Classification: Logistic Regression

Xiang Zhou

School of Data Science
Department of Mathematics
City University of Hong Kong

Statistical Decision Theory for Classification

- k-NN method
- Bayes classifier
- LDA and QDA

Review of Bayes Classifier

0-1 loss

We use 0-1 loss to evaluate the performance of classifiers.
The zero-one $(0\text{-}1)$ loss function h for the labelled class y and the predicted class $\hat{y}$ is defined [1],

$$\boxed{\ell_{01}(y,\hat{y}) = \mathbf{1}(y \neq \hat{y})} \triangleq \begin{cases} 1 & \text{if } y \neq \hat{y} \\ 0 & \text{if } y = \hat{y} \end{cases} \tag{1}$$

where the misclassifications are charged by a single positive unit.

Remark (other equivalent forms)

If the binary outcome is encoded as $\{-1,+1\}$*, then* $\ell_{01}(y,\hat{y}) = 1 - \textit{heaviside}(y\hat{y}) = (1 - \textit{sign}(y\hat{y}))/2$ *where* $\textit{heaviside}(t) = \begin{cases} 1 & \textit{if } \ t \geq 0 \\ 0 & \textit{if } \ t < 0 \end{cases}$ *and* $\textit{sign}(t) = \begin{cases} 1 & \textit{if } \ t \geq 0 \\ -1 & \textit{if } \ t < 0 \end{cases}$*. So 0-1 loss is equivalent to* $-\textit{heaviside}(y\hat{y})$ *and* $-\textit{sign}(y\hat{y})$*.*

[1] In logistic regression, it is h, the pdf, not the class label $\hat{y}$, that shows in the loss function

For any classifier $\phi : \mathcal{X} \to \{1, \ldots, K\}$, its 0-1 loss overall test error rate is

$$\begin{aligned} \mathbb{E}_{X,Y}\left[\ell_{01}(Y, \phi(X))\right] &= \mathbb{E}_X\left(\sum_{k=1}^{K} \ell_{01}(k, \phi(X)) \times \mathbb{P}(Y = k|X)\right) \\ &= 1 - \mathbb{E}_X\left[\mathbb{P}(Y = \phi(X)|X)\right] \quad \because \ell_{01} \text{ is 0-1 loss} \end{aligned} \tag{2}$$

So,

$$\inf_{\phi} \mathbb{E}_{X,Y}\left[\ell_{01}(Y, \phi(X))\right]$$

is equivalent to

$$\sup_{\phi} \mathbb{E}_X\left[\mathbb{P}(Y = \phi(X)|X)\right]$$

which has the following optimal solution defined point-wisely for x:

$$\phi^*(x) = \underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}} \ \mathbb{P}(Y = k|X = x)$$

Definition (Bayes classifier)

$$\boxed{\phi^*(x) = \underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}} \; h_k(x)}$$

where

$$h_k(x) := \mathbb{P}(Y = k | X = x)]$$

Definition (Gibbs classifier)

Given an input x, the predicted class is a random sample from $\{1, \ldots, K\}$ according to the prob mass fun $\{h_k(x), 1 \leq k \leq K\}$

This also works well.

Bayes classifier is optimal for misclassification error

Recall for regression, the conditional probability $f(x) = \mathbb{E}(Y|X = x)$ minimizes the squared error loss $\mathbb{E}[|Y - f(X)|^2]$ and the conditional median $f(x) = \text{median}(Y|X = x)$ minimizes the L_1 error loss $\mathbb{E}\,|Y - f(X)|$. For classification, we have the analogy for the Bayes classifier.

Theorem

Bayes classifier minimizes the expected 0-1 *loss.*

The 0-1 loss of Bayes classifier is called **Bayes error rate**:

$$1 - \mathbb{E}_X\left[\max_k \mathbb{P}(Y = k|X)\right] = 1 - \mathbb{E}_X\left[\max_k h_k(X)\right].$$

Bayes Theorem for Bayes Classifier

- The **Bayes theorem** is to view this as the *posterior* distribution of Y with the given observation $X = x$:

$$\begin{aligned} h_k(x) &= \mathbb{P}(Y = k | X = x) \\ &= \frac{\mathbb{P}(X = x | Y = k)\mathbb{P}(Y = k)}{\mathbb{P}(X = x)} \\ &=: \boxed{\frac{f_k(x)\pi_k}{\sum_{l=1}^{K} f_l(x)\pi_l}} \end{aligned} \tag{3}$$

- $f_k(x)$: **the class-conditional pdf of** X in class $Y = k$;
- π_k: the (prior) distribution of the class Y ;
- For any given x, the conditional pmf of Y is

$$h_k(x) \propto f_k(x)\pi_k.$$

- One might estimate $f_k(x)$ ("density estimation") and π_k (the fraction of training examples belong to class k) directly from the data.

