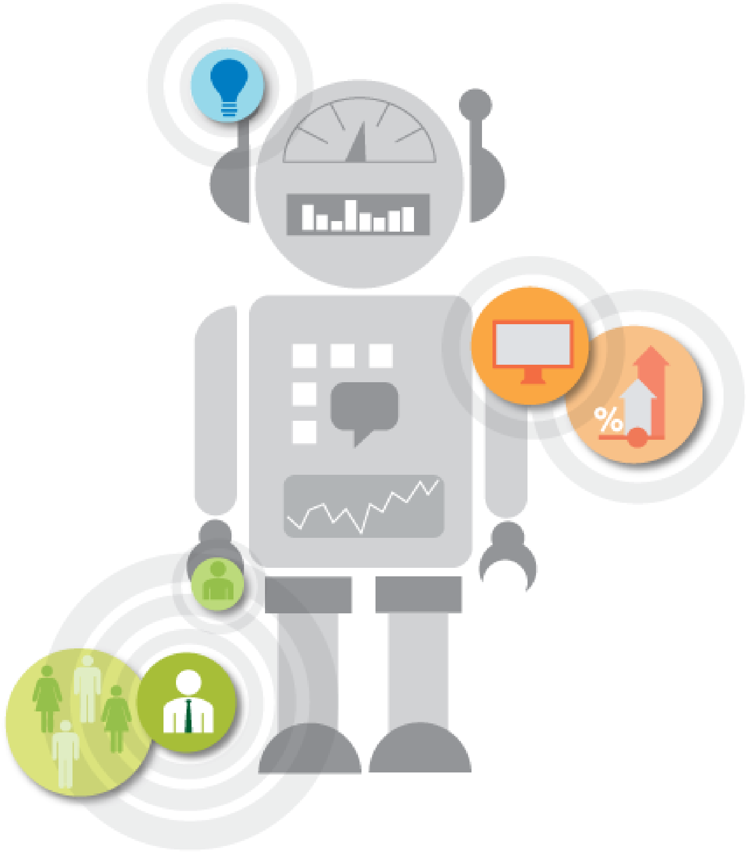
From Neural Networks to parametric modeling

- Cesare Alippi, Juergen Schmidhuber

What is machine learning

«Yes, it is a hot topic»

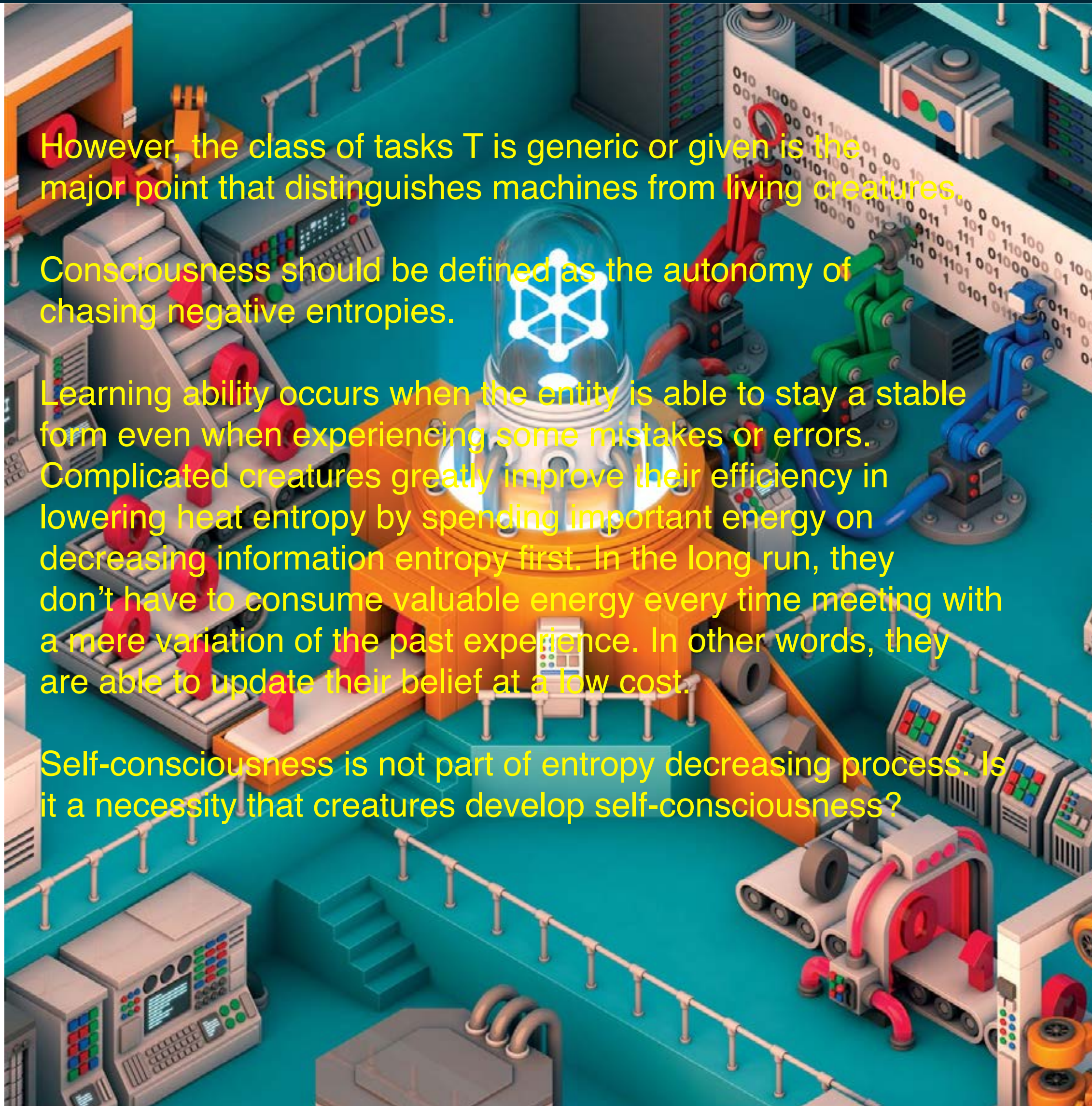


What does it mean “to learn”?

- Hastie, Tibshirani, Friedman:
  - “Vast amounts of data are being generated in many fields, and the statisticians’s job is to make sense of it all: to extract important patterns and trends, and to understand “what the data says”. We call this *learning from data.*”
- Mitchell:
  - “The field of machine learning is concerned with the question of how to construct computer programs that automatically improve with experience.”
- Alippi:
  - “The ultimate goal of machine learning is to provide the simplest consistent method able to explain past and future data without requesting an explicitly programmed algorithm.”

Mitchell formalization of the learning framework

A computer program is said to **learn** from **experience *E*** with respect to some class of **tasks *T*** and **performance measure *P***, if its performance at tasks in *T*, as measured by *P*, improves with experience *E*.



However, the class of tasks T is generic or given is the major point that distinguishes machines from living creatures.

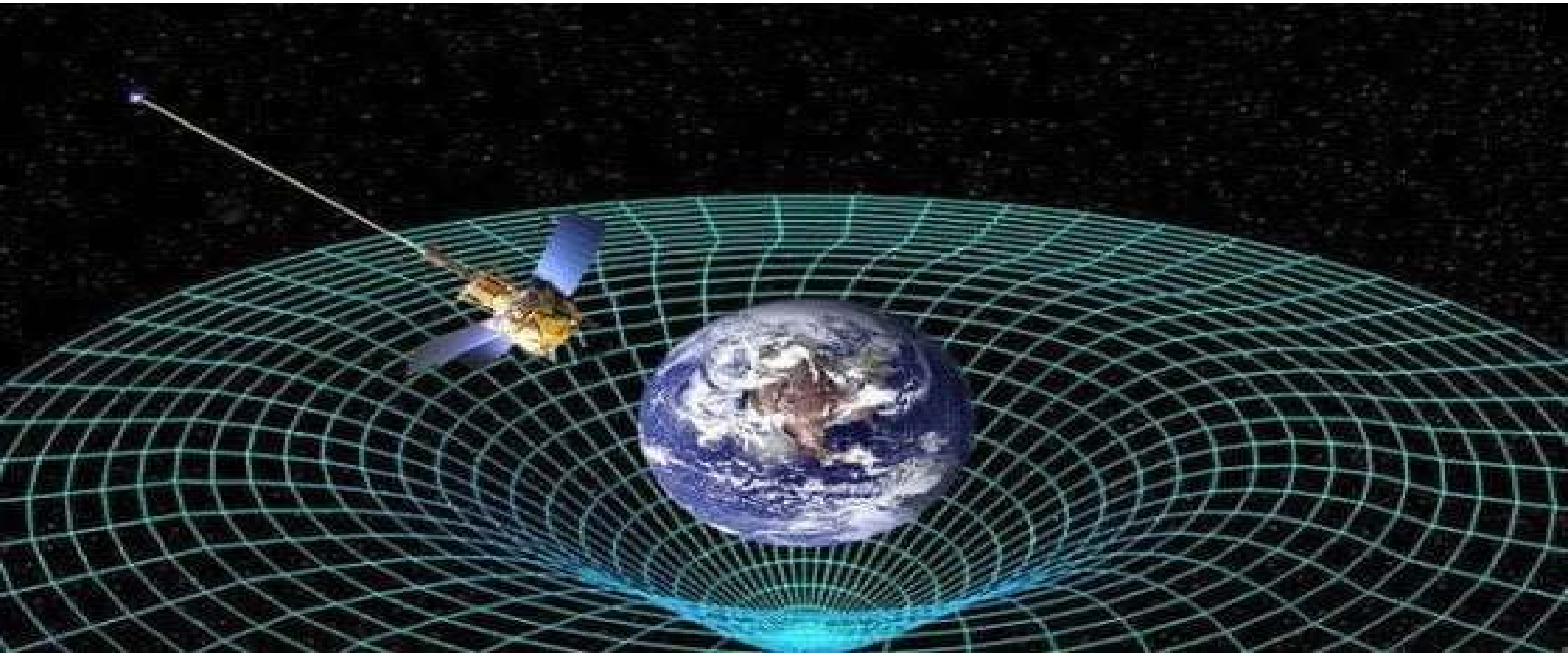
Consciousness should be defined as the autonomy of chasing negative entropies.

Learning ability occurs when the entity is able to stay a stable form even when experiencing some mistakes or errors. Complicated creatures greatly improve their efficiency in lowering heat entropy by spending important energy on decreasing information entropy first. In the long run, they don’t have to consume valuable energy every time meeting with a mere variation of the past experience. In other words, they are able to update their belief at a low cost.

Self-consciousness is not part of entropy decreasing process. Is it a necessity that creatures develop self-consciousness?

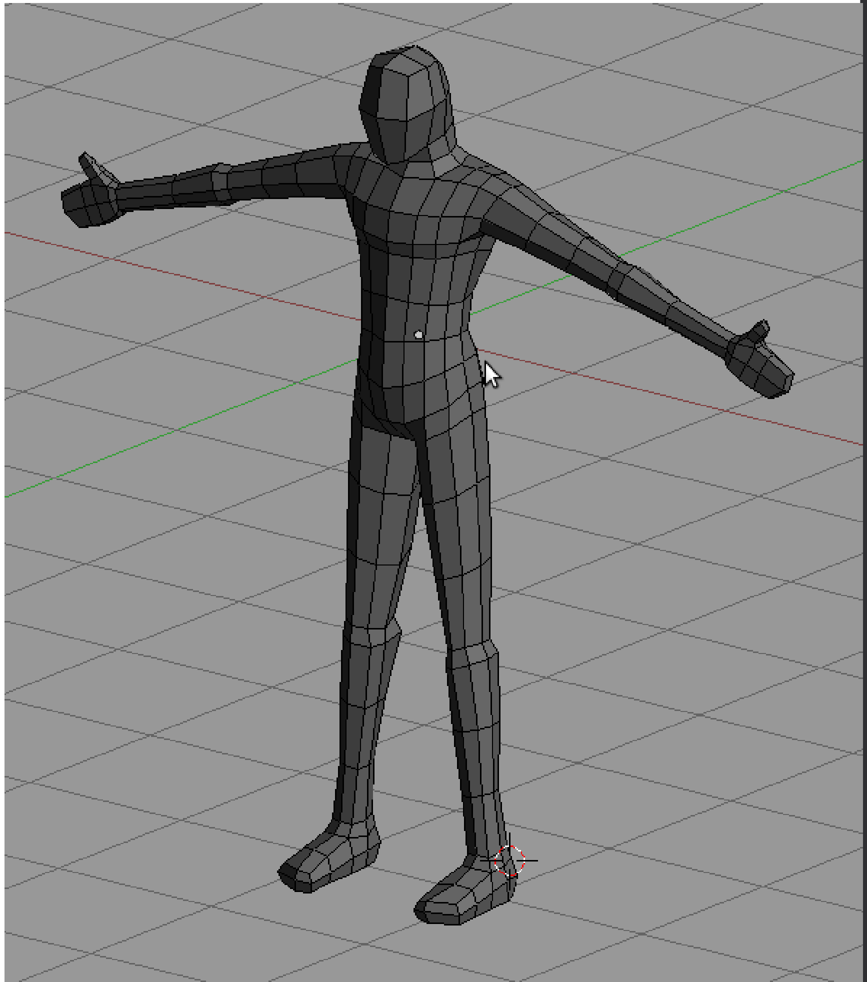
The regression problem

- **Linear regression**
- **Nonlinear regression**
- **Feed-forward neural networks**



