{Ber}(\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n))$	$\sim \mathcal{N}(\boldsymbol{w}^\top \boldsymbol{x}_n, \sigma^2)$
Gradient per sample	$\left(\sigma(\boldsymbol{x}_n^\top \boldsymbol{w}) - y_n\right) \boldsymbol{x}_n$	$\left(\boldsymbol{x}_n^\top \boldsymbol{w} - y_n\right) \boldsymbol{x}_n$

Cross-entropy loss function (logistic regression):

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

RSS loss function (linear regression):

$$RSS(\boldsymbol{w}) = \frac{1}{2} \sum_n (y_n - \boldsymbol{w}^\top \boldsymbol{x}_n)^2$$

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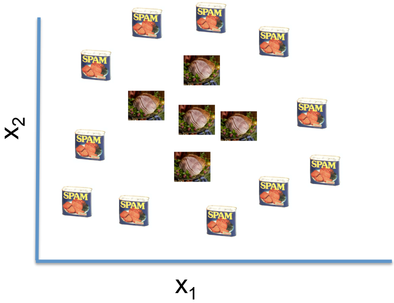
Non-linear Decision Boundaries

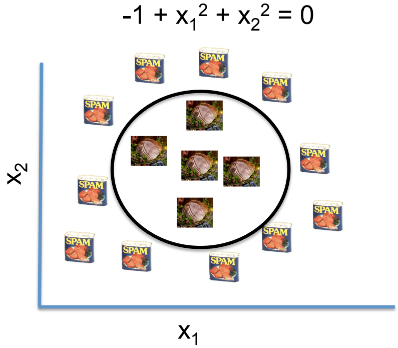
How to Handle More Complex Decision Boundaries?



- This data is not linearly separable...
- Use non-linear basis functions to add more features.

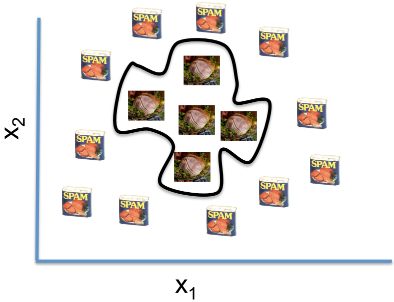
Adding Polynomial Features

- New feature vector is $\mathbf{x} = [1, x_1, x_2, x_1^2, x_2^2]$
- $\Pr(y = 1|\mathbf{x}) = \sigma(w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2)$
- If $\mathbf{w} = [-1, 0, 0, 1, 1]$, the boundary is $-1 + x_1^2 + x_2^2 = 0$
  - If $-1 + x_1^2 + x_2^2 \geq 0$ declare spam
  - If $-1 + x_1^2 + x_2^2 < 0$ declare ham



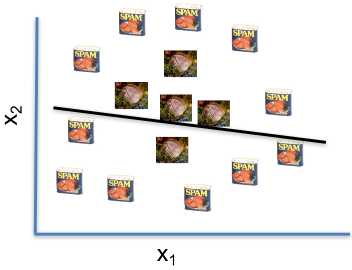
Adding Polynomial Features

- What if we add many more features and define $\mathbf{x} = [1, x_1, x_2, x_1^2, x_2^2, x_1^3, x_2^3, \ldots]$?
- We get a complex decision boundary

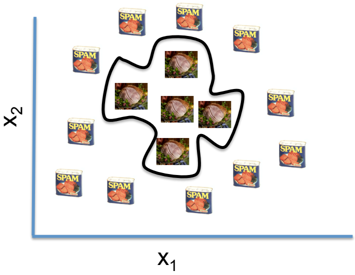


Can result in overfitting and bad generalization to new data points.

