Introduction to Machine Learning

Logistic Regression, Multi-class Classification

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Overview

- Classification: predicting a discrete-valued target
  - Binary classification: predicting a binary-valued target
  - Multiclass classification: predicting a discrete (> 2)-valued target
- Examples of binary classification:
  - predict whether a patient has a disease, given the presence or absence of various symptoms
  - classify e-mails as spam or non-spam
  - predict whether a financial transaction is fraudulent

Overview

- Binary linear classification
  - classification: given a D-dimensional input $\boldsymbol{x} \in \mathbb{R}^D$ predict a discrete-valued target
  - binary: predict a binary target $t \in \{0, 1\}$
    - Training examples with $t = 1$ are called positive examples, and training examples with $t = 0$ are called negative examples.
    - $t \in \{0, 1\}$ or $t \in \{+1, -1\}$ is for computational convenience.
  - linear: model prediction y is a linear function of $\boldsymbol{x}$, followed by a threshold r

$$z = \boldsymbol{w}^\top \boldsymbol{x} + b \tag{1}$$

$$y = \begin{cases} 1 & z \geq r \\ 0 & z < r \end{cases} \tag{2}$$

Some Simplification

- Eliminating the threshold
  - We can assume without loss of generality (WLOG) that the threshold $r = 0$:

$$\boldsymbol{w}^\top \boldsymbol{x} + b \geq r \iff \boldsymbol{w}^\top \boldsymbol{x} + b - r \geq 0 \tag{3}$$

- Eliminating the bias
  - Add a dummy feature x0 which always takes the value 1. The weight $w_0 = b$ is equivalent to a bias (same as linear regression)
- Simplified model
  - Receive input $\boldsymbol{x} \in \mathbb{R}^{D+1}$ with $x_0 = 1$:

$$z = \boldsymbol{w}^\top \boldsymbol{x} \tag{4}$$

$$y = \begin{cases} 1 & z \geq r \\ 0 & z < r \end{cases} \tag{5}$$

Some Examples

- Let's consider some simple examples to examine the properties of our model
- Let's focus on minimizing the training set error, and forget about whether our model will generalize to a test set.

Some Examples

NOT

x_0	x_1	t
1	0	1
1	1	0

- Suppose this is our training set, with the dummy feature x_0 included
- Which conditions on w0, w1 guarantee perfect classification?
  - When $x_1 = 0$, need: $z = w_0 x_0 + w_1 x_1 \geq 0 \iff w_0 \geq 0$
  - When $x_1 = 1$, need: $z = w_0 x_0 + w_1 x_1 < 0 \iff w_0 + w_1 < 0$
- Possible solution: $w_0 = 1, w_1 = -2$
- Is this the only solution?

Some Examples

AND

x_0	x_1	x_2	t
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

$$z = w_0 x_0 + w_1 x_1 + w_2 x_2$$

$$\text{need: } w_0 < 0$$

$$\text{need: } w_0 + w_2 < 0$$

$$\text{need: } w_0 + w_1 < 0$$

$$\text{need: } w_0 + w_1 + w_2 \geq 0$$

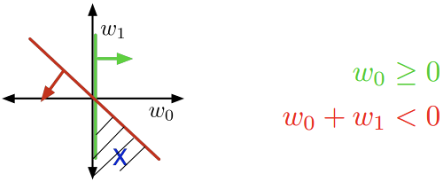
Example solution: $w_0 = -1.5,\ w_1 = 1,\ w_2 = 1$

The Geometric Picture

- Training examples are points
- Weights (hypotheses) $\boldsymbol{w}$ can be represented by half-spaces.
  $H_+ = \{\boldsymbol{x} : \boldsymbol{w}^\top \boldsymbol{x} \geq 0\}$, $H_- = \{\boldsymbol{x} : \boldsymbol{w}^\top \boldsymbol{x} < 0\}$
  - The boundaries of these half-spaces pass through the origin (why?)
  - Decision boundary: $\{\boldsymbol{x} : \boldsymbol{w}^\top \boldsymbol{x} = 0\}$
    - In 2-D, it's a line, but in high dimensions it is a hyperplane
- If the training examples can be perfectly separated by a linear decision rule, we say data is linearly separable.

