Classification

December 20, 2017

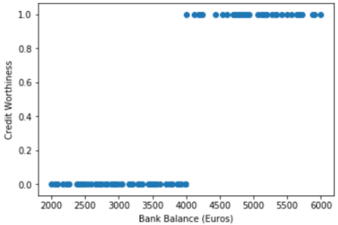
Classification

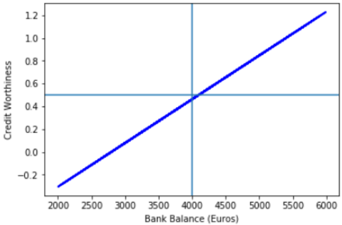
- Linear regression: the response variable y is quantitative.
- Classification: y is qualitative (takes on a number of discrete values).
- Classification problems seem to occur more often than regression problems:
  - spam classifiers (spam or ham)
  - classifying whether a bank transaction is fradulent or not
  - given a set of symptoms, determining which medical condition a person has
  - classifying whether a video is suitable or unsuitable for children
  - MNIST: given a handwritten digit, determine which digit it actually is

Why not Linear Regression?

Example 1

Consider the following (simplified) problem: given the bank balance x of an individual, determine whether they are credit worthy or not.



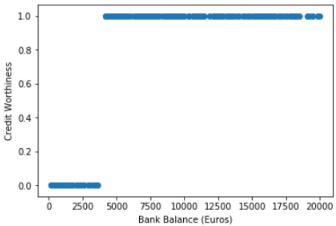


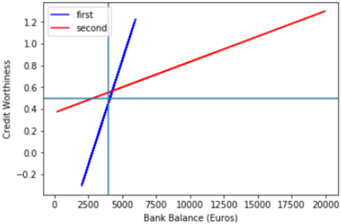
- Turns out that anyone with a balance of €4000 or more is credit worthy
- Classification: if $y(x) \geq 0.5$, then "credit worthy"; else "not"
- Slope of the regression line depends on the how many data points are in each of the two buckets

Why not Linear Regression?

Example 1

- With more data points in the "positive" bucket, the slope of the regression line is less steep.
- The threshold predicted also changes.

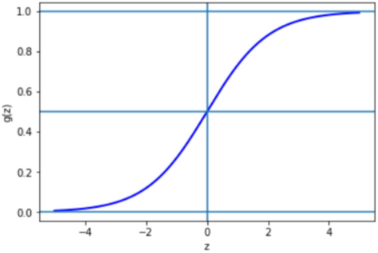




Binary Classification: Logistic Regression

- Two classes: 0 and 1
- Logistic regression models the probability that the response variable y belongs to a particular class: $P(y = 1 \mid x)$
- $P(y = 1 \mid x; \theta) = g(\theta^\intercal x) = \frac{1}{1+e^{-\theta^\intercal x}}$
- $g(z) = \frac{1}{1+e^{-\theta^\intercal x}}$ is the sigmoid function

The Sigmoid Function



- $g(z) \to 1$ as $z \to \infty$
- $g(z) \to 0$ as $z \to -\infty$
- $g'(z) = g(z)(1 - g(z))$

Logistic Regression: Learning the Model Parameters

In logistic regression, the probabilities are modeled as follows:

$$P(y = 1 \mid x; \theta) = g(\theta^\intercal x) = \frac{1}{1 + e^{-\theta^\intercal x}}$$
$$P(y = 0 \mid x; \theta) = 1 - g(\theta^\intercal x)$$

Logistic Regression: Learning the Model Parameters

In logistic regression, the probabilities are modeled as follows:

$$P(y = 1 \mid x; \theta) = g(\theta^{\intercal} x) = \frac{1}{1 + e^{-\theta^{\intercal} x}}$$

$$P(y = 0 \mid x; \theta) = 1 - g(\theta^{\intercal} x)$$

$$P(y \mid x; \theta) = (g(\theta^{\intercal} x))^{y} \cdot (1 - g(\theta^{\intercal} x))^{1-y}$$

Logistic Regression: Learning the Model Parameters

In logistic regression, the probabilities are modeled as follows:

$$P(y = 1 \mid x; \theta) = g(\theta^\top x) = \frac{1}{1 + e^{-\theta^\top x}}$$
$$P(y = 0 \mid x; \theta) = 1 - g(\theta^\top x)$$

$$P(y \mid x; \theta) = (g(\theta^\top x))^y \cdot (1 - g(\theta^\top x))^{1-y}$$

The Likelihood Function

Assume that the m training examples $(x^{(1)}, y^{(1)}), \ldots (x^{(m)}, y^{(m)})$ were generated *independently*.

$$\begin{aligned} L(\theta; \{(x^{(i)}, y^{(i)})\}_{i=1}^m) &= \prod_{i=1}^m P(y^{(i)} \mid x^{(i)}; \theta) \\ &= \prod_{i=1}^m \left(g(\theta^\top x^{(i)})\right)^{y^{(i)}} \cdot \left(1 - g(\theta^\top x^{(i)})\right)^{(1-y^{(i)})} \end{aligned}$$

Maximizing the Likelihood ...

... is equivalent to maximizing the log-likelihood:

$$
\begin{aligned}
l(\theta) &= \log L(\theta) \\
&= \sum_{i=1}^{m} y^{(i)} \log g(\theta^{\mathsf{T}} x^{(i)}) + (1 - y^{(i)}) \log(1 - g(\theta^{\mathsf{T}} \cdot x^{(i)}))
\end{aligned}
$$

- Use gradient ascent to maximize $l(\theta)$
- $\theta_{\text{new}} := \theta_{\text{old}} + \alpha \nabla_\theta l(\theta)$
- $\theta_j := \theta_j + \alpha \cdot \sum_{i=1}^{m} \left(y^{(i)} - g(\theta^{\mathsf{T}} x^{(i)}) \right) \cdot x_j^{(i)}$
- Stochastic gradient ascent: $\theta_j := \theta_j + \alpha \cdot (y^{(i)} - g(\theta^{\mathsf{T}} \cdot x^{(i)})) \cdot x_j^{(i)}$

Classifying New Data Points

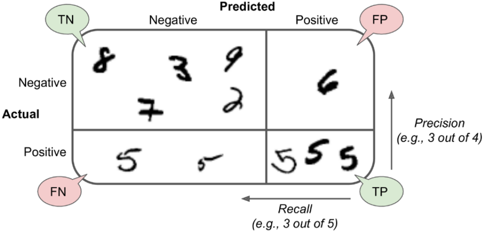
- Once θ has been estimated (using maximum likelihood, for instance), given x, $P(y = 1 \mid x) = g(\theta^\intercal \cdot x)$
- We could for instance classify x as belonging to class 1 iff $g(\theta^\intercal \cdot x) \geq 0.5$

Evaluating the Performance of a Classifier

Harder than evaluating a linear regressor.

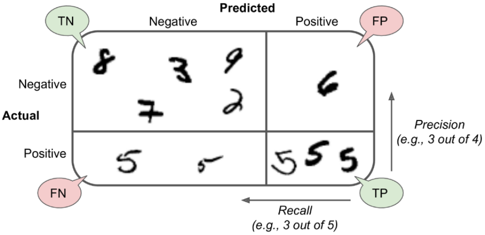
- Consider unbalanced data sets: let's say that 90% of customers in an online store are one-time customers.
- Want to determine whether a customer is a one-time customer.
- A "dumb" classifier that declares every customer as "bad" has 90% accuracy.

Precision and Recall



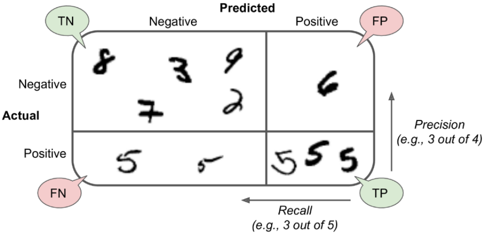
- Accuracy of positive predictions = Precision = $\frac{TP}{TP+FP}$
- Fraction of positive instances correctly classified = Recall = $\frac{TP}{TP+FN}$

Precision and Recall



- Accuracy of positive predictions = Precision = $\frac{\text{TP}}{\text{TP+FP}}$
- Fraction of positive instances correctly classified = Recall = $\frac{\text{TP}}{\text{TP+FN}}$
- A single score to compare different classifiers?