Bayesian classifier

- **Bayesian classifier** assigns each observation to the most likely class, given its predictor value x, i.e., classifies into the maximal posterior prob.

$$\phi^*(x) = \underset{1 \leq k \leq K}{\operatorname{argmax}} \mathbb{P}(Y = k | X = x) = \underset{1 \leq k \leq K}{\operatorname{argmax}} \; [f_k(x)\pi_k] \tag{4}$$

  This is called Brute Force MAP (*maximum a posterior*) Learner in Computer Science .

- *Bayes decision boundary* is the decision boundary determined by this Bayes classifier.
- The joint distribution of (X, Y) is $\mathbb{P}(X = x, Y = y) = \sum_{k=1}^{K} f_k(x)\pi_k$. Then this model is the typical mixture models: convex combination of K distributions of f_k: connection to missing data problem, EM algorithm.

Recall the posterior distribution in (3) $\mathbb{P}(Y=k|X=x) = \frac{f_k(x)\pi_k}{\sum_{l=1}^K f_l(x)\pi_l}$ where $f_k(x) \triangleq \mathbb{P}(X=x|Y=k)$ is the distribution of X conditioned on $Y=k$. Bayes classifier maximize this over k.

Exercise

Assume *that* $X \in \mathbb{R}^1$ *and* $f_k \sim \mathcal{N}(\mu_k, \sigma_k^2),\ 1 \le k \le K$.
Then the Bayes classifier corresponds to the maximizer k^* *of the following discriminant function*

$$\delta_k(x) = -\frac{x^2}{2\sigma_k^2} + x \cdot \frac{\mu_k}{\sigma_k^2} - \frac{\mu_k^2}{2\sigma_k^2} + \log \pi_k. \tag{5}$$

When $K=2$, *find the point corresponding to the Bayes decision boundary.*

Naive Bayesian Classifier:

If $\mathcal{X}$ has a dimensionality $d \gg 1$, then the class-conditional pdf $f_k(x)$ is a high dim fun of x. The "naive " idea in Naive Bayesian classifier is to **ASSUME** that each component is independent !

$$f_k(x) = f_k(x_1, \ldots, x_d) = \prod_{j=1}^{d} f_{kj}(x_j)$$

BENEFIT: decompose a high dim problem (intractable in density estimation) to low dim problems.
JUSTIFICATION: works surprisingly well in practice for **certain problems**.

> *"Along with decision trees, neural networks, k-nearest neighbours, the Naive Bayes Classifier is one of the most practical learning methods."*

If you are not happy, make the k class-conditional pdf dependency in the form of a network representing the conditional information (causal knowledge).

$$f_k(x_1, \cdots, x_d) = \mathbb{P}(X = (x_1, \cdots, x_d) | Y = k)$$

Linear/Quadratic Discriminant Analysis (LDA/QDA)

Recall the mixed Gaussian model (5) above but in d dimension,
Assuming $X|\ Y = k \sim \mathcal{N}_d(\mu_k, \Sigma_k)$, the d-dim Gaussian distribution, then

$$\delta_k(X) = \log(\pi_k) - (1/2)\log|\Sigma_k| - (1/2)(X - \mu_k)^T \Sigma_k^{-1}(X - \mu_k).$$

Classify x to class k with the largest $\delta_k(x)$.

- $\hat{\pi}_k = n_k/n$: the ratio of samples belonging to class k in totally n population;
- μ_k is estimated by the centroid in each class k
- Σ_k is estimated by sample covariance matrix with each class k

- **Assuming** that all Σ_k are equal (estimated by pooled sample variance matrix $\hat{\Sigma}$), we can reduce δ_k to a **linear** function in x ;
- The **QDA** method use the original **quadratic** function δ_k, but QDA need estimate the in-class variance σ_k or the covariance matrix $\hat{\Sigma}_k$ in high dim $\mathbb{R}^d$, $d > 1$. This requires more data than the LDA for better estimation.
- The decision boundary of QDA is (quadratically) curved.

Exercise

In LDA, consider the eigen-decompositon of the sample covariance matrix $\hat{\Sigma}$ and derive the reduced rank LDA.

k-NN (nearest neighboring) methods

a non-parametric approach to regression and classification

k-NN method [1]: directly estimate the conditional expectation/probability from the data $\mathtt{D} = \{(x_i, y_i) : 1 \leq i \leq n\}$.

- $$\text{For regression: } \mathbb{E}(Y|X = x) \approx \mathsf{AVE}(y_i|x_i \in N_k(x)) := \frac{1}{k} \sum_{i:x \in N_k(x)} y_i.$$
- $$\text{For classification: } \mathbb{P}(Y = class|X = x) \approx \frac{1}{k} \sum_{i \in N_k(x)} \mathbf{1}(y_i = class)$$

  where $N_k(x)$ is the collection of k points in $\{x_i\}$ *closest* to x.

[1] ⚠ k is the number of points in constructing a neighbourhood. Not to be confused with index previously used for the labels of K classes.

Logistic, LDA, QDA, k-NN ?

model selection – to be addressed later

[p154, [ISL]] "When the true decision boundaries are linear, then the LDA and logistic regression approaches will tend to perform well. When the boundaries are moderately non-linear, QDA may give better results. Finally, for much more complicated decision boundaries, a non-parametric approach such as KNN [1] can be superior. "

[1] with correct choice of k such as by the cross-validation

Logistic Regression

- Today, the logistic regression model is one of the most widely used binary models in the analysis of categorical data where $\mathcal{Y} = \{1, \ldots, K\}$.
- Logistic regression, an extension of the linear regression for classification, is based on modeling the *odds* of an outcome:
$$\mathbb{P}(Y = k|X = x),$$
in contrast to the outcome $Y = k$ itself.
- Before that, Fisher proposed *linear discriminant analysis* (**LDA**) in 1936. There are other methods based on the use of some discriminant function, which may not be $\mathbb{P}(Y = k|X = x)$.

We focus on the following four questions which we shall always follow for any machine learning problems

1. How to represent the "odds" ?
2. How to model the the cost/loss functions ?
3. How to minimize the cost function?
4. How to evaluate the performance of the trained model ?

Logistic regression model for binary classification

Now $\mathcal{Y} = \{0, 1\}$. Recall that in Bayes classifier, we introduced a function $h(x)$ as the **conditional probability** of $y = 1$ for a given input x:

$$h(x) = \mathbb{P}(Y = 1|X = x), \quad 1 - h(x) = \mathbb{P}(Y = 0|X = x)$$

- Assume that the logarithm of this probability, as a function of x, is a <u>linear</u> function: $\log h(x;\theta) = f(x, \theta) = \theta \cdot x$, we would have $h = e^{\theta \cdot x}$ which is always positive but has no upper bounds.
- The modification is to use the "0" class probability (i.e. $1 - h$) as a *reference value.* Then the logistic regression model is to assume that

$$\log h(x;\theta) - \log(1 - h(x;\theta)) = f(x;\theta)$$

or

$$h = \frac{1}{1 + e^{-f}}, \quad 1 - h = \frac{e^{-f}}{1 + e^{-f}}$$

Now, f can be any $\mathbb{R}$-valued continuous function on $\mathcal{X}$. You can propose any hypothesis space ($\subset \mathcal{X}$) you want to search the best f in this space.

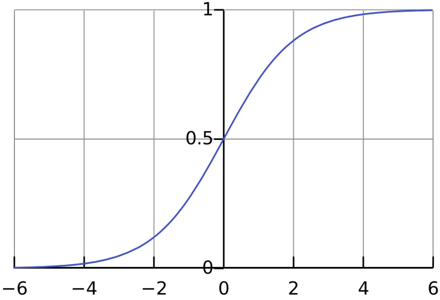
Definition

The **logit** function: $(0,1) \to \mathbb{R}^1$ is

$$h \to z = \log \frac{h}{1-h} =: \mathrm{logit}(h)$$

The inverse of logit function is the **sigmoid(logistic)** function: $\mathbb{R}^1 \to (0,1)$

$$z \to h = \boxed{\sigma(z) := \frac{1}{1+e^{-z}}}$$



activation function family

Why σ this form ?