Concept-check: Bias-Variance Trade-off



high bias



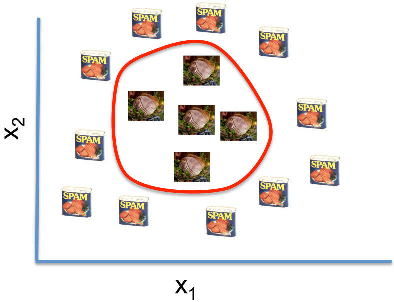
high variance

Solution to Overfitting: Regularization

- Add regularization term to be cross entropy loss function

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1-y_n) \log[1-\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\} + \underbrace{\frac{1}{2}\lambda \|w\|_2^2}_{\text{regularization}}$$

- Perform gradient descent on this regularized function
- Often, we do NOT regularize the bias term w_0



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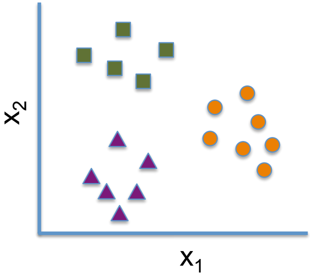
Multi-class Classification

What If There Are More than 2 Classes?

- Dog vs. cat. vs crocodile
- Movie genres (action, horror, comedy, ...)
- Part of speech tagging (verb, noun, adjective, ...)
- ...



Setup

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

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

$M =$number of classes

Methods we've studied for binary classification:

- Naïve Bayes
- Logistic regression

Do they generalize to multi-class classification?

Naïve Bayes Is Already Multi-class!

Formal Definition
Given a random vector $\mathbf{X} \in \mathbb{R}^{\mathrm{K}}$ and a dependent variable $Y \in [\mathrm{C}]$, the Naïve Bayes model defines the joint distribution

$$
\begin{aligned}
P(\mathbf{X} = \mathbf{x}, Y = c) &= P(Y = c) P(\mathbf{X} = \mathbf{x} | Y = c) && (1) \\
&= P(Y = c) \prod_{k=1}^{\mathrm{K}} P(\mathrm{word}_k | Y = c)^{x_k} && (2) \\
&= \pi_c \prod_{k=1}^{\mathrm{K}} \theta_{ck}^{x_k} && (3)
\end{aligned}
$$

where x_k is the number of occurrences of the kth word, π_c is the prior probability of class c (which allows multiple classes!), and θ_{ck} is the weight of the kth word for the cth class.

Learning Multi-class Naïve Bayes

Training data

$$\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{\mathsf{N}} \rightarrow \mathcal{D} = \{(\{x_{nk}\}_{k=1}^{\mathsf{K}}, y_n)\}_{n=1}^{\mathsf{N}}$$

Our goal
Learn $\pi_c, c = 1, 2, \cdots, \mathsf{C}$, and $\theta_{ck}, \forall c \in [\mathsf{C}], k \in [\mathsf{K}]$ under the constraints:

$$\sum_c \pi_c = 1$$

and

$$\sum_k \theta_{ck} = \sum_k P(\text{word}_k | Y = c) = 1$$

as well as π_c, $\theta_{ck} \geq 0$.

Our Hammer: Maximum Likelihood Estimation

- Find the log-likelihood of the training data

$$
\begin{aligned}
\mathcal{L} = \log P(\mathcal{D}) &= \log \prod_{n=1}^{\mathsf{N}} \pi_{y_n} P(\mathbf{x}_n | y_n) \\
&= \log \prod_{n=1}^{\mathsf{N}} \left(\pi_{y_n} \prod_k \theta_{y_n k}^{x_{nk}} \right) \\
&= \sum_n \left(\log \pi_{y_n} + \sum_k x_{nk} \log \theta_{y_n k} \right) \\
&= \sum_n \log \pi_{y_n} + \sum_{n,k} x_{nk} \log \theta_{y_n k}
\end{aligned}
$$

- Optimize it!

$$
(\pi_c^*, \theta_{ck}^*) = \arg\max \sum_n \log \pi_{y_n} + \sum_{n,k} x_{nk} \log \theta_{y_n k}
$$

Our Hammer: Maximum Likelihood Estimation

Optimization Problem

$$(\pi_c^*, \theta_{ck}^*) = \arg\max \left(\sum_n \log \pi_{y_n} + \sum_{n,k} x_{nk} \log \theta_{y_n k} \right)$$

Solution

$$\theta_{ck}^* = \frac{\#\text{of times word } k \text{ shows up in data points labeled as } c}{\#\text{total trials for data points labeled as } c}$$

$$\pi_c^* = \frac{\#\text{of data points labeled as c}}{\text{N}}$$

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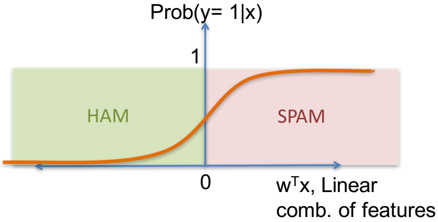
Logistic Regression for Predicting Multiple Classes?