Precision and Recall



- Accuracy of positive predictions = Precision = $\frac{\text{TP}}{\text{TP}+\text{FP}}$
- Fraction of positive instances correctly classified = Recall = $\frac{\text{TP}}{\text{TP}+\text{FN}}$
- A single score to compare different classifiers?
- **F1 score** = harmonic mean of the precision and recall = $\frac{2}{1/P+1/R}$
- F1 score penalizes classifiers with either small precision or recall

Stochastic Gradient Descent

In batch gradient descent, the update step for the jth component is:

$$\theta_j := \theta_j + \alpha \cdot \sum_{i=1}^{m} \left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)} \theta_j \right) \cdot x_j^{(i)}.$$

- Has to scan through the entire training set for a *single* update
- Costly operation if m is large

Stochastic Gradient Descent

In batch gradient descent, the update step for the jth component is:

$$\theta_j := \theta_j + \alpha \cdot \sum_{i=1}^{m} \left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)} \theta_j \right) \cdot x_j^{(i)}.$$

- Has to scan through the entire training set for a *single* update
- Costly operation if m is large
- **Stochastic Gradient Descent**: for every training instance (x, y), $x = (x_0, x_1, \ldots, x_n)^\mathsf{T}$, update the parameters:

$$\theta_j := \theta_j + \alpha \cdot \left(y - \sum_{j=0}^{n} x_j \theta_j \right) \cdot x_j.$$

Stochastic Gradient Descent: Features and Issues

- Doesn't have to look at the entire training set to make progress.
- Often gets close to the optimum much faster than batch gradient descent.
- May never converge to the optimum (can keep on oscillating between values near the optimum). This problem is alleviated by choosing α to be very small.

Analytic Solution

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)}\theta_j\right)^2$$

Want to find in closed-form a value of θ that minimizes $J(\theta)$

- Write $J(\theta)$ is matrix-vector form.

Analytic Solution

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)}\theta_j\right)^2$$

Want to find in closed-form a value of θ that minimizes $J(\theta)$

- Write $J(\theta)$ is matrix-vector form.
- **Design matrix.** An $m \times (n+1)$ matrix X defined by:

$$X = \begin{bmatrix} — & (x^{(1)})^\intercal & — \\ — & (x^{(2)})^\intercal & — \\ \vdots & \vdots & \vdots \\ — & (x^{(m)})^\intercal & — \end{bmatrix}$$

Analytic Solution

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}\left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)}\theta_j\right)^2$$

Want to find in closed-form a value of θ that minimizes $J(\theta)$

- Write $J(\theta)$ is matrix-vector form.
- **Design matrix.** An $m \times (n+1)$ matrix X defined by:

$$X = \begin{bmatrix} - & (x^{(1)})^\intercal & - \\ - & (x^{(2)})^\intercal & - \\ \vdots & \vdots & \vdots \\ - & (x^{(m)})^\intercal & - \end{bmatrix}$$

- $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$

Analytic Solution . . .

$$y - X \cdot \theta = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix} - \begin{bmatrix} (x^{(1)})^\intercal \cdot \theta \\ (x^{(2)})^\intercal \cdot \theta \\ \vdots \\ (x^{(m)})^\intercal \cdot \theta \end{bmatrix}$$

Matrix-form of $J(\theta)$:

$$\begin{aligned} J(\theta) &= \frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \sum_{j=0}^{n} x_j^{(i)} \theta_j \right)^2 \\ &= \frac{1}{2} (y - X\theta)^\intercal (y - X\theta) \end{aligned}$$

Analytic Solution . . .

Minimize $J(\theta)$ w.r.t θ:

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(y - X\theta)^\intercal (y - X\theta) \\
&= \text{see Andrew Ng's notes} \\
&= X^\intercal X\theta - X^\intercal y
\end{aligned}
$$

yielding:

$$
\boxed{\theta = (X^\intercal X)^{-1} \cdot X^\intercal y.}
$$

Analytic Solution ...

Minimize $J(\theta)$ w.r.t θ:

$$\begin{aligned}\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(y - X\theta)^\top (y - X\theta) \\ &= \text{see Andrew Ng's notes} \\ &= X^\top X\theta - X^\top y\end{aligned}$$

yielding:

$$\boxed{\theta = (X^\top X)^{-1} \cdot X^\top y.}$$

- **Assumption:** X has full column rank so that $X^\top X$ is invertible.

Analytic Solution . . .

Minimize $J(\theta)$ w.r.t θ:

$$\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(y - X\theta)^\intercal (y - X\theta) \\
&= \text{see Andrew Ng's notes} \\
&= X^\intercal X\theta - X^\intercal y
\end{aligned}$$

yielding:

$$\boxed{\theta = (X^\intercal X)^{-1} \cdot X^\intercal y.}$$

- **Assumption:** X has full column rank so that $X^\intercal X$ is invertible. *Proof.* Show that $X^\intercal X z = 0$ implies $z = 0$.

Analytic Solution . . .

Minimize $J(\theta)$ w.r.t θ:

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(y - X\theta)^\intercal (y - X\theta) \\
&= \text{see Andrew Ng's notes} \\
&= X^\intercal X\theta - X^\intercal y
\end{aligned}
$$

yielding:

$$\boxed{\theta = (X^\intercal X)^{-1} \cdot X^\intercal y.}$$

- **Assumption:** X has full column rank so that $X^\intercal X$ is invertible. *Proof.* Show that $X^\intercal X z = 0$ implies $z = 0$.
- If X does not have full column rank, the usual strategy is to remove redundant columns.

Probabilistic Interpretation

Assumptions

$$y^{(i)} = \theta^{\mathsf{T}} \cdot x^{(i)} + \epsilon^{(i)},$$

where the error terms $\epsilon^{(i)}$

- capture unmodeled effects and/or random noise
- are independent and identically distributed as $N(0, \sigma^2)$

Probabilistic Interpretation

Assumptions

$$y^{(i)} = \theta^{\mathsf{T}} \cdot x^{(i)} + \epsilon^{(i)},$$

where the error terms $\epsilon^{(i)}$

- capture unmodeled effects and/or random noise
- are independent and identically distributed as $N(0, \sigma^2)$

Given $x^{(i)}$,

- $E(y^{(i)} \mid x^{(i)}) = \theta^{\mathsf{T}} \cdot x^{(i)}$

Probabilistic Interpretation

Assumptions

$$y^{(i)} = \theta^{\mathsf{T}} \cdot x^{(i)} + \epsilon^{(i)},$$

where the error terms $\epsilon^{(i)}$

- capture unmodeled effects and/or random noise
- are independent and identically distributed as $N(0, \sigma^2)$

Given $x^{(i)}$,

- $E(y^{(i)} \mid x^{(i)}) = \theta^{\mathsf{T}} \cdot x^{(i)}$
- $\mathrm{Var}(y^{(i)} \mid x^{(i)}) = \mathrm{Var}(\epsilon^{(i)}) = \sigma^2$

Probabilistic Interpretation

Assumptions

$$y^{(i)} = \theta^{\mathsf{T}} \cdot x^{(i)} + \epsilon^{(i)},$$

where the error terms $\epsilon^{(i)}$

- capture unmodeled effects and/or random noise
- are independent and identically distributed as $N(0, \sigma^2)$

Given $x^{(i)}$,

- $E(y^{(i)} \mid x^{(i)}) = \theta^{\mathsf{T}} \cdot x^{(i)}$
- $\mathrm{Var}(y^{(i)} \mid x^{(i)}) = \mathrm{Var}(\epsilon^{(i)}) = \sigma^2$

Thus $y^{(i)} \mid x^{(i)} \sim N(\theta^{\mathsf{T}} x^{(i)}, \sigma^2)$:

$$p(y^{(i)} \mid x^{(i)}; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^{\mathsf{T}} \cdot x^{(i)})^2}{2\sigma^2} \right)$$

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \ldots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$?

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \dots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \dots, y^{(m)})^\intercal$?
- Since the $\epsilon^{(i)}$s are independent:

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \ldots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$?
- Since the $\epsilon^{(i)}$s are independent:

$$p(y \mid x; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \ldots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$?
- Since the $\epsilon^{(i)}$s are independent:

$$p(y \mid x; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$

- **Likelihood function.** $L(\theta) = p(y \mid x; \theta)$

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \ldots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$?
- Since the $\epsilon^{(i)}$s are independent:

$$p(y \mid x; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$

- **Likelihood function.** $L(\theta) = p(y \mid x; \theta)$

$$L(\theta) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{\left(y^{(i)} - \theta^\intercal x^{(i)}\right)^2}{2\sigma^2} \right\}$$

Maximum Likelihood Estimation

- Given $x = (x^{(1)}, \ldots, x^{(m)})^\intercal$ and θ, what is the joint distribution of the $y = (y^{(1)}, \ldots, y^{(m)})^\intercal$?
- Since the $\epsilon^{(i)}$s are independent:

$$p(y \mid x; \theta) = \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta)$$

- **Likelihood function.** $L(\theta) = p(y \mid x; \theta)$

$$L(\theta) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{\left(y^{(i)} - \theta^\intercal x^{(i)}\right)^2}{2\sigma^2} \right\}$$

- **Principle of Maximum Likelihood.** Choose the parameters to make the data as likely as possible. Choose θ to maximize $L(\theta)$.

Maximum Likelihood Estimation . . .

Maximizing $L(\theta)$ is equivalent to maximizing *any* strictly increasing function of $L(\theta)$.

Maximum Likelihood Estimation . . .

Maximizing $L(\theta)$ is equivalent to maximizing *any* strictly increasing function of $L(\theta)$.

- Usual to maximize the log likelihood $l(\theta) = \log L(\theta)$.
- $l(\theta) = m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^{\mathsf{T}} x^{(i)}\right)^2$.
- Maximizing $l(\theta)$ is equivalent to minimizing $\frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^{\mathsf{T}} x^{(i)}\right)^2$.

Maximum Likelihood Estimation . . .

Maximizing $L(\theta)$ is equivalent to maximizing *any* strictly increasing function of $L(\theta)$.

- Usual to maximize the log likelihood $l(\theta) = \log L(\theta)$.
- $l(\theta) = m \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^\intercal x^{(i)}\right)^2$.
- Maximizing $l(\theta)$ is equivalent to minimizing $\frac{1}{2} \sum_{i=1}^{m} \left(y^{(i)} - \theta^\intercal x^{(i)}\right)^2$.

Summary

Under the previous probabilistic assumptions: **least-squares regression** corresponds to finding the **maximum likelihood estimate** of θ.

The Goodness of Fit

- Residual Standard Error: standard deviation of the error terms $\epsilon^{(i)}$.

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}$$

The Goodness of Fit

- Residual Standard Error: standard deviation of the error terms $\epsilon^{(i)}$.

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2} \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2}$$

- R^2 Statistic:

$$R^2 = 1 - \frac{\sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2}{\sum_{i=1}^{m} \left(y^{(i)} - \bar{y}\right)^2}$$

The Goodness of Fit

- Residual Standard Error: standard deviation of the error terms $\epsilon^{(i)}$.

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}$$

- R^2 Statistic:

$$R^2 = 1 - \frac{\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}{\sum_{i=1}^{m}\left(y^{(i)} - \bar{y}\right)^2}$$

- Total sum of squares $= \sum_{i=1}^{m}\left(y^{(i)} - \bar{y}\right)^2$: variability inherent in the response
- Residual sum of squares $= \left(y^{(i)} - \hat{y}^{(i)}\right)^2$: variability left unexplained after performing the regression