- What kind of *activation* function mapping $\mathbb{R}^1$ onto $(0, 1)$?
  - Heaviside function $\sigma(x) = I_{\{x>0\}}$;
  - capped linear function $\sigma(x) = \max\{\min(kx + c, 1), 0\}$ with $k > 0$, $c \in \mathbb{R}$;
  - $\sigma(x) = \frac{1}{\pi}\arctan(x) + \frac{1}{2}$
  - $\sigma(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-x^2} dx$ ......
- The considerations of choosing the feature variable and the activation function:
  - simple
  - computational concerns in minimizing the loss
  - Inverse function
  - some certain stat/prob. interpretation (*log-odds* by G. A. Barnard,1949)

Sigmoid logistic function

- The logistic function was invented for the purpose of describing the population growth (history). Logistic map: $x_{n+1} = rx_n(1 - x_n)$. Logistic function was given its name by a Belgian mathematician, P.F. Verhulst (1838). So, the logistic function is used in areas far beyond the classification.
- The logistic function is an offset and scaled **hyperbolic tangent function**: $\sigma(x) = \frac{1}{2} + \frac{1}{2}\tanh(z)$ because $\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$.
- $\sigma(x)$ is smooth and symmetric in the sense

$$\sigma(x) + \sigma(-x) = 1$$

Exercise

Show that the sigmoid function satisfies the logistic equation

$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$

and show that if $h(x;\theta) = \sigma(z(\theta, x))$ *for a general bi-variate function* $z(\cdot,\cdot)$ *of* θ *and* x, *then the gradient* $\nabla_\theta h(x;\theta) = \sigma'(z)\nabla_\theta z$, *and the Hessian matrix* $\nabla_\theta^2 h(x;\theta) = \sigma''(z)\nabla_\theta z \nabla_\theta z^T + \sigma'(z)\nabla_\theta^2 z$

Exercise (softplus function)

Show that the derivative of the so called **softplus** *function*

$$\textit{softplus}(x) = \ln(1 + e^x)$$

is the sigmoid function $\sigma(x) = 1/(1 + e^{-x})$. *Equivalent* $\int_{-\infty}^{x} \sigma(x')\mathrm{d}x' = \textit{softplus}(x)$. *In addition, show that*

$$-\log(\sigma(z)) = \textit{softplus}(-z) \ \text{ and } \ -\log(1 - \sigma(z)) = \textit{softplus}(z)$$

So, softplus function is connected to the negative log likelihood function.

Softplus function is a smooth function close to the RELU: RELU$(x) = \max(0, x)$

framework

We now have a general framework for classification problem by working on the log-odd, z:

$$\boxed{x \in \mathcal{X} \xrightarrow{f(x;\theta)} z \in \mathbb{R}^1 \xrightarrow{\sigma(\cdot)} h \in (0,1) \xrightarrow[h>0.5]{h<0.5} y \in \mathcal{Y} = \{0,1\}}$$

The decision boundary $\{x : h(x) = 0.5\}$ becomes the set where $z = f(x;\theta) = 0$ since $\sigma(0) = 0.5$

- $z = f(x) > 0 \iff h(x) > 0.5$: classifies x as "1".
- $z = f(x) < 0 \iff h(x) < 0.5$: classifies x as "0".
- $z = f(x) = 0$ gives the decision boundary.

In summary, the classifier given by f is to assigne x to the class $=$ heaviside$(f(x)) =$ heaviside$(h(x) - 0.5)$

What remains is to select a model class (hypothesis space $\mathcal{H}$) for representing

$$x \in \mathcal{X} \xrightarrow{f(x;\theta)} z \in \mathbb{R}^1$$

- Linear function $z = \beta \cdot x + \beta_0 \longrightarrow$ logistic regression linear decision

Logistic regression model for $K > 2$ classes

Softmax regression (multinomial logistic regression)

Generalize to the K-class where the labels $y \in \{1, \ldots, K\}$ by assuming that the conditional prob. takes the form

$$\mathbb{P}(Y = k|X = x) = h_k(x; \theta) \tag{6}$$

But we have the constraint

$$\sum_k h_k(x; \theta) = \sum_k \mathbb{P}(Y = k|X = x)) = 1.$$

WLOG, we use the last one $h_K(x; \theta)$. Define z_k, the **logit**,

$$z_k := \log h_k(x; \theta) - \log h_K(x; \theta), \quad k = 1, 2, \ldots, K - 1.$$

Then $h_k = h_K e^{z_k}$ and $z_K = 0$. The constraint $\sum_k h_k = 1$ leads to $h_K = \left(\sum_{k=1}^K e^{z_k}\right)^{-1}$ and

$$\boxed{h_k(x; \theta) = \frac{e^{z_k}}{\sum_{k=1}^K e^{z_k}}}, \quad k = 1, 2, \ldots K \tag{7}$$

Softmax function

Definition

The **softmax** function is the following nonlinear mapping $\mathbb{R}^K \to (0,1)^K$:

$$z = (z_1, \ldots, z_K) \mapsto h = (h_1, \ldots, h_K) = \texttt{softmax}(z)$$

where

$$\boxed{h_k = \frac{e^{z_k}}{\mathcal{Z}}, \quad \text{where} \quad \mathcal{Z} := \sum_{i=1}^{K} e^{z_i}}$$

i.e., $\log h_k = z_k - c$ where c is a constant such that $\sum_{k=}^{K} h_k = 1$.

