Data-Driven Problem Solving in Mechanical Engineering

Model Development & Linear Regression

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ME 364 - Spring 2022

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The Cooper Union for the Advancement of Science and Art

March, 2022

Learning from Data

The basic premise of learning from data is the use of a set of observations to uncover an underlying process. That is a very broad premise and it is difficult to fit into a single framework.

(a) **Supervised Learning:** Training data contains explicit examples of what the correct output should be for given inputs, i.e. pairs of (input, correct output)

(b) **Unsupervised Learning:** Training data does not contain any output information. Can be viewed as the task of finding patterns and structure in input data.

(c) **Reinforcement Learning:** is concerned with the problem of finding suitable actions to take in a given situation in order to maximize a reward. Here the learning algorithm is not given examples of optimal outputs, but must instead discover them by a process of trial and error. See Gym platform.

Modeling

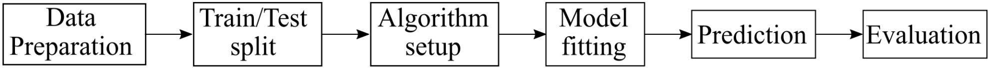
The process of encapsulating information into a tool which can forecast and make predictions.

"*All models are wrong, but some models are useful*" -George Box

To develop a model, we split the data into *training data* and *test data*, typically 80/20.

- **Training Data:** data used to fit your models or the set used for learning
- **Test Data:** data used to evaluate how good your model is.

General procedure



Linear Regression

Given a collection of m points, linear regression seeks to find the line which best approximates or *fits* the points.

There are two main reasons why we want to do this:

- Use it as simplification and compression. We can see the trend and highlight the location and magnitude of outliers
- Use it for value predicting and forecasting.

Linear Regression

Linear Regression seeks the line $y = f(\mathrm{x})$ which minimizes the sum of the squared errors over all points, i.e. the coefficient vector w that minimizes the following squared error function:

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

with $f(\mathrm{x}) = \omega_o + \sum_{i=1}^{n-1} \omega_i x_i$

where, $\hat{y}^{(i)}$ is the estimated value at $\mathrm{x}^{(i)}$ and m is the number of samples.

Linear Regression can be divided into two types:

- <u>Simple Linear Regression</u>: $f(\mathrm{x}) = \omega_o + \omega_1 x_1$
- <u>Multiple Linear Regression</u>: $f(\mathrm{x}) = \omega_o + \omega_1 x_1 + \omega_2 x_2 + \omega_3 x_3 + \ldots + \omega_{n-1} x_{n-1}$

Multiple Linear Regression

Multiple linear regression refers to multiple independent variables to make a prediction.

Generally, we seek to find the best values for ω's in $f(\mathrm{x}) = \omega_o + \omega_1 x_1 + \omega_2 x_2 + \omega_3 x_3 + ...$

$\rightarrow f(\mathrm{x}) = \mathrm{w}^T \mathrm{x}$

$\mathrm{w}^T = [\omega_o, \omega_1, \omega_2, \omega_3, ...]$ and $\mathrm{x} = [1, x_1, x_2, x_3, ...]^T$

These coefficients (weights) can be found using:

- Solving the model parameters analytically using closed-form equations (see here)

- An optimization algorithm such as Gradient Descent (see here)

Evaluation Metrics for Regression

Mean Absolute Error (MAE) $= \frac{1}{m}\sum_{i=1}^{m}\left|y^{(i)} - \hat{y}^{(i)}\right|$

Mean Squared Error (MSE) $= \frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$

Root Mean Squared Error (RMSE) $= \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}$

Relative Absolute Error (RAE) $= \frac{\sum_{i=1}^{m}\left|y^{(i)} - \hat{y}^{(i)}\right|}{\sum_{i=1}^{m}\left|y^{(i)} - \bar{y}\right|}$

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

R-squared (R^2) = 1-RSE

R^2 is not error, but is a popular metric for accuracy of the model. It represents how close the data are to the fit regression line. The higher the R^2, the better the model fits your data. Best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse).