

MSc - Data Mining

Topic 01 : Module Overview

Part 05 : Optimisation Overview

Dr Bernard Butler and Dr Kieran Murphy

Department of Computing and Mathematics, WIT.
(bbutler@tssg.org and kmurphy@wit.ie)

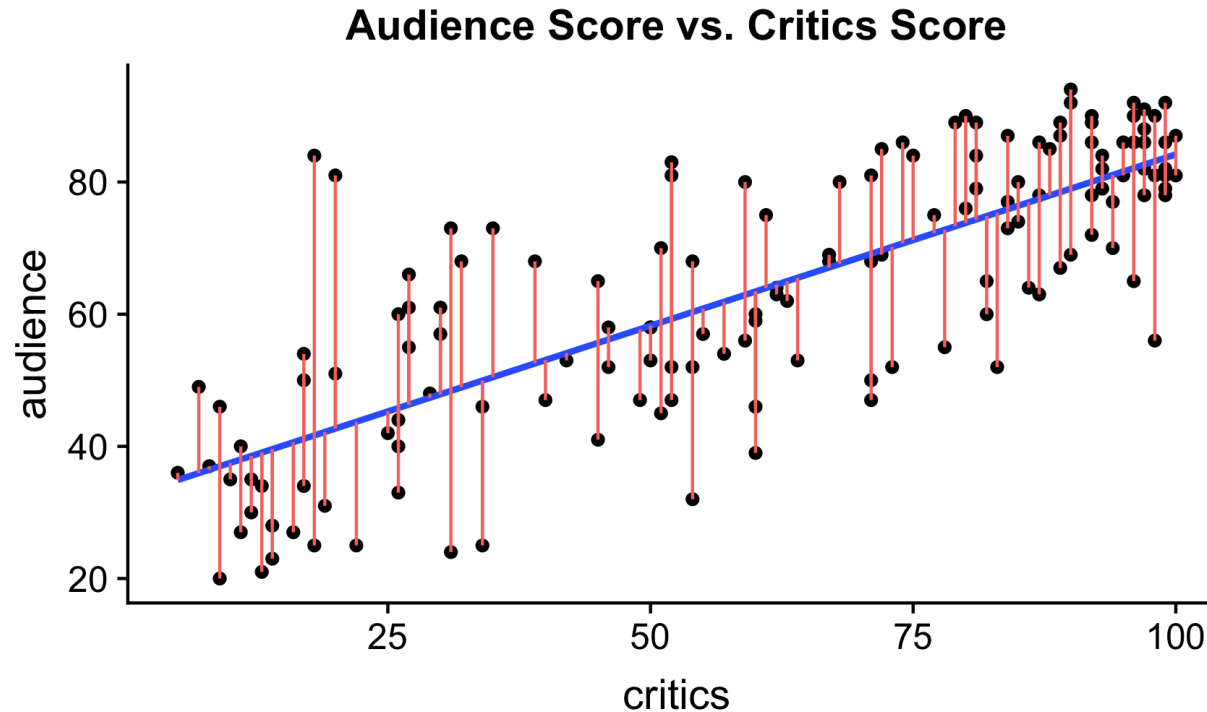
Spring Semester, 2021

Outline

Machine learning meta-model: The Loss Function

- Machine learning is a large part of this module, but how does it 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 properties
- Often that function is referred to as a *loss function* $L \equiv L(M(\{D_i\}, \mathbf{a}), \{\varepsilon_i\})$, where
 - $\{D_i\}$, with $i = 1, \dots, m$ represents the *training* data (observations) used by the learner;
 - $\{\varepsilon_i\}$ represents the (unknown) errors in that training data;
 - $M(\{D_i\}, \mathbf{a})$ represents the model used to represent the data;
 - \mathbf{a} represents one or more variables, that each take a special value when a given 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



Source: towardsdatascience.com

- 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 $M : y^* = a_0 + a_1x$ is assumed and the errors are estimated by the difference between the predicted values (on the line) and the corresponding data values.
- 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 error 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.

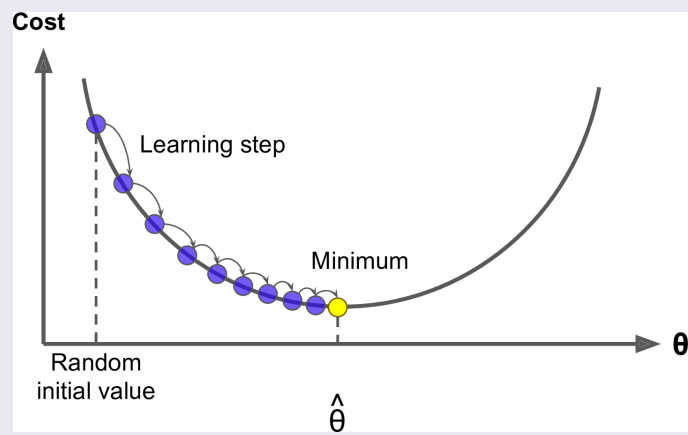
Solving the optimisation problem

- 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!

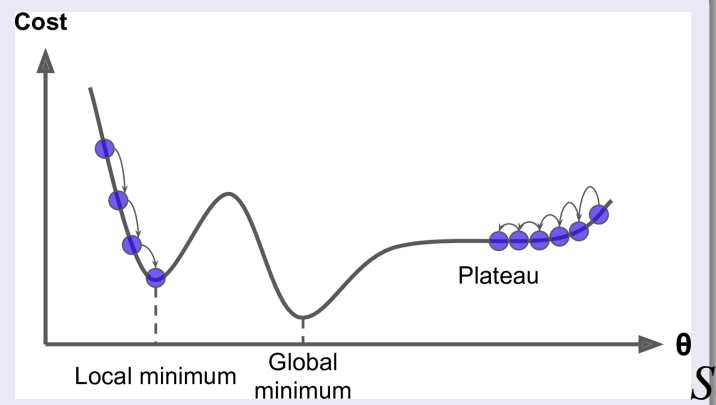
Spotlight on Gradient Descent

Basic Operation



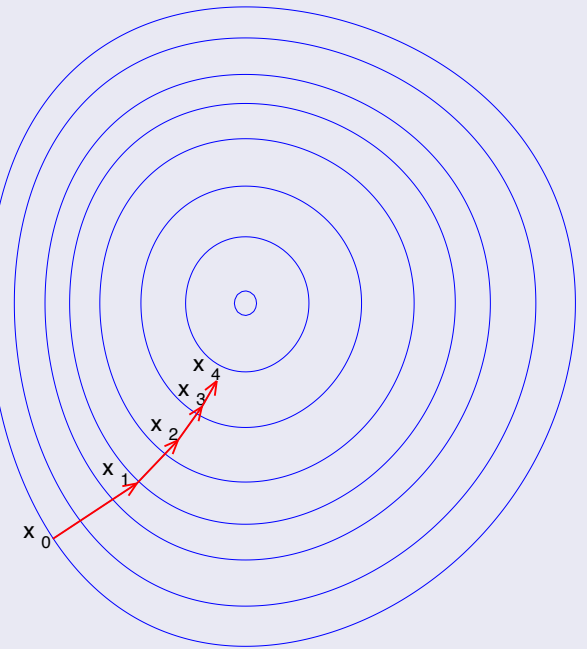
Hands-on machine learning

Challenges



Hands-on machine learning

Two dimensions - Contours



Wikipedia