Remark

The name "softmax" comes from the fact $\lim_{\delta \to 0}$ *softmax*$(z/\delta) = (0, \ldots, 0, 1, 0, \ldots, 0)$ *where the position of* 1 *entry corresponds to* $\operatorname{argmax}_k \{z_k\}$ *.*

It takes a vector of arbitrary real-valued scores and squashes the vector to a new vector with values between 0 and 1 and with zero sum.

Exercise

- *If* $z_1 < z_2$*, then* $h_1 < h_2$*. So* h *keeps the order of* z *(and magnifies the difference among the values* $\{z_k\}$*)*
- $\texttt{softmax}(z + c) = \texttt{softmax}(z)$ *for any scalar* c*. If choose* $c = -\max\{z_1, \ldots, z_K\}$*, then every elements in the vector* $z + c$ *is not positive. The calculation of* $\texttt{softmax}(z + c)$ *is more stable than that directly on* $\texttt{softmax}(z)$*. (*$\exp(1000)$ *gives you* `NaN` *on computers.)*
- *When* $z_k = \theta_k \cdot x$*, show that the shift* $\theta \to \theta - c$ *does not change the value of* $h(x; \theta)$*. So the softmax regression's* K *parameters are redundant. In learning* θ*, we can simply set* $\theta_K = 0$ *or adding the linear constraint* $\sum \theta_k = 0$*.*

Linear model assumption for z_k

- With the aid of softmax, the representation of the function $\{h_k(x)\}$ becomes the representation of $\mathbb{R}^K$-value functions $z_k(x) = f_k(x; \theta)$.
- The softmax (logistic) regression assume the linear form $z_k = f_k(x; \theta_k) = \theta_k \cdot x$, with K parameters $\theta_k \in \mathbb{R}^d$ [1]. For convenience, we still use $\theta = \{\theta_1, \ldots, \theta_K\}$ to denote all the parameters of our model .
- Like in nonlinear regression, all same techniques can be applied here to represent the function $x \to z_k$. (sparse, kernel, spline ,.....)
- Recently, the DNN (deep neural network) models the function $x \to z_k$ by neural network. The result is a huge success.

[1] Effectively, $K - 1$ parameters, since $z_K = 0$.

Decision rule of softmax regression

$$\boxed{x \in \mathcal{X} \xrightarrow[k=1,\ldots,K]{f_k(x;\theta)} z_k \in \mathbb{R}^1 \xrightarrow{\texttt{softmax}} h_k \in (0,1) \xrightarrow[y=k^*]{\max_k h_k(x)} y \in \mathcal{Y} = \{0,1\}}$$

$h(x;\theta) = \texttt{softmax}(z)$ i.e., $h_k(x;\theta) = \frac{e^{z_k}}{\sum_{k=1}^K e^{z_k}}, k = 1, 2, \ldots K$ and $z_k = f_k(x;\theta) = \theta_k \cdot x$. Then for an input x, we assign it to the class which is

$$\begin{aligned} k^*(x) &= \operatorname*{argmax}_{1\leq k\leq K} h_k(x;\theta) = \operatorname*{argmax}_k e^{z_k} \\ &= \operatorname*{argmax}_k z_k = \operatorname*{argmax}_k f_k(x) \\ &= \operatorname*{argmax}_k (\theta_k \cdot x) \end{aligned}$$

The last step shows that it is a linear classifier since z_k is linear in x.

Exercise: For example, $K = 3$, and $d = 2$, $\theta_1 = (1,0), \theta_2 = (1,1), \theta_3 = (0,0)$. draw the three domains where x are classified as $1, 2, 3$, respectively.