The Geometric Picture

- Weight space



- Weights (hypotheses) $\boldsymbol{w}$ are points
- Each training example $\boldsymbol{x}$ specifies a half-space $\boldsymbol{w}$ must lie in to be correctly classified: $\boldsymbol{w}^\top \boldsymbol{x} \geq 0$ if $t = 1$.
- For NOT example:
  - $x_0 = 1, x_1 = 0, t = 1 \Longrightarrow (w_0, w_1) \in \boldsymbol{w} : w_0 \geq 0$
  - $x_0 = 1, x_1 = 1, t = 0 \Longrightarrow (w_0, w_1) \in \boldsymbol{w} : w_0 + w_1 < 0$
- The region satisfying all the constraints is the feasible region; if this region is nonempty, the problem is feasible, otherwise it is infeasible.

Summary — Binary Linear Classifiers

- Summary: Targets $t \in \{0, 1\}$, inputs $\boldsymbol{x} \in \mathbb{R}^{D+1}$ with $x_0 = 1$, and model is defined by weights $\boldsymbol{w}$ and

$$z = \boldsymbol{w}^\top \boldsymbol{x} \tag{6}$$

$$y = \begin{cases} 1 & z \geq r \\ 0 & z < r \end{cases} \tag{7}$$

- How can we find good values for $\boldsymbol{w}$?
- If the training set is linearly separable, we could solve for $\boldsymbol{w}$ using linear programming
  - We could also apply an iterative procedure known as the perceptron algorithm (but this is primarily of historical interest).
- If it's not linearly separable, the problem is harder
  - Data is almost never linearly separable in real life.

Towards Logistic Regression

Loss Function

- Instead: define loss function then try to minimize the resulting cost function
  - Recall: cost is loss averaged (or summed) over the training set
- Seemingly obvious loss function: 0-1 loss

$$\mathcal{L}_{0,1}(y,t) = \begin{cases} 1 & y = t \\ 0 & y \neq t \end{cases} \tag{8}$$

$$\mathcal{L}_{0,1}(y,t) = \mathbb{I}(y \neq t) \tag{9}$$

Attempt 1: 0-1 loss

- Usually, the cost $\mathcal{J}$ is the averaged loss over training examples; for 0-1 loss, this is the misclassification rate:

$$\mathcal{J} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(y^{(i)} \neq t^{(i)}) \tag{10}$$

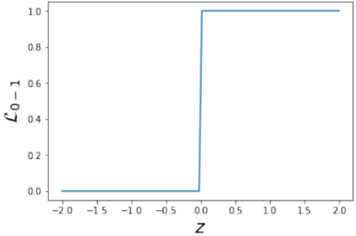
- Problem: how to optimize? In general, a hard problem (can be NP-hard)
- This is due to the step function (0-1 loss) not being nice (continuous/smooth/convex etc)

Attempt 1: 0-1 loss

- Minimum of a function will be at its critical points.
- Let's try to find the critical point of 0-1 loss
- Chain rule:

$$\frac{\partial \mathcal{L}_{0,1}}{\partial w_j} = \frac{\partial \mathcal{L}_{0,1}}{\partial z} \frac{\partial z}{\partial w_j} \tag{11}$$

- But $\frac{\partial \mathcal{L}_{0,1}}{\partial z}$ is zero everywhere it's defined!



- $\frac{\partial \mathcal{L}_{0,1}}{\partial w_j} = 0$ means that changing the weights by a very small amount probably has no effect on the loss $\Longrightarrow$ Almost any point has 0 gradient!

Attempt 2: Linear Regression

- Sometimes we can replace the loss function we care about with one which is easier to optimize. This is known as relaxation with a smooth surrogate loss function.
- One problem with $\mathcal{L}_{0,1}$: defined in terms of final prediction, which inherently involves a discontinuity
- Instead, define loss in terms of $\boldsymbol{w}^\top \boldsymbol{x}$ directly
    - Redo notation for convenience: $z = \boldsymbol{w}^\top \boldsymbol{x}$

Attempt 2: Linear Regression

- We already know how to fit a linear regression model. Can we use this instead?

