Classification

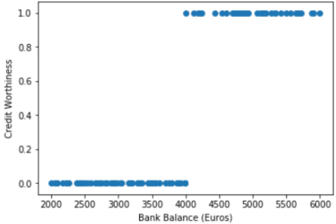
December 17, 2017

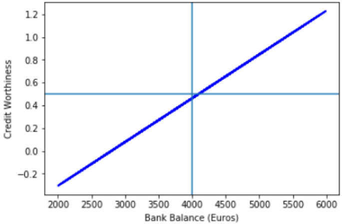
Classification

- 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

Example 1

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



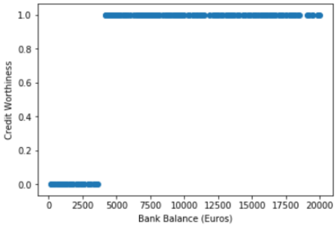


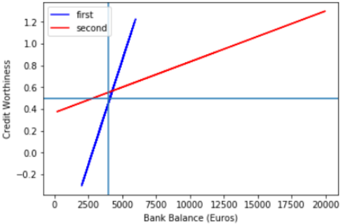
- Turns out that anyone with a balance of €4000 or more is credit worthy
- Classification: if $y(x) \geq 0.5$, then "credit worthy"; else "not"
- Slope of the regression line depends on the how many data points are in each of the two buckets

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.





Linear Regression Models and Least Squares ...

- Typical situation: we have training data

$$(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$$

  from which to estimate the parameters θ.

- Least squares: pick parameters $\theta = (\theta_0, \ldots, \theta_n)^\mathsf{T}$ to minimize

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

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- Gradient descent
- Analytical solution
- Probabilistic interpretation

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where α is the learning rate.

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- Gradient descent is susceptible to **local minima** in general; in this case, J is a **convex** function and has a **unique global minimum**.

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

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

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

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 $J(\theta)$:

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

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Minimize $J(\theta)$ w.r.t θ:

$$\begin{aligned}\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(y - X\theta)^\mathsf{T}(y - X\theta) \\ &= \text{see Andrew Ng's notes} \\ &= X^\mathsf{T}X\theta - X^\mathsf{T}y\end{aligned}$$

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- 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 $\epsilon^{(i)}$

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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

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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:

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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