How to choose loss function

- A criterion must be set to define the loss function ℓ in order to find the optimal parameter θ in $h_k(x;\theta)$.
- We first recall that the 0-1 loss is defined for the classification outcome: $\mathcal{Y} \times \mathcal{Y} \to \{0,1\}$.
- The predicted class $\hat{y}(x) = \operatorname{argmax}_k h_k(x;\theta)$, then $\ell_{01}(y,\hat{y}) = I(y = \operatorname{argmax}_k h_k(x;\theta))$
- The empirical risk from the data $\mathtt{D} = \{(x_i, y_i)\}$ is
$$\sum_{i=1}^{N} I(y_i = \operatorname*{argmax}_k h_k(x_i;\theta)) = \sum_{k=1}^{K} \sum_{(x_i, y_i = k)} I(k = \operatorname*{argmax}_{k'} h_{k'}(x_i;\theta))$$
- For the binary case where $\mathcal{Y} = \{0,1\}$, with $h(x;\theta) = h_1(x;\theta)$,
$$\begin{aligned}
&\sum_{i=1}^{N} I(y_i = \operatorname*{argmax}_k h_k(x_i;\theta)) \\
= &\sum_{(x_i, y_i = 1)} I(h(x_i;\theta) > 0.5) + \sum_{(x_i, y_i = 0)} (1 - I(h(x_i;\theta) > 0.5)).
\end{aligned}$$

- The above 0-1 loss only used the sign of $h(x) - 0.5$; the prob. meaning of $h(x)$ is not used. In addition, the minimization for the above empirical 0-1 loss is hard.
- The key difference of logistic regression from most machine learning methods based on linear separating hyperplane (SVM) is that logistic regression attempt to model and estimate $\mathbb{P}(Y = k|X = x)$ for each k directly .

Two Main Principles to Build Loss functions

- Statistical Learning Approach:
  - Maximize Likelihood
  - Bayesian = Prior $\times$ Likelihood
- Information Theory Approach: Minimize the “distance” between prob. measures.

Loss function of logistic regression = negative log-likelihood

coursera video.

- In linear regression, the squared error $l(y, \hat{y}) = (y - \hat{y})^2$, has the interpretation of negative log likelihood for Gaussian-type residuals. The same idea of taking negative log likelihood as the loss for classification is as follows.
- For a given data point (x, y), in binary case, the probability $\mathbb{P}(Y = y|X = x) = h(x; \theta)$ if $y = 1$ and $\mathbb{P}(Y = y|X = x) = 1 - h(x; \theta)$ if $y = 0$, which can be unified in one expression for the likelihood function:

$$\mathbb{P}(Y = y|X = x) = h^y(1 - h)^{1-y},$$

Then the negative log-likelihood is

$$-y \log h - (1 - y) \log(1 - h)$$

which is will be defined as ℓ. Thus, MLE is equivalent to minimizing ℓ.

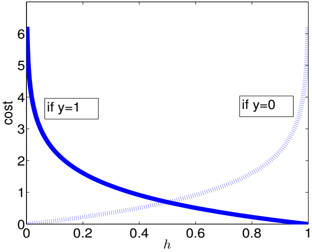
Loss function for Binary classification

Definition

The loss function for the binary logistic regression is the function $(0,1) \times \{0,1\} \to \mathbb{R}^+$ in the form

$$\ell(h,y) = -y \log h - (1-y)\log(1-h) = \begin{cases} -\log h & \text{if } y=1 \\ -\log(1-h) & \text{if } y=0 \end{cases} \quad (8)$$

Note that this form of this loss function is unlike the regression loss where the two input argument are both $\mathcal{Y}$-valued.



`Homework` ℓ is convex in h.
`discussion`: Why this cost fun makes sense from the viewpoint of minimizers at different values of y?
Derivative $\partial l / \partial h$

Then the objective function [1] on the training dataset $\mathtt{D} = \left\{(X^{(i)}, Y^{(i)})\right\}$ is the sum of loss from all individual examples

$$\begin{aligned} J(\theta) &= \frac{1}{n}\sum_{i=1}^{n} \ell(h(X^{(i)};\theta), Y^{(i)}) \\ &= \frac{1}{n}\left(\sum_{i:Y^{(i)}=1} -\log h(X^{(i)};\theta) + \sum_{i:Y^{(i)}=0} -\log(1-h(X^{(i)};\theta))\right) \\ &= \frac{1}{n}\left(\sum_{i:Y^{(i)}=1} \log\left(1+e^{-f(X^{(i)};\theta)}\right)\right. \\ &\qquad \left. + \sum_{i:Y^{(i)}=0} \log\left(1+e^{+f(X^{(i)};\theta)}\right)\right). \end{aligned} \tag{9}$$

In logistic regression, $f(x;\theta) = \theta \cdot x$.

Exercise

Show that J is convex in θ for logistic regression.

[1] sometimes, we drop the $\frac{1}{n}$ factor in J since it does not affect the minimizers.

The following exercise shows that the binomial deviance loss is just the loss in logistic regression, written in terms of f rather than of h.

Exercise

Recall the relation that the odd $h = \sigma(z)$, σ is the sigmoid function, and $z = f(x;\theta)$. Then the logistic loss ℓ in (8) can be written in terms of f, [a]

$$\ell(f,y) = \begin{cases} -\log h(x;\theta) = \log(1+e^{-f}) = \textit{softplus}(-f) & \textit{if } y = 1 \\ -\log(1-h(x;\theta)) = \log(1+e^{f}) = \textit{softplus}(f) & \textit{if } y = 0 \end{cases} \tag{10}$$

Change the binary coding of $\mathcal{Y}$ to $\{\pm 1\}$ (i.e, "0" class is named as "-1" class now), then $\ell(f,y)$ has a convenient expression:

$$\boxed{\ell_{\textit{bd}}(f,y) := \textit{softplus}(-yf(x)), \quad y \in \mathcal{Y} = \{-1,1\}, f : \mathcal{X} \to \mathbb{R}.} \tag{11}$$

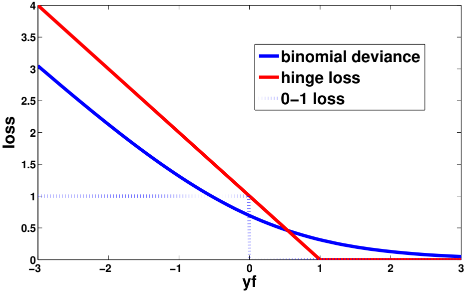
which is __the product of y and f__. This loss $\ell_{\textit{bd}}(f,y)$ has the name **binomial deviance loss**, *which arises from* deviance *statistics for binormal distribution.* [b]

---

[a] We here abused the use of ℓ. The definition domain of ℓ function here is $\mathbb{R} \times \{0,1\}$, not $(0,1) \times \{0,1\}$.

In this page, we use $\{\pm 1\}$-encoded $\mathcal{Y}$ and compare the 0-1 loss and the binomial deviance loss.

- Note that the classifier with a given f is equal to sign$(f(x))$. Then the 0-1 loss can be rewritten as $\ell_{01}(y, f(x)) =$ heaviside$(-yf(x))$.
- Logistic regression: $\ell_{bd}(y, f(x)) =$ softplus$(-yf(x))$.
- The third loss: hinge loss $\ell_{\text{hinge}}(y, f) = (1 - yf)_+$ is used in support vector classifier (to be discussed later)



Exercise

Recall in Topic 1, we have $\mathcal{E}$ defined as the expected loss (the generalized error):

$$\mathcal{E}_{bd}(f) = \mathbb{E}\,\ell_{bd}(Y, f(X)) = \mathbb{E}_{X,Y}\left[\textit{softplus}(-Y f(X))\right]$$

Denote $\pi_\pm = \mathbb{P}(Y = \pm 1)$ *the distribution of* Y *and* $\rho_\pm = p_{X|Y=\pm}(x)$*, the conditional distribution of* X *given* Y*. Solve the variational problem*

$$\inf_f \mathcal{E}_{bd}(f)$$

Show that the optimal f_* *is*

$$\sigma(f_*(x)) = \frac{\pi_+\rho_+(x)}{\pi_+\rho_+(x) + \pi_-\rho_-(x)} = \frac{\mathbb{P}(X = x, Y = +)}{p_X(x)} = \mathbb{P}(Y = +|X = x)$$

This expression of f^* is consistent to the fact that $h(x) = \sigma(z) = \sigma(f(x))$.

Loss function of K-classification

- The loss function as the negative log likelihood for K-classification on an input-output (x, y) is

$$\ell(\mathbf{h}, y) = \begin{cases} -\log h_1(x;\theta) & \text{if } y = 1 \\ -\log h_2(x;\theta) & \text{if } y = 2 \\ \cdots\cdots & \\ -\log h_K(x;\theta) & \text{if } y = K \end{cases} = \boxed{-\log h_y(x;\theta)} \tag{12}$$

where $\mathbf{h} = (h_1, \ldots h_K) = \text{softmax}(z)$ with $z_k = f_k(x) = x \cdot \theta_k$.