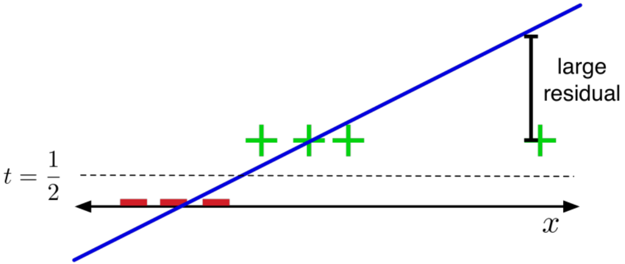
$$z = \boldsymbol{w}^\top \boldsymbol{x} \tag{12}$$

$$\mathcal{L}_{SE} = \frac{1}{2}(z - t)^2 \tag{13}$$

- Doesn't matter that the targets are actually binary. Treat them as continuous values.
- For this loss function, it makes sense to make final predictions by thresholding z at 0.5

Attempt 2: Linear Regression

- The problem:



- The loss function hates when you make correct predictions with high confidence!
- If $t = 1$, it's more unhappy about $z = 10$ than $z = 0$.

Attempt 3: Logistic Activation Function

- There's obviously no reason to predict values outside $[0, 1]$. Let's squash y into this interval.
- The logistic function is a kind of sigmoid, or S-shaped function:

$$\sigma(z) = \frac{1}{1 + e^{-z}} \tag{14}$$

- A linear model with a logistic nonlinearity is known as log-linear:

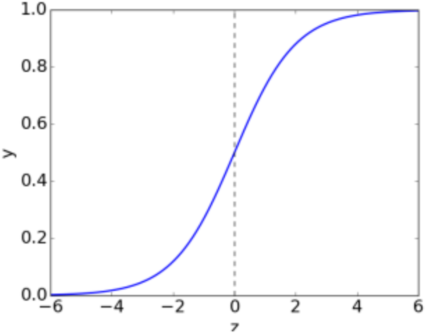
$$z = \mathbf{w}^\top \mathbf{x} \tag{15}$$

$$y = \sigma(z) \tag{16}$$

$$\mathcal{L}_{SE} = \frac{1}{2}(y - t)^2 \tag{17}$$

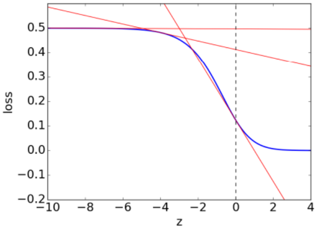
- Used in this way, σ is called an activation function.

Attempt 3: Logistic Activation Function



Attempt 3: Logistic Activation Function

- The problem: (plot of $\mathcal{L}_{SE}$ as a function of z, assuming $t = 1$)



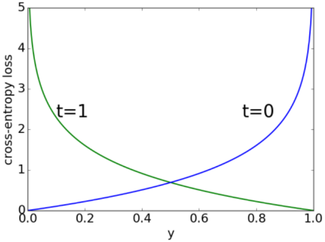
$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

- For $z \ll 0$, we have $\sigma(z) \approx 0$.
- $\frac{\partial \mathcal{L}}{\partial z} \approx 0$ (check!) $\Longrightarrow \frac{\partial \mathcal{L}}{\partial w_j} \approx 0 \Longrightarrow$ derivative w.r.t. w_j is small $\Longrightarrow w_j$ is like a critical point
- If the prediction is really wrong, you should be far from a critical point (which is your candidate solution).

