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

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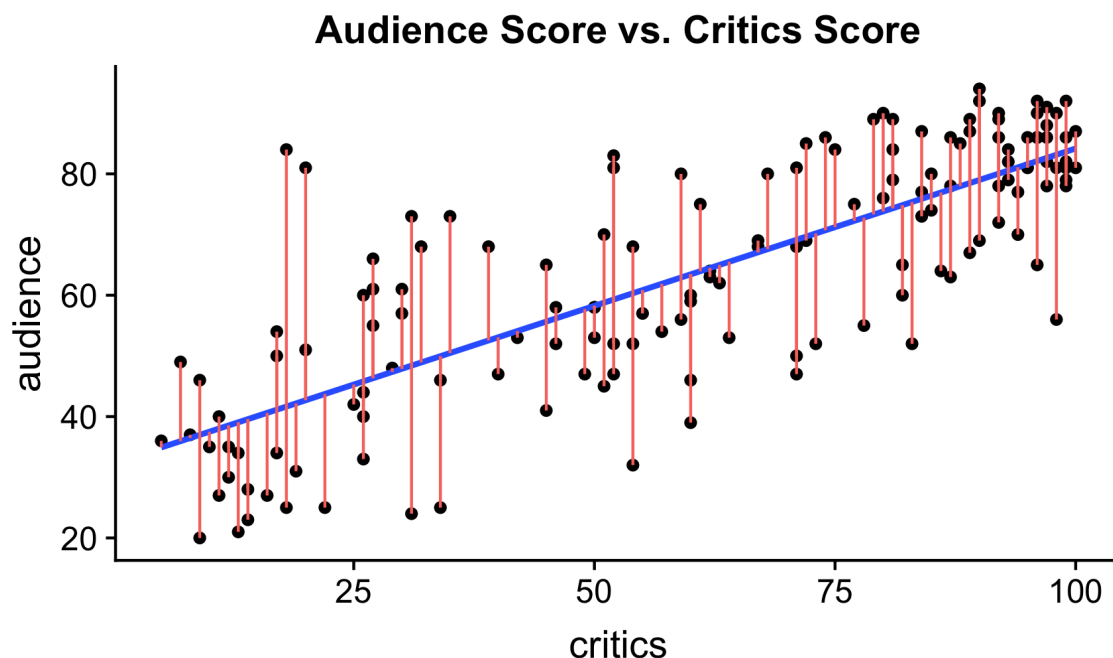
Here the training data is $\{D_i\} = \{x_i, y_i\}$ where x_i is the ith critics score and y_i is the corresponding audience score. A linear relationship $M : y^* = a_0 + a_1 x$ is assumed and the errors are estimated by the difference between the predicted values (on the line) and the corresponding data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

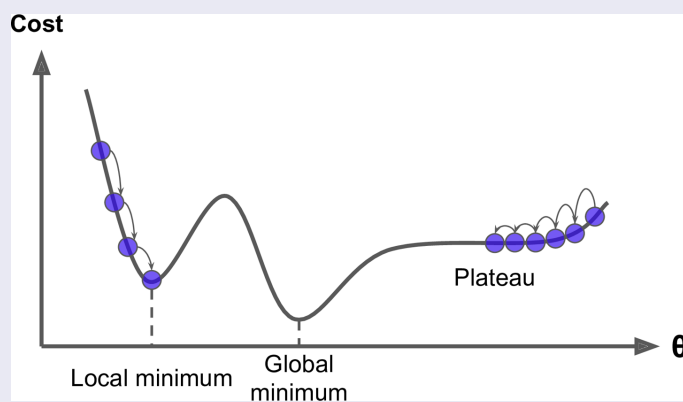*Enhancement*: Apply constraints, e.g., when predicting weight, it cannot take negative values!
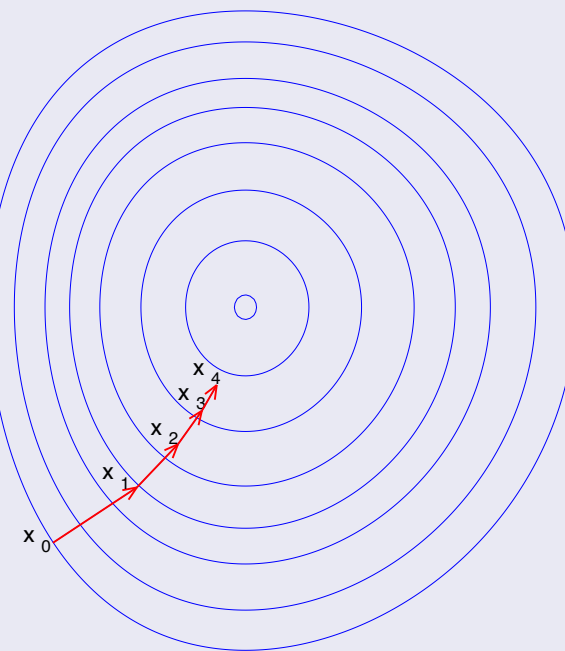
Spotlight on Gradient Descent

Basic Operation

Cost

Learning step

Minimum

Random
initial value

$\hat{\theta}$

θ
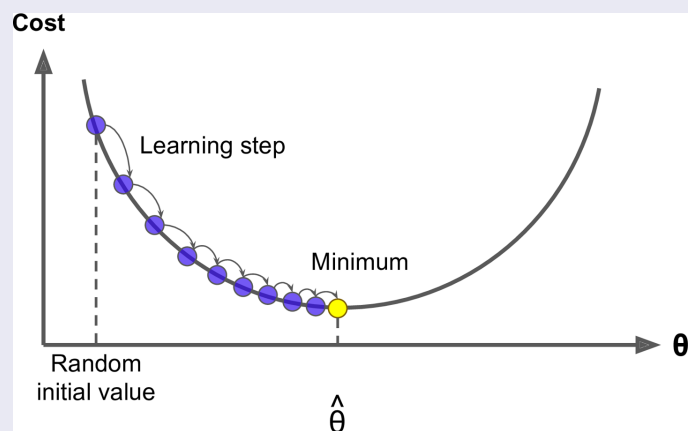
Source: Hands-on machine learning

Challenges

Cost

Plateau

Local minimum

Global minimum

θ

Source: Hands-on machine learning

Two dimensions - Contours

x_4

x_3

x_2

x_1

x_0

Source: Wikipedia