Splines and Linear and Polynomial Regression

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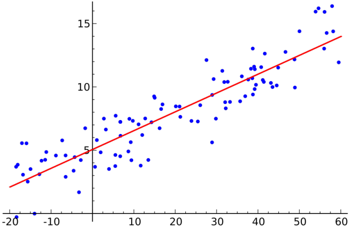
Regression

- Unsupervised learning: data (a subset from a larger distribution) is labeled, and we attempt to generalize to (predict) the larger distribution.
- Regression: predicts a continuous value output (i.e. estimates relationship among variables).

Regression: Examples



- Given data about square footage, age, zip code, and housing demand, predict the selling price of a house.
- Predict the percentage increase or decrease in the price of an equity.

Recall

$$X = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & \dots & x_1^{(m)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} & \dots & x_2^{(m)} \\ \vdots & & & \ddots & \vdots \\ x_n^{(1)} & x_n^{(2)} & x_n^{(3)} & \dots & x_n^{(m)} \end{bmatrix}, y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- Data is stored in matrices and vectors.
- Given n (training) data points and m features (per data point).
- Given labeled data vector y.

Recall

$$X_{test} = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & \dots & x_1^{(m)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} & \dots & x_2^{(m)} \\ \vdots & & & \ddots & \vdots \\ x_k^{(1)} & x_k^{(2)} & x_k^{(3)} & \dots & x_k^{(m)} \end{bmatrix}, \hat{y}_{test} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_k \end{bmatrix}$$

- Given k testing data points and m features (per data point).
- $\hat{y}_{test} = f(X_{test})$ contains *predictions* of the regression algorithm, where $f(\cdot)$ is learned by the algorithm.
- How do we define $f(\cdot)$, and how does the algorithm "learn" it?

Simple Linear Regression

$$y = \alpha + \beta x + \epsilon$$

$$\hat{y} = f(x) = \alpha + \beta x$$

- Goal: predict y from a single feature x.
- Allow α to be some *bias* not explained by x, and β the dependence of y on x.
- ϵ accounts for the "error" not explained by the model, and hence our estimate is $\hat{y}$.

Loss Function

$$\min \ell(f(x), y)$$
$$= \min \ell(\hat{y}, y) = \min \ell(\alpha + \beta x, y)$$

- We want our estimates $\hat{y}$ to be as accurate as possible for our choices of α and β.
- Allow ℓ to be some loss function, which gives a notion of the "distance" between $\hat{y}$ and y.

Least-squares Error

$$\ell(f(x), y) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}\epsilon_i^2$$

- We will minimize the least-squares error, which is common in regression analysis for several reasons.
- Choices of α and β that minimize the loss, over the training data, will be used.

Multiple Linear Regression

$$y = \beta_0 + \beta_1 x^{(1)} + \beta_2 x^{(2)} + \cdots + \beta_m x^{(m)} + \epsilon$$

$$\hat{y} = f(x) = \beta_0 + \beta_1 x^{(1)} + \beta_2 x^{(2)} + \cdots + \beta_m x^{(m)}$$

- Goal: predict y from multiple features $x^{(1)}, \ldots, x^{(m)}$.
- Allow β_0 to be some *bias* not explained by the features, and β_i the dependence of y on feature $x^{(i)}$.
- ϵ accounts for the "error" not explained by the model, and hence our estimate is $\hat{y}$.

Compact Notation

$$y = \beta^T x + \epsilon$$

$$\hat{y} = f(x) = \beta^T x$$

- $\beta = (\beta_0, \beta_1, \ldots, \beta_m)^T$ and $x = (1, x^{(1)}, x^{(2)}, \ldots, x^{(m)})^T$.
- We can further extend this to allow for more data points.

Compact Notation

$$X = \begin{bmatrix} 1 & x_1^{(1)} & x_1^{(2)} & x_1^{(3)} & \dots & x_1^{(m)} \\ 1 & x_2^{(1)} & x_2^{(2)} & x_2^{(3)} & \dots & x_2^{(m)} \\ \vdots & & & & \ddots & \vdots \\ 1 & x_n^{(1)} & x_n^{(2)} & x_n^{(3)} & \dots & x_n^{(m)} \end{bmatrix}, y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$y = X\beta + \epsilon$$

$$\hat{y} = f(X) = X\beta$$

- $\beta = (\beta_0, \beta_1, \dots, \beta_m)^T$ as before.