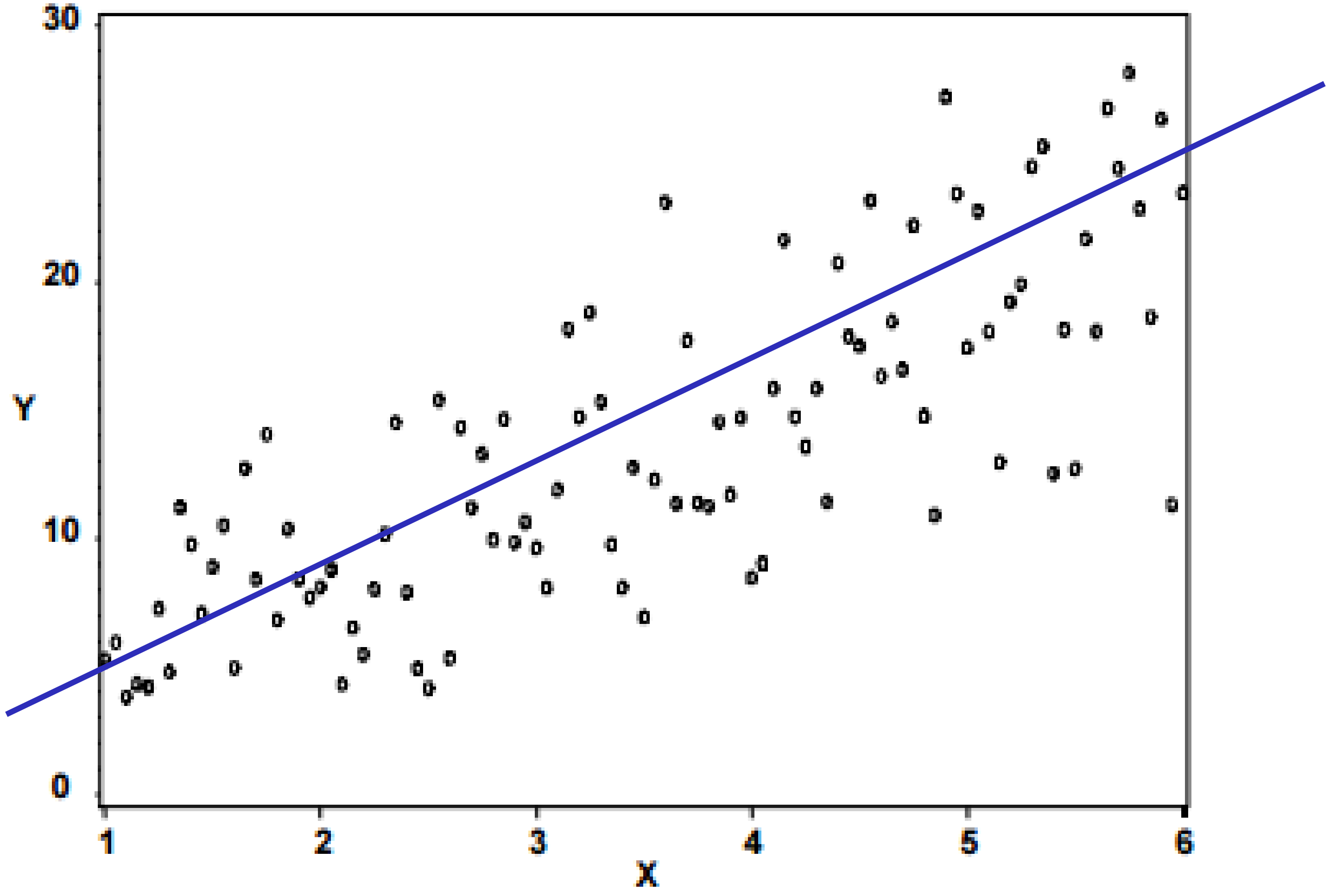
Linear regression

«Keep the model simple»



Some examples

- linear regression: least mean square algorithm



Multiple Linear regression (as they taught you)

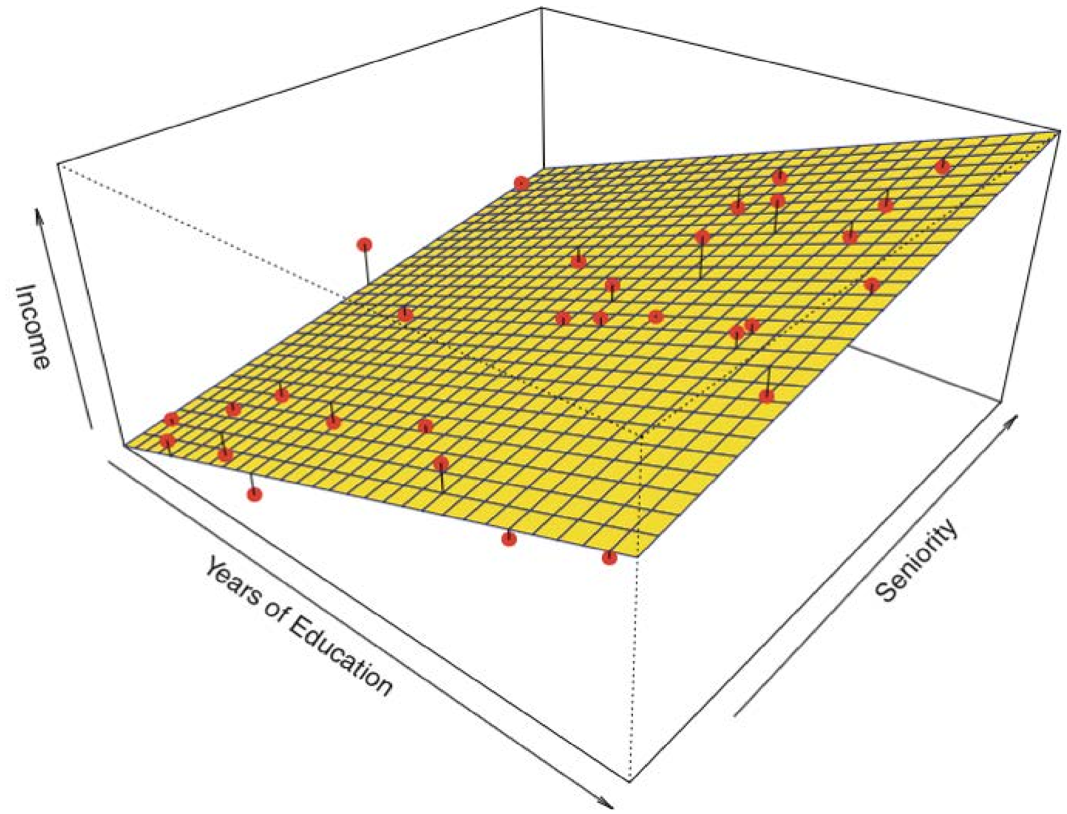
A set of n data couples (training set)