Logistic Regression

- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$. If $t = 0$, then we want to heavily penalize $y \approx 1$.
- The people who were 99% confident a certain presidential candidate would win were much more wrong than the ones who were only 90% confident, given that the person didn't win.
- Cross-entropy loss (aka log loss) captures this intuition:

$$\mathcal{L}_{\mathrm{CE}}(y,t) = \begin{cases} -\log y & \text{if } t = 1 \\ -\log(1-y) & \text{if } t = 0 \end{cases}$$
$$= -t\log y - (1-t)\log(1-y)$$

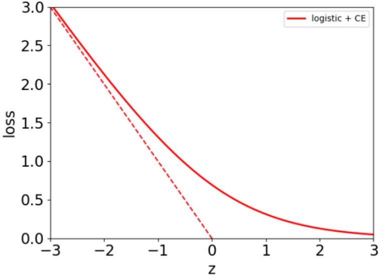


Logistic Regression

- Logistic regression:

$$
\begin{aligned}
z &= \mathbf{w}^\top \mathbf{x} \\
y &= \sigma(z) \\
&= \frac{1}{1+e^{-z}} \\
\mathcal{L}_{\text{CE}} &= -t \log y - (1-t)\log(1-y)
\end{aligned}
$$

Plot is for target $t = 1$.



Logistic Regression - Numerical Instabilities

- If we implement logistic regression naively, we can end up with numerical instabilities.
- Consider: $t = 1$ but you're really confident that $z \ll 0$
- If y is small enough, it may be numerically zero. This can cause very subtle and hard-to-find bugs.

$$y = \sigma(z) \Rightarrow y \approx 0 \tag{18}$$

$$\mathcal{L}_{CE} = -t \log y - (1 - t) \log(1 - y) \tag{19}$$

Logistic Regression - Numerical Stable Version

- Instead, we combine the activation function and the loss into a single logistic-cross-entropy function

$$\mathcal{L}_{LCE} = \mathcal{L}_{CE}(\sigma(z), t) = -t\log(\frac{1}{1+e^{-z}}) - (1-t)\log(\frac{1}{1+e^{-z}}) \quad (20)$$

Gradient Descent for Logistic Regression

- How do we minimize the cost $\mathcal{J}$ for logistic regression? No direct solution.
  - Taking derivatives of $\mathcal{J}$ w.r.t. $\boldsymbol{w}$ and setting them to 0 doesn't have an explicit solution.
- However, the logistic loss is a convex function in $\boldsymbol{w}$, so let's consider the gradient descent method/
  - Recall: we initialize the weights to something reasonable and repeatedly adjust them in the direction of the steepest descent.
  - A standard initialization is $w = 0$.

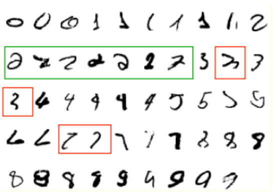
Multiclass Classification and Softmax Regression

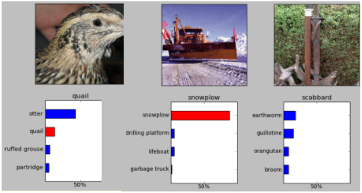
Overview

- Classification: predicting a discrete-valued target
  - Binary classification: predicting a binary-valued target
  - Multiclass classification: predicting a discretev(> 2)-valued target
- Examples of multi-class classification
  - predict the value of a handwritten digit
  - classify e-mails as spam, travel, work, personal

Multiclass Classification

- Classification tasks with more than two categories:





Multiclass Classification

- Targets form a discrete set $\{1, ..., K\}$.
- It's often more convenient to represent them as one-hot vectors, or a one-of-K encoding:
  - Entry k is 1, the other entries are all 0's.
  - k is not to be confused with K.

$$\boldsymbol{t} = (0, ..., 0, 1, 0, ..., 0) \in \mathbb{R}^K \tag{21}$$

Multiclass Linear Classification

- We can start with a linear function of the inputs.
- Now there are D input dimensions and K output dimensions, so we need $K \times D$ weights, which we arrange as a weight matrix W.
- Also, we have a K-dimensional vector b of biases.
- A linear function of the inputs:

$$z_k = \sum_{j=1}^{D} w_{kj} x_j + b_k \text{ for } k = 1, 2, ..., K \tag{22}$$

- We can eliminate the bias b by taking $W \in \mathbb{R}^{K \times (D+1)}$ adding a dummy variable x0 = 1. So, vectorized:

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}, \text{or with dummy } x_0 = 1, \boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} \tag{23}$$

Multiclass Linear Classification

- How can we turn this linear prediction into a one-hot prediction?
- We can interpret the magnitude of z_k as a measure of how much the model prefers k as its prediction.
- If we do this, we should set

$$y_i = \begin{cases} 1 & i = \underset{k}{\operatorname{argmax}}\, z_k \\ 0 & \text{otherwise} \end{cases} \tag{24}$$

- Exercise: how does the case of $K = 2$ relate to the prediction rule in binary linear classifiers?

Softmax Regression

- We need to soften our predictions for the sake of optimization.
- We want soft predictions that are like probabilities, i.e., $0 \le y_k \le 1$ and $\sum_k y_k = 1$.
- A natural activation function to use is the softmax function, a multivariable generalization of the logistic function:

$$y_k = \text{softmax}(z_1, ..., z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}} \tag{25}$$

  - Outputs can be interpreted as probabilities (positive and sum to 1)
  - If z_k is larger than the others, then $\text{softmax}(z)_k \approx 1$ and it behaves like argmax.
- The inputs z_k are called the logits.

Softmax Regression

- If a model outputs a vector of class probabilities, we can use cross-entropy as the loss function, where the log is applied elementwise.

$$\mathcal{L}_{CE}(\boldsymbol{y}, \boldsymbol{t}) = -\sum_{k-1}^{K} t_k \log y_k = -\boldsymbol{t}^\top (\log \boldsymbol{y}) \tag{26}$$

- Just like with logistic regression, we typically combine the softmax and cross-entropy into a softmax-cross-entropy function

Softmax Regression

- Softmax regression (with dummy $x_0 = 1$):

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} \tag{27}$$

$$\boldsymbol{y} = \text{softmax}(\boldsymbol{z}) \tag{28}$$

$$\mathcal{L}_{CE} = -\boldsymbol{t}^\top(\log \boldsymbol{y}) \tag{29}$$

- Gradient descent updates can be derived for each row of $\boldsymbol{W}$:

$$\frac{\partial \mathcal{L}_{CE}}{\partial \boldsymbol{w}_k} = \frac{\partial \mathcal{L}_{CE}}{\partial z_k}\frac{\partial z_k}{\partial \boldsymbol{w}_k} = (y_k - t_k) \cdot \boldsymbol{x} \tag{30}$$

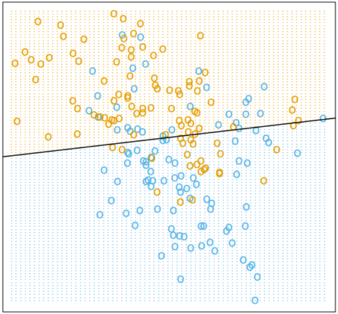
$$\boldsymbol{w}_k \longrightarrow \boldsymbol{w}_k - \frac{\alpha}{N}\sum_{i=1}^{N}(y_k^{(i)} - t_k^{(i)})\boldsymbol{x}^{(i)} \tag{31}$$

Linear Classifiers vs. KNN

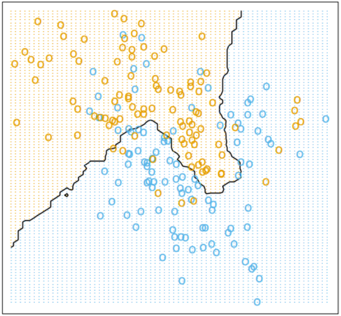
Linear Classifiers vs. KNN

- Linear classifiers and KNN have very different decision boundaries:

Linear Classifier



K Nearest Neighbours



Linear Classifiers vs. KNN

- Advantages of linear classifiers over KNN?
  - Robustness to irrelevant features
    - Linear classifiers are generally robust to irrelevant or redundant features.
  - Scalability
    - Linear classifiers can handle high-dimensional feature spaces efficiently and are more scalable as the number of features increases.
    - The curse of dimensionality!
  - Easy updates of the model
- Advantages of KNN over linear classifiers?
  - No assumption of data distribution
    - It is a non-parametric method, which means it does not assume any specific functional form for the decision boundaries.
  - Non-linearity
    - KNN can capture complex, non-linear decision boundaries
  - Robustness to imbalanced data
    - It relies on the local neighborhood and not global statistics.