- The linear decision boundary that we optimized was specific to binary classification.
  - If $\sigma(\mathbf{w}^\top \mathbf{x}) \geq 0.5$ declare $y = 1$ (spam)
  - If $\sigma(\mathbf{w}^\top \mathbf{x}) < 0.5$ declare $y = 0$ (ham)
- How to extend it to multi-class classification?

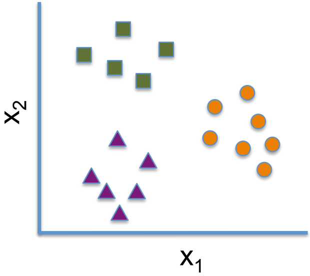


$y = 1$ for spam, $y = 0$ for ham

Idea: Express as multiple binary classification problems

The One-versus-Rest or One-versus-All Approach

- For each class c, change the problem into binary classification
  1. Relabel training data with label c, into POSITIVE (or '1').
  2. Relabel all the rest data into NEGATIVE (or '0').
- Repeat this multiple times: Train C binary classifiers, using logistic regression to differentiate the two classes each time.



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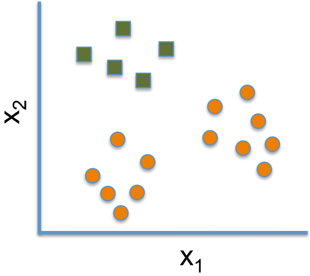

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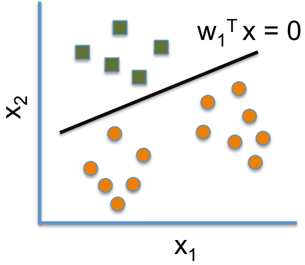
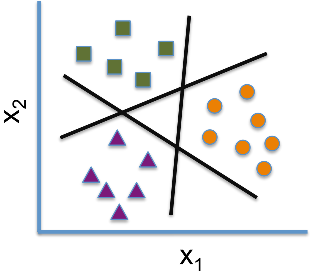


The One-versus-Rest or One-versus-All Approach

How to combine these linear decision boundaries?

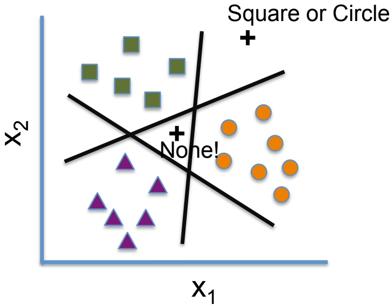
- There is ambiguity in some of the regions (the 4 triangular areas).



The One-versus-Rest or One-versus-All Approach

How to combine these linear decision boundaries?

- There is ambiguity in some of the regions (the 4 triangular areas).
- How do we resolve this?

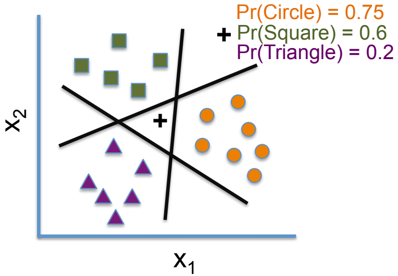


The One-versus-Rest or One-versus-All Approach

How to combine these linear decision boundaries?

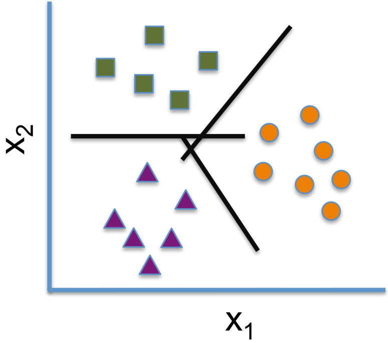
- Use the confidence estimates $\Pr(y = 1|\mathbf{x}) = \sigma(\mathbf{w}_1^\top \mathbf{x})$, $\ldots \Pr(y = C|\mathbf{x}) = \sigma(\mathbf{w}_C^\top \mathbf{x})$
- Declare class c^* that maximizes

$$c^* = \arg \max_{c=1,\ldots,C} \Pr(y = c|\mathbf{x}) = \sigma(\mathbf{w}_c^\top \mathbf{x})$$