$$\{(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)\}$$

is given

$$x \in \mathbb{R}^d, y \in \mathbb{R}$$

x is column vector



Multiple linear regression

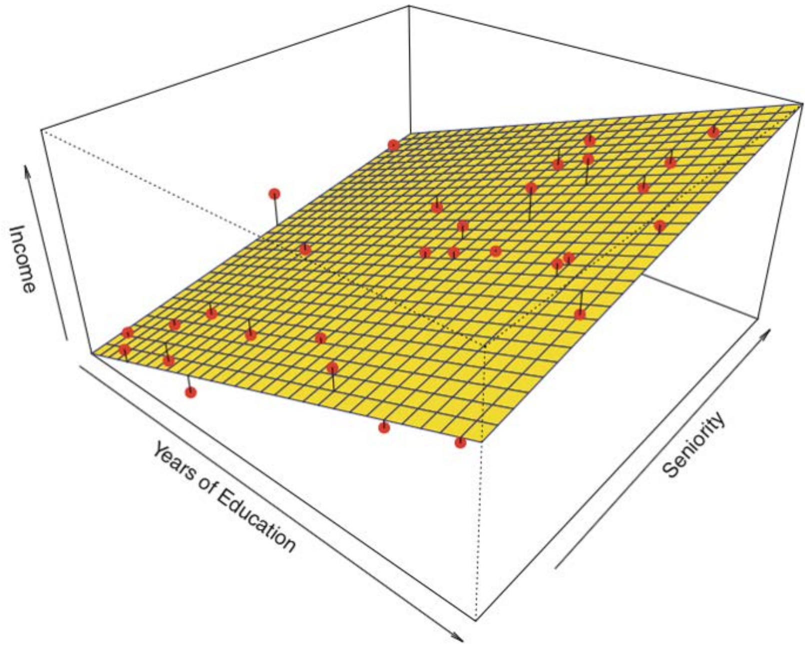
Assume that the unknown function that generates the data is linear and that there is a gaussian uncertainty affecting measurements in an additive way

$$y(x) = \theta_1^o + \theta_2^o x_2 + \cdots \theta_d^o x_d + \eta$$

Canonical form for system model

$$y(x) = x^T \theta^o + \eta$$

$$\theta^o \in \mathbb{R}^d \qquad \eta = N(0, \sigma_\eta^2)$$



Optimal parameters, grouped in a column vector, are unknown, as it is the variance of noise

Multiple linear regression

We know that the unknown system model is linear. Which family of models should we consider to best fit the available data?

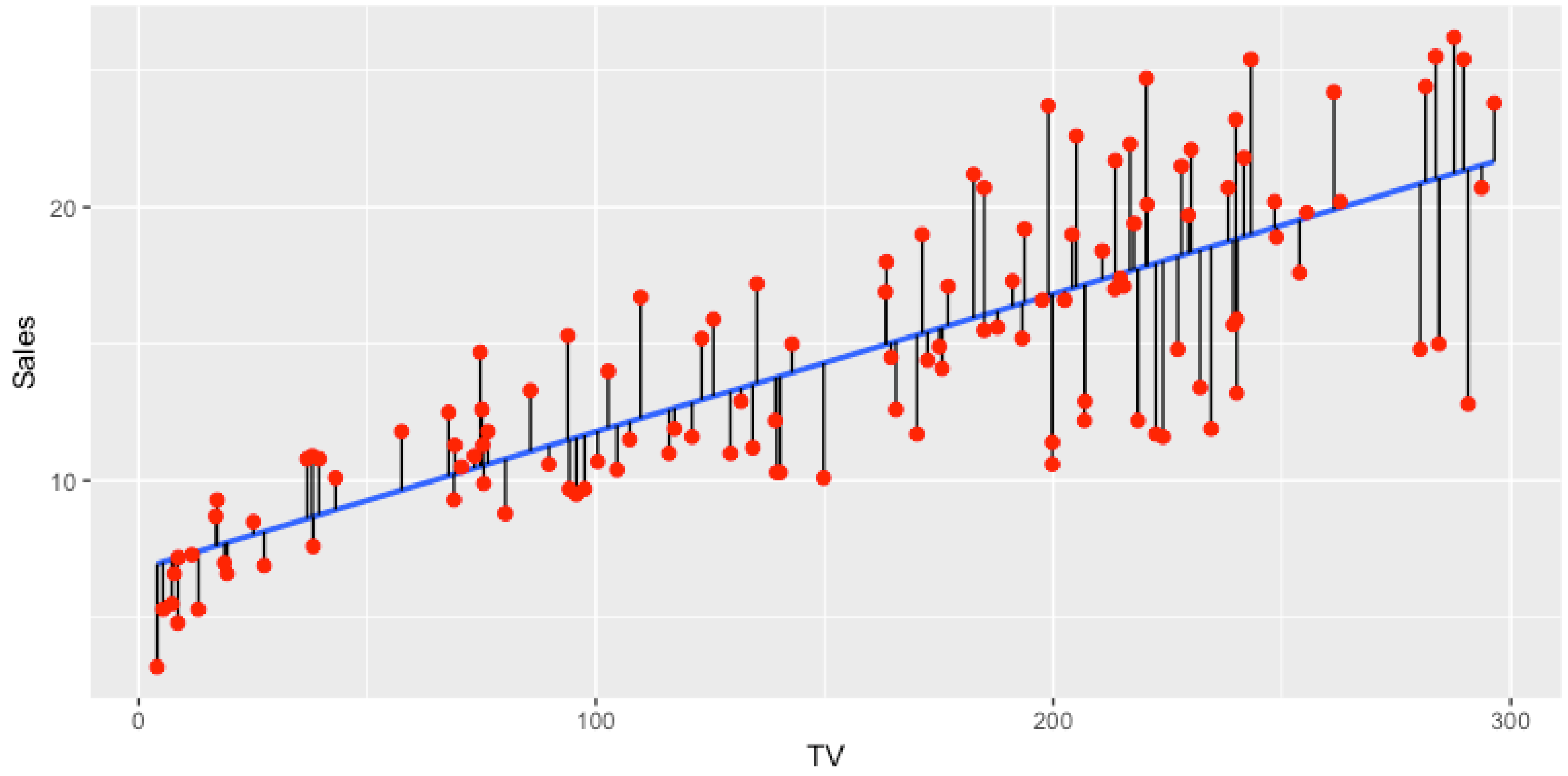
$$\hat{y}(x) = f(\theta, x) = x^T \theta$$

How to determine the best estimated parameter $\hat{\theta}$ so that we generate the model

$$f(\hat{\theta}, x) = x^T \hat{\theta}$$

approximating unknow function $x^T \theta^o$?

