Logistic Regression

UNIVERSITY OF LIVERPOOL

Binary Classification

- Given an instance $\mathbf{x}$, we must classify it to either positive (1) or negative (0) class.
  - We can use $\{1, -1\}$ instead of $\{1, 0\}$
  - (but we will use $1, 0$ as it simplifies the notation in subsequent derivations)
- Binary classification can be seen as learning a function f such that $f(x)$ returns either 1 or 0 indicating the predicted class.

Some terms in Machine Learning

- Training dataset with N instances
  - $\{(x_1,t_1), ..., (x_N,t_N)\}$ This can also be written as $\{(x_n,t_n)\}^N_{n=1}$
- Target label (class)
  - t: The class labels in the training dataset
  - Annotated by humans (supervised learning)
- Predicted label
  - Labels predicted by our model $f(x)$

From Naive Bayes to Logistic Regression

- Recall Naive Bayes Classifier
  - Predict:

$$\hat{Y} = \underset{y}{\operatorname{argmax}}\, P(\mathbf{X} \mid Y) = \underset{y}{\operatorname{argmax}}\, P(\mathbf{X} \mid Y)P(Y)$$

  - We use independence assumption:

$$P(\mathbf{X} \mid Y) = P(X_1, X_2, \ldots X_m \mid Y)P(Y) = \prod_{i=1}^{m} P(X_i \mid Y)$$

- Can we model $P(Y \mid \mathbf{X})$ directly?

From Naive Bayes to Logistic Regression

- Can we model $P(Y \mid \mathbf{X})$ directly?
  - We use logistic regression model to achieve this
  - Given $X, \mathbf{W}$ we compute $P(Y = 1 \mid X)$

$$\begin{matrix} [0, 1, 1, 1] \\ [-4, 2, 1, 2] \end{matrix} \longrightarrow 0.74$$

From Naive Bayes to Logistic Regression

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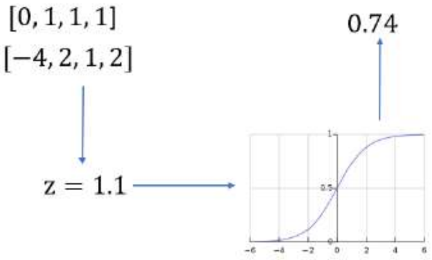


Generative vs. Discriminative Classifier

Generative

- goal of understanding how dogs look and cats look
- model can 'generate' (draw) a dog
- given a test image, choose the closest model as 'label'

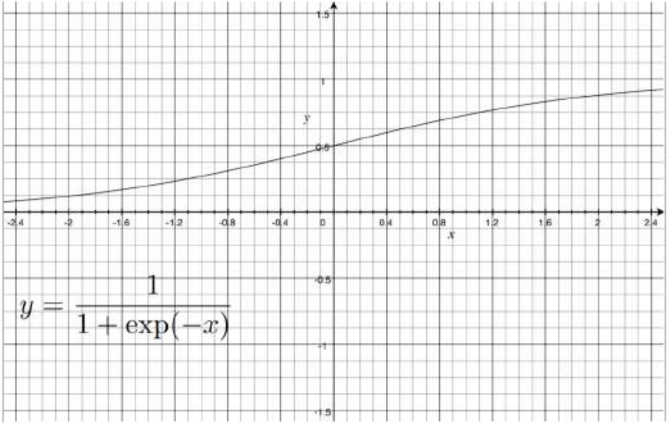
Discriminative

- trying to learn to distinguish the classes (not learning much about them)
- If one feature neatly separates the classes, the model is satisfied.
- e.g., dogs wearing collars and cat aren't

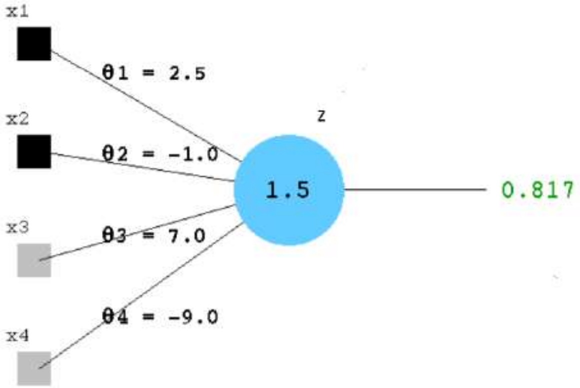
Logistic Regression

- is not a *regression* model
- is a *classification* model
- is a **Discriminative** classifier and not a **Generative** classifier
- is the basis of many advanced machine learning methods
  - neural networks, deep learning, conditional random fields, ...
- try to fit a logistic Sigmoid function to predict the class labels

Logistic Sigmoid Function



Logistic Regression Example



How to find Parameters of the Model

- In logistic regression, given $\mathbf{x}, \mathbf{w}$ we compute $P(Y = y \mid \mathbf{x})$
- How to compute $\mathbf{w}$?

- Maximum Likelihood Estimate/Principle (MLE): parameter estimation method to find parameters of the model

- The parameter values are found such that the values maximise the *likelihood* of making the observations given the parameters.

MLE Example

- Consider a bag containing 3 balls.
- Each ball is either red or blue (we have no other information)
- number of blue balls (θ) might be 0, 1, 2, or 3
- we are allowed to choose 4 balls at random with replacement.
- the random variables X_1, X_2, X_3 and X_4 are defined as follows:

$$X_i = \begin{cases} 1 & \text{if the } i\text{th chosen ball is blue} \\ 0 & \text{if the } i\text{th chosen ball is red} \end{cases}$$

MLE Example

- X_i's are i.i.d and $X_i \sim Bernoulli(\frac{\theta}{3})$.
- let us say the following values for X_i's are observed:

$$x_1 = 1, x_2 = 0, x_3 = 1, x_4 = 1$$

- Given the above:
  - For each possible value of θ, can we compute the probability of the observed sample
  - Can we find the value of θ for which the probability of the observed sample is the largest?

MLE Example

- Since $X_i \sim Bernoull(\frac{\theta}{3})$, we have:

$$P_{X_i}(x) = \begin{cases} \frac{\theta}{3} & \text{for } x = 1 \\ 1 - \frac{\theta}{3} & \text{for } x = 0 \end{cases}$$

- Since X_i's are independent, the joint PMF of X_1, X_2, X_3 and X_4, can be written as:

$$P_{X_1X_2X_3X_4}(x_1, x_2, x_3, x_4) = P_{X_1}(x_1)P_{X_2}(x_2)P_{X_3}(x_3)P_{X_4}(x_4)$$

MLE Example

- Thus:

$$P_{X_1X_2X_3X_4}(1,0,1,1) = \frac{\theta}{3} \cdot \left(1 - \frac{\theta}{3}\right) \cdot \frac{\theta}{3} \cdot \frac{\theta}{3}$$
$$= \left(\frac{\theta}{3}\right)^3 \left(1 - \frac{\theta}{3}\right).$$

θ	$P_{X_1X_2X_3X_4}(1,0,1,1;\theta)$
0	0
1	0.0247
2	0.0988
3	0

Log Likelihood

- Parameters of logistic regression model are chosen using maximum likelihood estimation (MLE) method.
- There are two steps:
  1. write the log-likelihood function (define cross entropy function)
  2. find the values of $\mathbf{w}$ that maximise the log-likelihood function

Logistic Regression Model

- for an individual training instance $(\mathbf{x}_i, t_i)$:

$$P(t_i = 1 \mid \mathbf{x}_i) = y_i = \sigma(\mathbf{w}^\top \mathbf{x}_i) = \frac{1}{1+\exp^{(-\mathbf{w}^\top \mathbf{x}_i)}}$$

$$P(t_i = 0 \mid \mathbf{x}_i) = 1 - y_i$$

- using the equation form of the PMF of Bernoulli distribution, where $t_n \in \{0, 1\}$, the probability of a single instance can be written as:

$$P(t_i = t \mid \mathbf{x}_i) = y_i^{t_i} \, \{1 - y_i\}^{(1-t_i)}$$

Likelihood

- for a dataset $\{x_n, t_n\}$, where where $t_n \in \{0, 1\}$, with $n = 1, \ldots, N$, the likelihood function can be written as:

$$L(\mathbf{w}) = P(\mathbf{t} \mid \mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \left\{1 - y_n\right\}^{(1-t_n)}$$

where $\mathbf{t} = (t_1, \ldots, t_N)^\top$ and $y_n = p(t_n = 1 \mid x_n)$

Cross Entropy

- define a negative logarithm of the likelihood to get *cross entropy* error function $E(w)$:

$$L(\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} \{1 - y_n\}^{(1-t_n)}$$

$$LL(\mathbf{w}) = E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

Derivation of the Gradient

- differentiating $E(w)$ w.r.t $\mathbf{w}$, we get the gradient $\nabla E(w)$:

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N}\left\{t_n \frac{1}{y_n}\frac{\partial y_n}{\partial w} + (1-t_n)\frac{1}{1-y_n}\left(-\frac{\partial y_n}{\partial w}\right)\right\}$$

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N}\left\{\frac{t_n}{y_n} - \frac{1-t_n}{1-y_n}\right\}\left(\frac{\partial y_n}{\partial w}\right)$$

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N}\left\{\frac{tn(1-y_n) - (1-t_n)y_n}{y_n(1-y_n)}\right\}\left(\frac{\partial y_n}{\partial w}\right)$$

Derivation of the Gradient

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ \frac{t_n(1-y_n) \; - \; (1-t_n)y_n}{y_n(1-y_n)} \right\} \left(\frac{\partial y_n}{\partial w} \right)$$

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ \frac{(t_n - y_n)}{y_n(1-y_n)} \right\} \left(\frac{\partial y_n}{\partial w} \right) \tag{1}$$

Derivation of the Gradient

- differentiating y_n w.r.t $\mathbf{w}$:

$$\frac{\partial y_n}{\partial w} = \frac{\partial}{\partial w}\left\{\frac{1}{1+\exp^{-wx_n}}\right\}$$

$$\frac{\partial y_n}{\partial w} = \frac{(1+\exp^{-wx_n})\frac{\partial(1)}{\partial w} - 1.\frac{\partial}{\partial w}(1+\exp^{-wx_n})}{(1+\exp^{-wx_n})^2}$$

$$\frac{\partial y_n}{\partial w} = \frac{-(\exp^{-wx_n})\,(-x_n)}{(1+\exp^{-wx_n})^2}$$

$$\frac{\partial y_n}{\partial w} = \frac{1}{1+\exp^{-wx_n}}\;\frac{\exp^{-wx_n}\;x_n}{1+\exp^{-wx_n}}$$

Derivation of the Gradient

- differentiating y_n w.r.t $\mathbf{w}$:

$$\frac{\partial y_n}{\partial w} = \frac{1}{1+\exp^{-wx_n}} \; \frac{\exp^{-wx_n} \;\; x_n}{1+\exp^{-wx_n}}$$

$$\frac{\partial y_n}{\partial w} = \frac{1}{1+\exp^{-wx_n}} \; \frac{(1+\exp^{-wx_n})-1}{1+\exp^{-wx_n}} \; x_n$$

$$\frac{\partial y_n}{\partial w} = \frac{1}{1+\exp^{-wx_n}} \left(\frac{1+\exp^{-wx_n}}{1+\exp^{-wx_n}} - \frac{1}{1+\exp^{-wx_n}} \right) x_n$$

$$\frac{\partial y_n}{\partial w} = \frac{1}{1+\exp^{-wx_n}} \left(1 - \frac{1}{1+\exp^{-wx_n}} \right) x_n$$

$$\frac{\partial y_n}{\partial w} = y_n(1-y_n)x_n \tag{2}$$

Derivation of the Gradient

- Substituting (2) in (1), we get:

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ \frac{(t_n - y_n)}{y_n(1 - y_n)} \right\} y_n(1 - y_n) x_n$$

- Simplifying further:

$$\nabla E(\mathbf{w}) = -\sum_{n=1}^{N} (t_n - y_n) x_n$$

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) x_n \tag{3}$$

Updating the weight vector

- Generic update rule

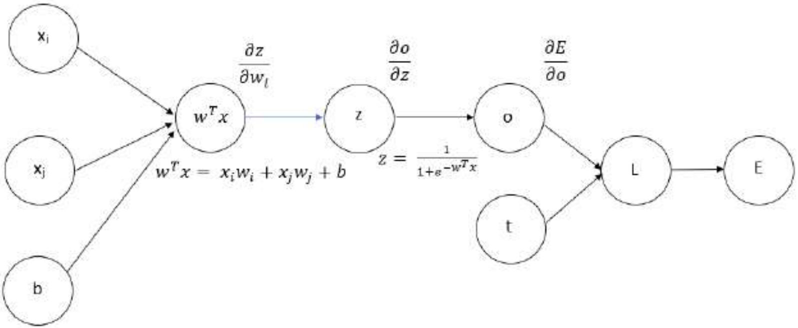
$$\mathbf{w}^{(r+1)} = \mathbf{w}^{(r)} - \eta \nabla E(\mathbf{w})$$

- Update rule with cross-entropy error function

$$\mathbf{w}^{(r+1)} = \mathbf{w}^{(r)} - \eta (y_n - t_n)\mathbf{x}_n$$

  - the contribution of the gradient from a data point n is given by the error $(y_n - t_n)$ times the feature vector $\mathbf{x}_n$

Updating Weight Vector



Logistic Regression Algorithm

- Given a set of training instances $\{(x_1, t_1), \ldots, (x_N, t_N)\}$, learning rate ($\eta$) and iterations T:
- Initialise weight vector $\mathbf{w} = \mathbf{0}$
- For j in $1, \ldots, T$
  - for n in $1, \ldots, N$
    - if pred($\mathbf{x}_i \neq t_i$) #misclassification
    - $\mathbf{w}^{(r+1)} = \mathbf{w}^{(r)} - \eta(y_n - t_n)\mathbf{x}_n$
- Return the final weight vector $\mathbf{w}$

Prediction Function (*pred*)