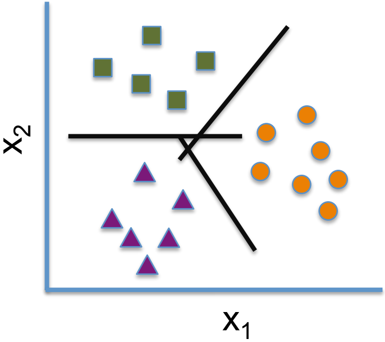
The One-versus-One Approach

- For each **pair** of classes c and c', change the problem into binary classification.
  1. Relabel training data with label c, into POSITIVE (or '1')
  2. Relabel training data with label c' into NEGATIVE (or '0')
  3. **Disregard** all other data



The One-versus-One Approach

- How many binary classifiers for C classes? $C(C-1)/2$
- How to combine their outputs?
- Given $\boldsymbol{x}$, count the $C(C-1)/2$ votes from outputs of all binary classifiers and declare the winner as the predicted class.
- Use confidence scores to resolve ties.



Contrast These Approaches

Number of binary classifiers to be trained

- One-versus-All: C classifiers.
- One-versus-One: $C(C-1)/2$ classifiers – bad if C is large

Effect of relabeling and splitting training data

- One-versus-All: imbalance in the number of positive and negative samples can cause bias in each trained classifier.
- One-versus-One: each classifier trained on a small subset of data (only data in two classes), which can result in high variance.

Any other ideas?

- Hierarchical classification – we will see this in decision trees
- Multinomial logistic regression – directly output probabilities of y being in each of the C classes.

First Try

So, can we define the following conditional model?

$$P(y = c|\boldsymbol{x}) = \sigma[\boldsymbol{w}_c^\top \boldsymbol{x}].$$

This would **not** work because:

$$\sum_c P(y = c|\boldsymbol{x}) = \sum_c \sigma[\boldsymbol{w}_c^\top \boldsymbol{x}] \neq 1,$$

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

But we are close!
Learn the C linear models jointly to ensure this property holds!

Multinomial Logistic Regression

- **Model:** For each class c, we have a parameter vector $\boldsymbol{w}_c$ and model the posterior probability as:

$$P(c|\boldsymbol{x}) = \frac{e^{\boldsymbol{w}_c^\top \boldsymbol{x}}}{\sum_{c'} e^{\boldsymbol{w}_{c'}^\top \boldsymbol{x}}} \qquad \leftarrow \qquad \textit{This is called the softmax function.}$$

- **Decision boundary:** Assign $\boldsymbol{x}$ with the label that is the maximum of posterior:

$$\arg\max_c P(c|\boldsymbol{x}) \rightarrow \arg\max_c \boldsymbol{w}_c^\top \boldsymbol{x}.$$

How Does the Softmax Function Behave?

Suppose we have

$$\boldsymbol{w}_1^\top \boldsymbol{x} = 100, \quad \boldsymbol{w}_2^\top \boldsymbol{x} = 50, \quad \boldsymbol{w}_3^\top \boldsymbol{x} = -20.$$

We would pick the winning class label 1.

Softmax translates these scores into well-formed conditional probabilities

$$P(y = 1|\boldsymbol{x}) = \frac{e^{100}}{e^{100} + e^{50} + e^{-20}} < 1$$

- Preserves relative ordering of scores.
- Maps scores to values between 0 and 1 that also sum to 1.

Sanity Check

Multinomial model reduces to binary logistic regression when $C = 2$.

$$P(1|\boldsymbol{x}) = \frac{e^{\boldsymbol{w}_1^\top \boldsymbol{x}}}{e^{\boldsymbol{w}_1^\top \boldsymbol{x}} + e^{\boldsymbol{w}_2^\top \boldsymbol{x}}} = \frac{1}{1 + e^{-(\boldsymbol{w}_1 - \boldsymbol{w}_2)^\top \boldsymbol{x}}}$$
$$= \frac{1}{1 + e^{-\boldsymbol{w}^\top \boldsymbol{x}}}$$

when we define $\boldsymbol{w} = \boldsymbol{w}_1 - \boldsymbol{w}_2$. Multinomial logistic regression thus generalizes the (binary) logistic regression to deal with multiple classes.