- Then we have the objective function

$$J(\theta) := \frac{1}{n}\sum_{i=1}^{n} -\log h_{Y^{(i)}}(X^{(i)};\theta) = \frac{1}{n}\sum_{k=1}^{K}\left(\sum_{\substack{i\in\{1,\ldots,n\} \\ Y^{(i)}=k}} -\log h_k(X^{(i)};\theta)\right) \tag{13}$$

- cross-entropy

Information Theory view: Loss function as the cross-entropy

Definition

- The (Shannon) **entropy** of a prob. distribution p is

$$H(p) = H(p,p) = -\mathbb{E}_{Y\sim p}[\log p(Y)] = -\sum_y p(y)\log p(y).$$

- The **cross-entropy** between a distribution p and another distribution q is defined as:

$$H(p,q) \triangleq -\sum_y p(y)\log q(y) = -\mathbb{E}_{Y\sim p}[\log q(Y)]$$

- The **Kullback-Leibler divergence** is defined as

$$D_{\mathrm{KL}}(p\|q) \triangleq -\sum_x p(x)\,\log\frac{q(x)}{p(x)} = H(p,q) - H(p)$$

- $D_{\mathrm{KL}}(p\|q)$ is non-negative and is the measurement of how far from q to p. Note that $D_{\mathrm{KL}}(p\|q) \neq D_{\mathrm{KL}}(q\|p)$ in general. But $D_{\mathrm{KL}}(p\|q) = 0$ iff $p = q$.
- For fixed p, minimizing $D_{\mathrm{KL}}(p\|q)$ over q is equivalent to minimizing $H(p, q)$.

How to choose p and q for classification problem ?

- In the above logistic regression for the K classification, *given* x, q is a Bernoulli distribution $q(k) = \mathbb{P}(Y = k|X = x) = h_k(x; \theta), 1 \leq k \leq K$.
- p is from one given sample $(x, y) \in \mathcal{X} \times \{1, \ldots, K\}$, it is the delta distribution (**one hot distribution**): $p(k) = 1$ if $k = y$ and $p(k) = 0$ if $k \neq y$, i.e., $p(k) = \delta_{k,y}$
- So, $H(p, q) = -\sum_k p(k) \log q(k) = -\log h_y(x; \theta)$, which is identical to the loss (12)

This is why (12) called the **cross-entropy loss** or *log* loss.

Recall that $\ell(h(x;\theta), y) = -y \log h(x;\theta) - (1-y)\log(1-h(x;\theta))$ and $h(x;\theta) = \sigma(z)$ where $z = f(x;\theta) = \theta \cdot x$.

$$\begin{aligned}\nabla_\theta \ell &= -y/\sigma(z) \cdot \sigma'(z)\nabla_\theta z + (1-y)/(1-\sigma(z)) \cdot \sigma'(z)\nabla_\theta z \\ &= -y(1-\sigma(z))\nabla_\theta z + (1-y)\sigma(z)\nabla_\theta z \\ &= (\sigma(z) - y)\nabla_\theta z = (h(x;\theta) - y)x\end{aligned}$$

Exercise

Show that the Hessian matrix of ℓ is

$$\nabla^2_\theta \ell = (h(x;\theta) - y)\nabla^2_\theta z + \sigma'(z)(\nabla_\theta z)(\nabla_\theta z)^T = h(1-h)xx^T.$$

Show that this matrix has the rank 1 and is positive semi-definite.

$$J(\theta) = \sum_{i=1}^{n} \ell(h(x^{(i)}; \theta), y^{(i)})$$

$$\nabla_\theta J = \sum_{i=1}^{n} (h(x^{(i)}; \theta) - y^{(i)}) x^{(i)} = \mathbf{X}(\sigma(\mathbf{z}) - \mathbf{y})$$

$$\text{where} \quad \mathbf{z} = \mathbf{X}\theta$$

Here, the matrix $\mathbf{X} \triangleq [x^{(1)}, x^{(2)}, \ldots, x^{(n)}] \in \mathbb{R}^{d \times n}$ whose n *columns* corresponding to n data points. θ and $\mathbf{y} = (y^{(1)}, y^{(2)}, \ldots, y^{(n)})^\mathsf{T}$ are column vectors. σ function acts on the vector in the element-wise sense. Then the gradient descent is

$$\theta^{new} = \theta^{old} + \text{learning rate} \times \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - h(x^{(i)}; \theta^{old})) x^{(i)}$$

Now consider the displacement $\Delta\theta := \theta^{new} - \theta^{old}$ on the projection of $x^{(i)}$, then $\Delta z^{(i)} = \Delta\theta \cdot x^{(i)} = \eta(y^{(i)} - h(x^{(i)}; \theta^{old})) \left\| x^{(i)} \right\|^2$. So, $y^{(i)} = 1$ means $\Delta z^{(i)} > 0$ and $y^{(i)} = 0$ means $\Delta z^{(i)} < 0$. Recall the decision boundary in $\mathcal{Z}$ space.