Multiple linear regression



Idea: select the linear function that minimizes the average distance between given points and the linear function: we obtain the **Least Mean Square –LMS-** procedure

Multiple linear regression

Performance function

$$V_n(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y(x_i) - f(\theta, x_i)\right)^2$$

The parameter vector to be chosen is

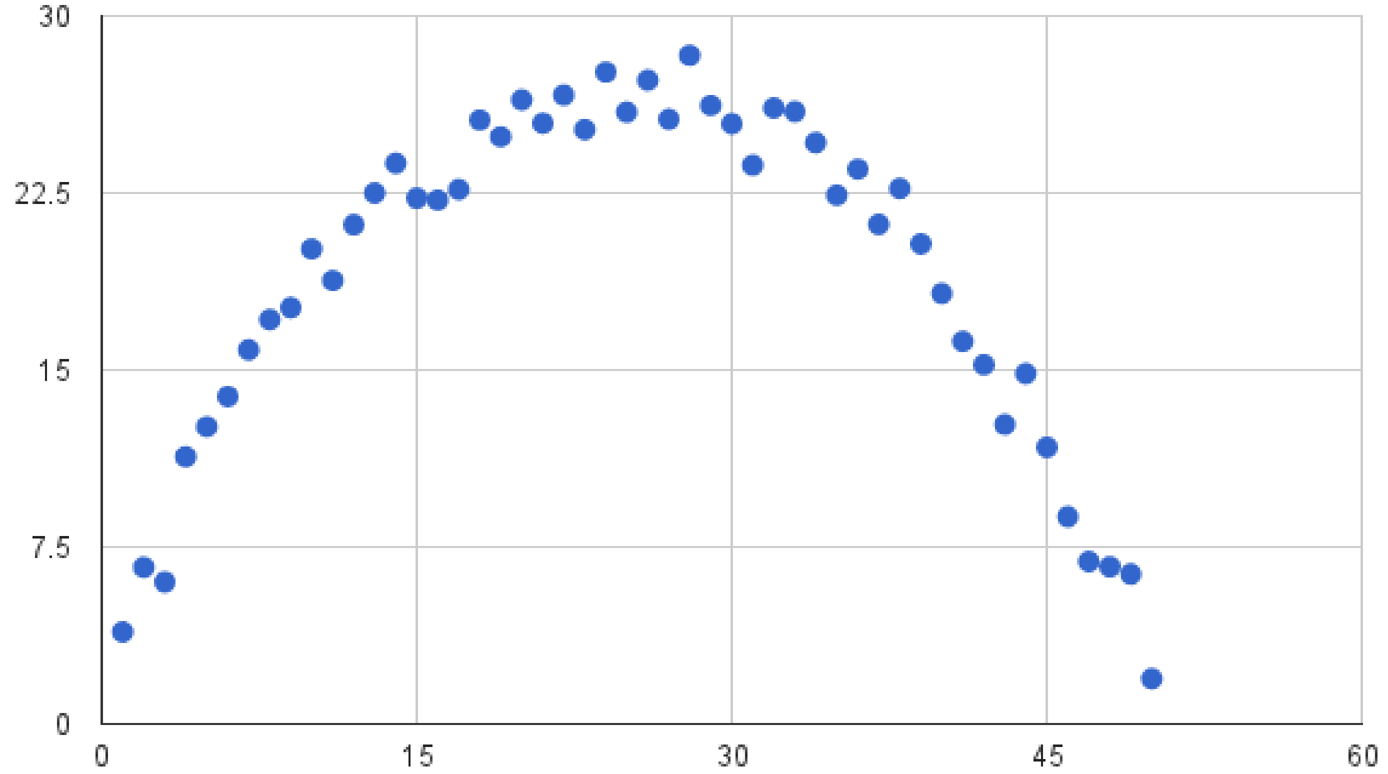
$$\hat{\theta} = \arg\min_{\theta \in \Theta} V_n(\theta)$$

Linearity must be intended according to the parameters!!!

- Linear regression

$$y = a + bz + cz^2 + dz^3$$

$$\theta = [a, b, c, d]; x = [1, z, z^2, z^3]$$



Multiple linear regression: how to estimate parameters

By grouping data as

$$Y = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \mathbf{y}_3 \\ \cdots \\ \mathbf{y}_n \end{bmatrix} \qquad X = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \mathbf{x}_3^T \\ \cdots \\ \mathbf{x}_n^T \end{bmatrix}$$

We can rewrite the loss function in a canonical form

$$V_n^*(\theta) = \sum_{i=1}^{n} \left(y(x_i) - x_i^T \theta\right)^2 = (Y - X\theta)^T (Y - X\theta)$$

Multiple linear regression

Stationary points are those for which

$$\frac{\partial V_n^*(\theta)}{\partial \theta} = -2X^T Y + 2X^T X\theta = 0$$

Therefore, the parameter vector minimizing the performance function is

$$\hat{\theta} = (X^T X)^{-1} X^T Y$$

and the best approximating model is

$$f(\hat{\theta}, x) = x^T \hat{\theta}$$

Multiple linear regression

- A computer program is said to **learn** from experience *E* with respect to some class of tasks *T* and performance measure *P*, if its performance at tasks in *T*, as measured by *P*, improves with experience *E*.
- Let's list the different actors

  - Task *T*: regression
  - Experience *E*: $\{(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)\}$
  - Performance measure *P*: Mean square error
  - Performance at task: $V_n(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y(x_i) - f(\theta, x_i))^2$

Performance at task: mmh….