Parameter Estimation for Multinomial Logistic Regression

Discriminative approach: Maximize conditional likelihood

$$\log P(\mathcal{D}) = \sum_n \log P(y_n | \boldsymbol{x}_n)$$

We will change y_n to $\boldsymbol{y}_n = [y_{n1} \ y_{n2} \ \cdots \ y_{nC}]^\top$, a C-dimensional vector using 1-of-C encoding.

$$y_{nc} = \begin{cases} 1 & \text{if } y_n = c \\ 0 & \text{otherwise} \end{cases}$$

Ex: if $y_n = 2$, then, $\boldsymbol{y}_n = [0 \ 1 \ 0 \ 0 \ \cdots \ 0]^\top$.

$$\Rightarrow \sum_n \log P(y_n | \boldsymbol{x}_n) = \sum_n \log \prod_{c=1}^{C} P(c|\boldsymbol{x}_n)^{y_{nc}} = \sum_n \sum_c y_{nc} \log P(c|\boldsymbol{x}_n)$$

Cross-entropy Error Function

Definition: negative log-likelihood

$$\begin{aligned}\mathcal{E}(\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_C) &= -\sum_n \sum_c y_{nc} \log P(c|\boldsymbol{x}_n) \\ &= -\sum_n \sum_c y_{nc} \log \left(\frac{e^{\boldsymbol{w}_c^\top \boldsymbol{x}_n}}{\sum_{c'} e^{\boldsymbol{w}_{c'}^\top \boldsymbol{x}_n}} \right)\end{aligned}$$

Properties of cross-entropy

- Convex in the **w** vectors, therefore local minimum = global optimum
- Optimization requires numerical procedures, analogous to those used for binary logistic regression.

Finding the Gradient

$$\mathcal{E}(\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_C) = -\sum_n \sum_c y_{nc} \log P(c|\boldsymbol{x}_n)$$
$$= -\sum_n \sum_c y_{nc} \log \left(\frac{e^{\boldsymbol{w}_c^\top \boldsymbol{x}_n}}{\sum_{c'} e^{\boldsymbol{w}_{c'}^\top \boldsymbol{x}_n}} \right)$$

- Need to find the gradient w.r.t. $\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_C$ and update

$$\boldsymbol{w}_c \leftarrow \boldsymbol{w}_c - \eta \frac{\partial \mathcal{E}}{\partial \boldsymbol{w}_c}, \qquad c = 1, \ldots, C$$

Can you find the gradient? (Hint: what is the gradient of the softmax function?)

Evaluating Classification Methods

Loss Functions

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n) + (1 - y_n) \log[1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)]\}$$

- Easy to optimize!
- Average loss over the (training, validation, test) dataset
- ...but what does it mean?

Interpretable Classification Metrics

True positive	False positive
False negative	True negative

- Measure the accuracy within each class
- Accounts for imbalance between classes

- Sensitivity: true positive rate

$$\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

- Specificity: true negative rate

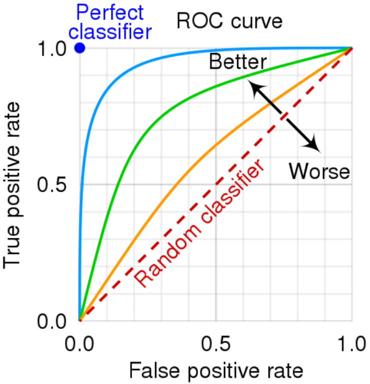
$$\mathrm{TNR} = \frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}}$$

- Precision: positive predictive value

$$\mathrm{PPV} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

These metrics are difficult to optimize directly, but they have the advantage of being easily interpretable.

Combining These Metrics: the ROC Curve



Receiver Operating Characteristic (ROC)

- Define a "threshold" for the positive/negative split
- Increasing the threshold: more samples are predicted to be positive
- Area Under the ROC Curve: want this as large as possible

You Should Know

- How to generalize logistic regression to handle nonlinear decision boundaries.
- How to handle multiclass classification: one-versus-all, one-versus-one, multinomial regression.
- How to measure classification accuracy