MSc Data Mining

Topic 01 : Module Overview

Part 05 : Optimisation Overview

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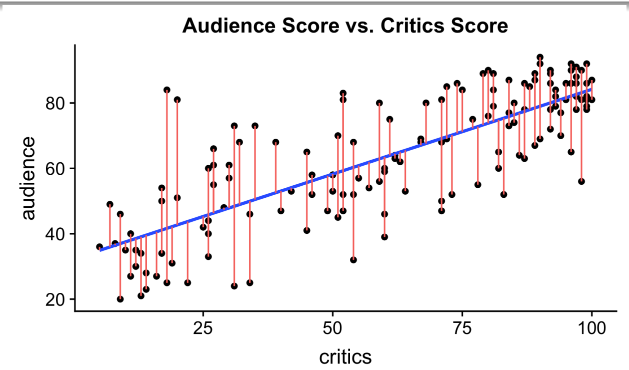
Outline

Machine learning meta-model: The Loss Function

- Machine learning is a large part of this module, but how does it actually work?
- Mathematically, we have a *function*, of one or more variables.
- Most machine learning problems can be formulated as finding values of that function that satisfy certain desirable properties
- Often that function is referred to as a *loss function* $L \equiv L(M(\{D_i\}, \boldsymbol{a}), \{\varepsilon_i\})$, where
  - $\{D_i\}$, with $i = 1, \ldots, m$ represents the *training* data (observations) used by the learner;
  - $\{\varepsilon_i\}$ represents the (unknown) errors in that training data;
  - $M(\{D_i\}, \boldsymbol{a})$ represents the model used to represent the data;
  - $\boldsymbol{a}$ represents one or more variables, that each take a special value when the required property holds
- Generally, the property we are looking for is that the value of the Loss Function should be as small as possible.

Example Loss Function



Here the training data is $\{D_i\} = \{x_i, y_i\}$ where x_i is the i^{th} critics score and y_i is the corresponding audience score. A linear relationship $M : y^* = a_0 + a_1 x$ is assumed and the errors are estimated by the difference between the predicted values (on the line) and the corresponding data values.

Source: towardsdatascience.com

- The loss function is an expression computed from all the error estimates, giving a scalar output (a single number) with the property that the loss function decreases when the overall error decreases.
- So: minimising the loss function has the effect of fitting the line as close to the data as possible, equivalent to searching for the "best" values of a_0 and a_1 above.
- Many machine learning algorithms can be formulated in this way.

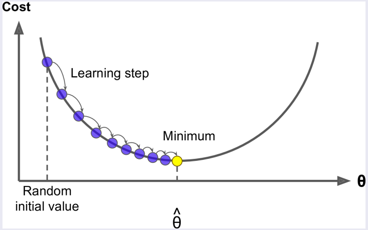
Solving the optimisation problem

1. Use trial and error - unworkable unless there is a small, finite set to check
2. Use function values only, compare them and use heuristics to guide the search
3. Use derivatives and head downhill until you reach a valley (gradient descent)
4. Use higher order derivatives to make more informed decisions

Enhancement: Apply constraints, e.g., when predicting weight, it cannot take negative values!

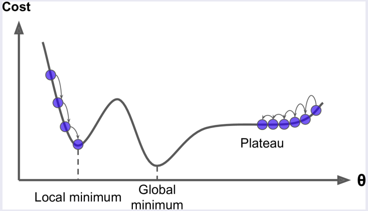
Spotlight on Gradient Descent

Basic Operation



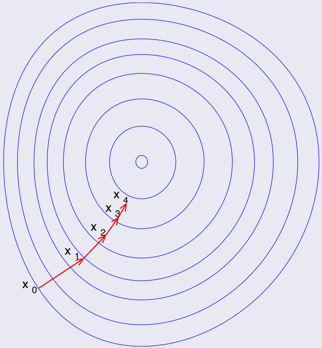
Source: Hands-on machine learning

Challenges



Source: Hands-on machine learning

Two dimensions - Contours



Source: Wikipedia