Classification

December 18, 2017

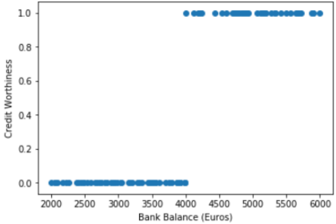
Classification

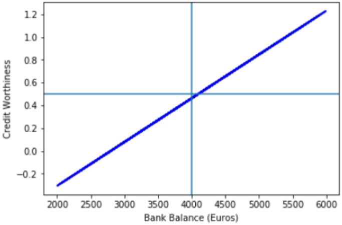
- Linear regression: the response variable y is quantitative.
- Classification: y is qualitative (takes on a number of discrete values).
- Classification problems seem to occur more often than regression problems:
  - spam classifiers (spam or ham)
  - classifying whether a bank transaction is fradulent 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.

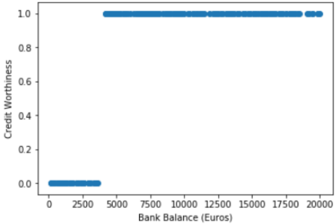


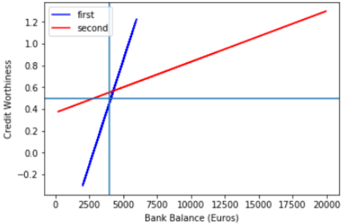


- Turns out that anyone with a balance of €4000 or more is credit worthy
- Classification: if $y(x) \geq 0.5$, then "credit worthy"; else "not"
- Slope of the regression line depends on the how many data points are in each of the two buckets

Example 1

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

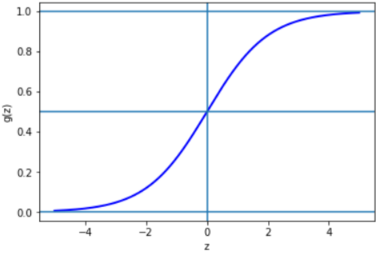




Binary Classification: Logistic Regression

- 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:

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

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

Maximizing the Likelihood

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

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

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 $g(\theta^\intercal) \geq 0.5$

Stochastic Gradient Descent

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

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

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- 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.

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- **Design matrix.** An $m \times (n+1)$ matrix X defined by:

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

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

Analytic Solution . . .

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

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

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

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:

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- **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 $N(0, \sigma^2)$

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

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

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

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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 $\epsilon^{(i)}$.

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

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- R^2 Statistic:

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

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- 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