Limitations of Linear Classification

A Few Basic Concepts

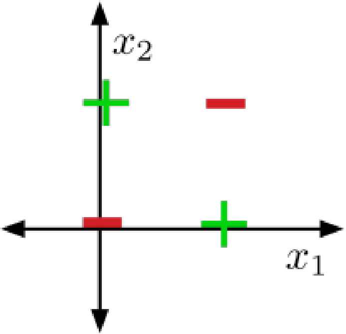
- A hypothesis is a function $f : \mathcal{X} \to \mathcal{T}$ that we might use to make predictions (recall $\mathcal{X}$ is the input space and $\mathcal{T}$ is the target space).
- The hypothesis space $\mathcal{H}$ for a particular machine learning model or algorithm is a set of hypotheses that it can represent.
  - E.g., in linear regression, $\mathcal{H}$ is the set of functions that are linear in the data features
  - The job of a machine learning algorithm is to find a good hypothesis $f \in \mathcal{H}$
- The members of $\mathcal{H}$, together with an algorithm's preference for some hypotheses of $\mathcal{H}$ over others, determine an algorithm's inductive bias.
  - Inductive biases can be understood as general natural patterns or domain knowledge that helps our algorithms to generalize;
    - E.g., linearity, continuity, simplicity (L_2 regularization) ...
  - The so-called No Free Lunch (NFL) theorems assert that if datasets/problems were not naturally biased, no ML algorithm would be better than another

A Few Basic Concepts

- If an algorithm's hypothesis space $\mathcal{H}$ can be defined using a finite set of parameters, denoted $\boldsymbol{\theta}$, we say the algorithm is parametric.
  - In linear regression, $\boldsymbol{\theta} = (\boldsymbol{w}, b)$
  - Other examples: logistic regression, neural networks, k-means and Gaussian mixture models
- If the members of $\mathcal{H}$ are defined in terms of the data, we say that the algorithm is non-parametric.
  - In k-nearest neighbors, the learned hypothesis is defined in terms of the training data
  - Other examples: Gaussian processes, decision trees, support vector machines, kernel density estimation
  - These models can sometimes be understood as having an infinite number of parameters

Limits of Linear Classification

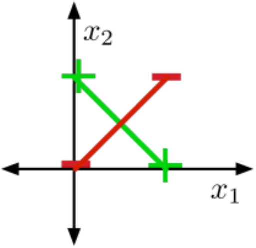
- Some datasets are not linearly separable, e.g. XOR,



- Visually obvious, but how to show this?

Showing that XOR is not linearly separable (proof by contradiction)

- If two points lie in a half-space, the line segment connecting them also lies in the same half-space.
- Suppose there were some feasible weights (hypothesis). If the positive examples are in the positive half-space, then the green line segment must be as well.
- Similarly, the red line segment must line within the negative half-space



- But the intersection can't lie in both half-spaces. Contradiction!

Limits of Linear Classification

- Sometimes we can overcome this limitation using feature maps, just like for linear regression. E.g., for XOR:

$$\boldsymbol{\psi}(\mathbf{x}) = \begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}$$

x_1	x_2	$\psi_1(\mathbf{x})$	$\psi_2(\mathbf{x})$	$\psi_3(\mathbf{x})$	t
0	0	0	0	0	0
0	1	0	1	0	1
1	0	1	0	0	1
1	1	1	1	1	0

- This is linearly separable.

In the Future

- Feature maps are hard to design well, so next time we'll see how to learn nonlinear feature maps directly using neural networks...
- The basics of NN will be covered in this class.

...