Multiple Linear Regression

$$\min \ell(f(x), y) = \min \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

- Again, we want our estimates $\hat{y}$ to be as accurate as possible for our choice of β.
- Utilize the least-squares error as the loss function.
- Closed form solution: $\beta = (X^T X)^{-1} X^T y$ (over the training data).

Multiple Polynomial Regression

- y may not necessarily have a linear dependence on x.
- Solution: simply create new "features" $(x^{(i)})^2, (x^{(i)})^3, \ldots$ for each feature $x^{(i)}$ (polynomial regression).
  - Closed form solution: $\beta = (X^T X)^{-1} X^T y$ (remains same).
  - High degree polynomials may lead to overfitting: choose degree via cross-validation (discussed later).

Practicalities

- Closed form solution $\beta = (X^T X)^{-1} X^T y$ may not be possible, as $(X^T X)^{-1}$ may not exist: use *pseudoinverse* instead.
- Still, computing the pseudoinverse (which uses the *singular value decomposition*) takes $O(\min(mn^2, m^2 n))$ running time.
- May need to use *gradient descent* instead, with some learning rate α.
  - Choose some initial value of β.
  - Compute gradient of loss function, and move in direction of steepest (negative) change with step size α (chosen carefully).
  - Update β, and repeat until convergence.

Gradient Descent

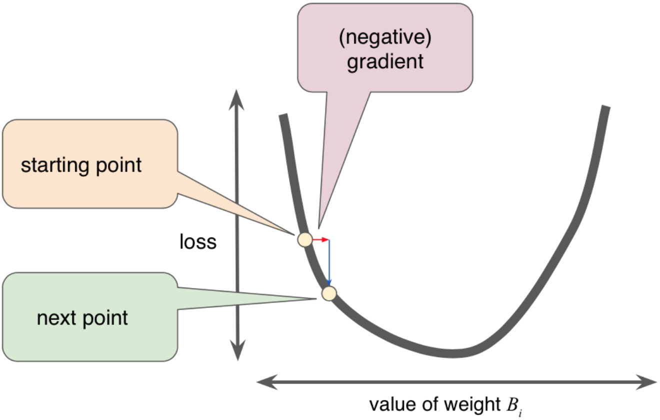


Image source: Google Developers

Feature Scaling

- In general, it is important to scale features such that $\mu^{(j)} = 0$ and $\sigma^{(j)} = 1$.
- Allows for proper convergence (in gradient descent) and assigns equal weight to features (in other applications and algorithms).

Regularization

- Goal is to prevent overfitting.
- General form: $\min \ell(f(x), y) + \lambda R(f)$, where ℓ is the loss function, R is the regularization function, and λ is the regularization coefficient.
  - Ordinary least squares regression: $\lambda = 0$.
  - Choose λ via cross-validation (discussed later).
- Has applications beyond linear and polynomial regression.

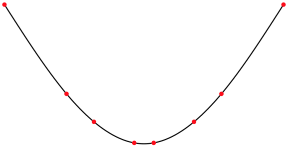
LASSO vs. Ridge Regression

- LASSO regression: $\min \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda|\beta|_1$
  - Used for variable section: certain coefficients β_j can be 0.
  - Does not have a closed form solution.
- Ridge regression: $\min \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda|\beta|_2^2$
  - Closed form solution: $\beta = (X^TX + \lambda I)^{-1}X^Ty$.

Interpolation

- Keeps "training" set of data points fixed and constructs a function around these data points.
- Note that, by construction, we are "overfitting" on the training data.
- Not very useful in machine learning, but applicable to other disciplines, and important nevertheless.
  - Used to estimate values *within* the range of data we have.
  - Regression is used to *extrapolate* to outside data points.

Spline Interpolation



- Create piecewise polynomials between each pair of consecutive points.
- Usually cubic polynomials (“splines”) to make the first and second derivatives continuous.

Image source: Wikipedia

Notebook

- Today's notebook will work through an example of regression, including simple, multiple, and polynomial regression.
- We'll also look at utilizing regularization.