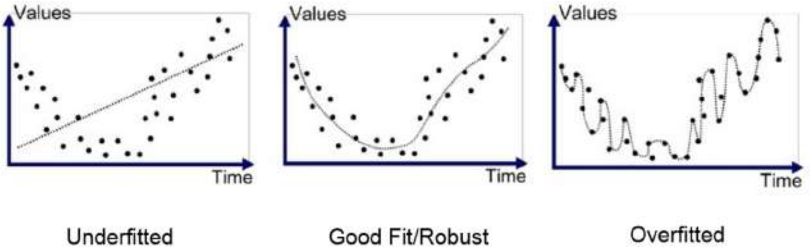
- Given the weight vector **w**, returns the class label for an instance **x**
  - if $\mathbf{w}^T\mathbf{x} > 0$:
    - predicted label = +1 # positive class
  - else:
    - predicted label = 0 # negative class

Online vs. Batch

- Online vs. Batch Logistic Regression
  - The algorithm we discussed in the previous slides is an *online algorithm* because it considers only one instance at a time and updates the weight vector
    - Referred to as the Stochastic Gradient Descent (SGD) update
  - In the batch version, we will compute the cross-entropy error over the *entire* training dataset and then update the weight vector
    - Popular optimisation algorithm for the batch learning of logistic regression is the Limited Memory BFGS (L-BFGS) algorithm
- Batch version is slow compared to the SGD version. But shows slightly improved accuracies in many cases
- SGD version can require multiple iterations over the dataset before it converges (if ever)
- SGD is a technique that is frequently used with large scale machine learning tasks (even when the objective function is non-convex)

Regularisation

Overfitting



Regularisation

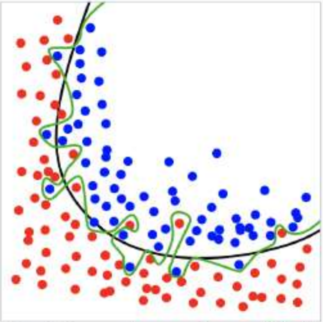


Figure 1. The green line represents an overfitted model and the black line represents a regularized model. While the green line best follows the training data, it is too dependent on that data and it is likely to have a higher error rate on new unseen data, compared to the black line.

How to reduce overfitting?

Without adding any regularisation

- Train on more data
- Data augmentation
- Early stopping

  stop training when validation error starts increasing or validation error stops improving

Regularisation

- Regularisation
  - Reducing overfitting in a model by constraining it (reducing the complexity/no. of parameters)
  - For classifiers that use a weight vector, regularisation can be done by minimising the norm (length) of the weight vector.
  - Several popular regularisation methods exist
    - L2 regularisation (ridge regression or Tikhonov regularisation)
    - L1 regularisation (Lasso regression)
    - L1+L2 regularisation (mixed regularisation)

L2 Regularisation

- Let us denote the Loss of classifying a dataset D using a model represented by a weight vector **w** by L(D,**w**) and we would like to impose L2 regularisation on **w**.
- The overall objective to minimise can then be written as follows (here λ is called the regularisation coefficient and is set via cross-validation)

$$J(D, \boldsymbol{w}) = L(D, \boldsymbol{w}) + \lambda \, ||\boldsymbol{w}||_2^2$$

- The gradient of the overall objective simply becomes the addition of the loss-gradient and the scaled weight vector **w**.

$$\frac{\partial J(D, \boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{\partial L(D, \boldsymbol{w})}{\partial \boldsymbol{w}} + 2\lambda \boldsymbol{w}$$

Examples

- Note that SGD update for minimising a loss multiplies the loss gradient by a negative learning rate (η). Therefore, the L2 regularised update rules will have a -2ηλ**w** term as shown in the following examples
- L2 regularised Perceptron update (for a misclassified instance we do)

$$\boldsymbol{w}^{(k+1)} = \boldsymbol{w}^{(k)} + t\boldsymbol{x} - 2\lambda \boldsymbol{w}^{(k)}$$

- L2 regularised logistic regression

$$\begin{aligned}\boldsymbol{w}^{(k+1)} &= \boldsymbol{w}^{(k)} - \eta((y-t)\boldsymbol{x} + 2\lambda \boldsymbol{w}^{(k)}) \\ &= (1 - 2\lambda\eta)\boldsymbol{w}^{(k)} - \eta(y-t)\boldsymbol{x}\end{aligned}$$

How to set λ

- Split your training dataset into training and validation parts (eg. 80%-20%)
- Try different values for λ (typically in the logarithmic scale). Train a different classification model for each λ and select the value that gives the best performance (eg. accuracy) on the validation data.
  - $\lambda = 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1, 0, 10^{1}, 10^{2}, 10^{3}, 10^{4}, 10^{5}$

References

- Bishop (Pattern Recognition and Machine Learning) Section 4.3.2
- Software
  - Scikit-learn (Python)
    - https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html