- In a typical classroom the teacher provides solution examples/instances related to a concept, e.g., what a cat is.

- However, at exam time, the problems the teacher provides you to test your understanding are not identical to the ones you saw during the course. E.g.,

Performance at target: mmh….

- Instead, we propose different instances

- Why?
- Performance at task assessed according to

$$V_n(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y(x_i) - f(\theta, x_i)\right)^2$$

is biased to the training set

How to measure performance at task?

- Much more to come later in the course
- For now, based on our exam experience, we consider another data set, called test set,

$$\{(\bar{x}_1, \bar{y}_1), (\bar{x}_2, \bar{y}_2), \cdots, (\bar{x}_l, \bar{y}_l)\}$$

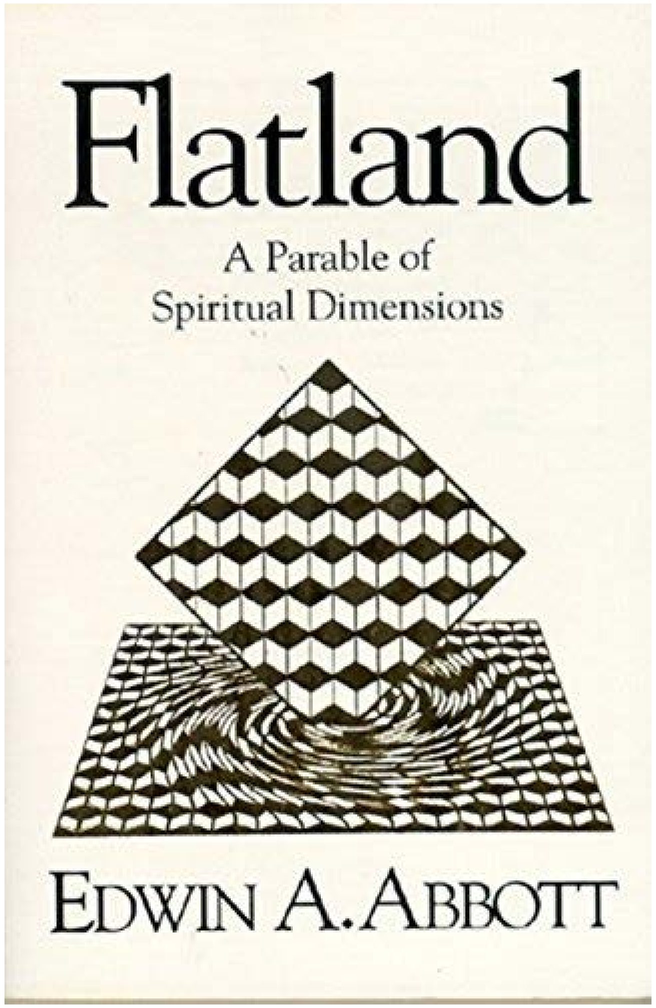
- and evaluate performance on it

$$V_l(\hat{\theta}) = \frac{1}{l} \sum_{i=1}^{l} \left(\bar{y}_i - \bar{x}^T \hat{\theta}\right)^2$$

The procedure is named cross-validation

Nonlinear regression

«I like straight lines but sometimes curves are appreciable»



Non-linear regression: formalization

The *stationary* process generating the data

$$y = g(x) + \eta$$

provides, given input x_i output

$$y_i = g(x_i) + \eta_i$$

Collect a set of couples (training set)

$$Z_N = \{(x_1, y_1), \ldots, (x_N, y_N)\}$$

The goal of supervised learning is to design the simplest approximating model able to explain past Z_N data and future instances provided by the data generating process.

Non-linear regression: formalization

Model unknown function $g(x)$

with parameterized family of models $f(\theta, x)$

Consider loss function

$$L(y(x), f(\theta, x))$$

e.g.,

$$L(y(x), f(\theta, x)) = (y(x) - f(\theta, x))^2$$

The traditional statistical approach

The structural risk

$$\bar{V}(\theta) = \int L(y, f(\theta, x))\, p_{x,y} dxy$$

$$\theta^o = \arg\min_{\theta \in \Theta} \bar{V}(\theta)$$

The empirical risk

$$V_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(\theta, x_i))$$

$$\hat{\theta} = \arg\min_{\theta \in \Theta} V_N(\theta)$$

Non-linear regression: formalization

Determine the parameter estimate through a minimization problem

$$\hat{\theta} = \arg\min_{\theta \in \Theta} V_N(\theta)$$

carried out by a learning procedure

$$\theta_{i+1} = \theta_i - \varepsilon_L \frac{\partial V_N(\theta)}{\partial \theta}\Big|_{\theta_i}$$

and get model $f(\hat{\theta}, x)$

characterized by performance $\bar{V}(\hat{\theta})$

The classification case

In the classification case, by considering the empirical risk as the ratio of correct classification on the training set and defined d_{VC} as the Vapnik Chervonenkis dimension, we have

$$\Pr\left(\bar{V}(\hat{\theta}) \leq V_N(\hat{\theta}) + \sqrt{\frac{1}{N}\left[d_{VC}\left(log(\frac{2N}{d_{VC}})+1\right) - log(\frac{\delta}{4})\right]}\right) \geq 1-\delta$$

