Linear Regression

December 15, 2017

Linear Regression

- Simple approach to supervised learning when the target variable is **continuous**.
- Assumes a linear relationship between the input variables $x_1, \ldots, x_n$ and the target variable y.
- When the target variable is discrete, the problem is a **classification** problem.

Linear Regression Models and Least Squares

- input vector $x^\mathsf{T} = (x_1, \ldots, x_n)$, output/response y
- linear model: $y = \theta_0 + \sum_{j=1}^{n} x_j \theta_j = \sum_{j=0}^{n} x_j \theta_j$, where $x_0 = 1$
- θs are unknown parameters
- variables x_j can come from different sources:
  - quantitative inputs
  - transformations of quantitative inputs: $\log$, $\sqrt{}$ etc
  - basis functions: $x_2 = x_1^2$, $x_3 = x_1^3$
  - numeric encoding of the levels of qualitative inputs
  - interactions between variables $x_3 = x_1 \cdot x_2$

The model is **linear in the parameters** θ.

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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$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta),$$

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:

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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:

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

yielding:

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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 $\epsilon^{(i)}$

- capture unmodeled effects and/or random noise
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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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Maximum Likelihood Estimation ...

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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

Predicting House Prices

	longitude	latitude	median_age	median_income	ocean_proximity	rooms	bedrooms_fraction	people_per_house	price_Dollars
18139	-122.01	37.34	31.0	6.3052	<1H OCEAN	5.292096	0.170779	2.565292	344200.0
202	-122.23	37.78	43.0	1.9338	NEAR BAY	3.242009	0.332394	3.438356	112500.0
9150	-118.52	34.44	26.0	5.3209	<1H OCEAN	5.765432	0.158458	3.203704	185000.0
7519	-118.26	33.91	39.0	2.4375	<1H OCEAN	4.844560	0.224599	3.683938	101900.0
13996	-117.02	34.88	18.0	3.0313	INLAND	5.304239	0.208275	2.912718	80000.0
18665	-121.96	36.99	23.0	2.7375	NEAR OCEAN	4.818318	0.233094	2.136637	238000.0
14303	-117.14	32.72	34.0	2.1199	NEAR OCEAN	3.255784	0.340308	2.584833	160400.0
15726	-122.45	37.78	43.0	4.1319	NEAR BAY	3.694656	0.273416	2.282443	322700.0
7460	-118.19	33.92	36.0	2.0785	<1H OCEAN	4.520000	0.231563	4.896667	139800.0
14633	-117.20	32.79	16.0	5.0958	NEAR OCEAN	5.428198	0.189514	1.947781	300000.0
20382	-118.85	34.14	16.0	8.1064	<1H OCEAN	7.337500	0.132149	2.516071	423400.0
20540	-121.72	38.54	16.0	3.1908	INLAND	4.386792	0.223656	2.179245	194300.0