The above holds when $d_{VC} << N$

d_{VC} measures the expressive power of a classification model family

Uniform Convergence of Empirical Mean (UCEM) property

The Empirical mean converges to its expectation uniformely as N goes to infinity and for each element of an arbitrarily selected finite sequence of parameter estimates (finite number of models). From the Hoeffding inequality we have

$$\Pr\left(\sup_{L\in A}|V_N(L(\theta))-E_x[L(\theta,x)]|>\varepsilon\right)\leq 2me^{-2N\varepsilon^2}$$

$$A=\{L(\hat{\theta}_1,x),\cdots,L(\hat{\theta}_m,x)\}$$

In other words, the right terms goes to zero as N tends to infinity

The traditional statistical approach

The UCEM property can also hold for a family of function with infinite models

$$A = \{L(\theta, x), \theta \in \Theta\}$$

provided that the Pollard dimension of family A is finite (the dimension extends the VC one to the real case).

For deep learning (feedforward networks) the VC-dim is O(m log m)

Comments

The risk associated with the model (generalization ability, performance at task) can be decomposed in three terms

$$\bar{V}\left(\hat{\theta}\right) = \left(\bar{V}\left(\hat{\theta}\right) - \bar{V}\left(\theta^{o}\right)\right) + \left(\bar{V}\left(\theta^{o}\right) - V_{I}\right) + V_{I}$$

Comments

The inherent risk

$$V_I$$

depends only on the structure of the learning problem. This term can be improved only by improving the problem itself (e.g., by reducing the instrumentation noise)

Comments

The approximation risk

$$\bar{V}(\theta^o) - V_I$$

depends only on how close the approximating model family is to the process generating the data. As such, a more appropriate model family reduces the risk

Comments

The estimation risk

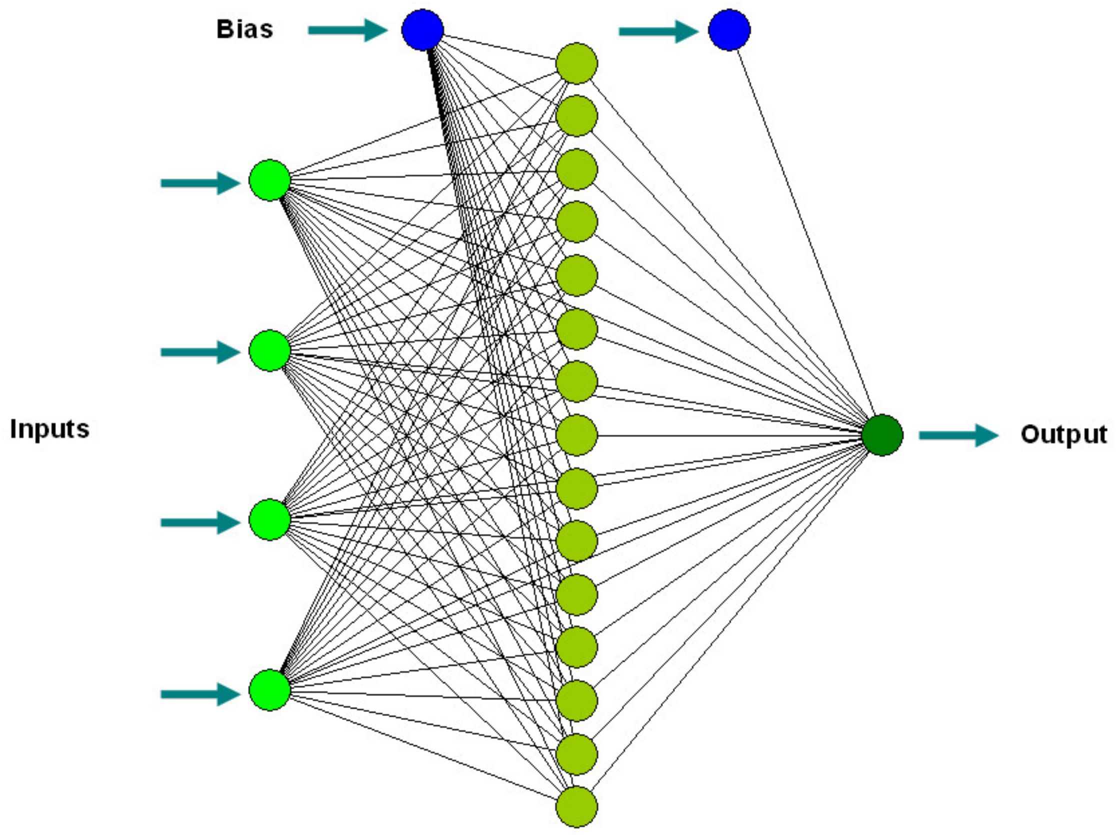
$$\bar{V}(\hat{\theta}) - \bar{V}(\theta^o)$$

depends on the effectiveness of the learning procedure. As such, a more effective learning algorithm reduces the risk

All consistent learning procedures are equally effective

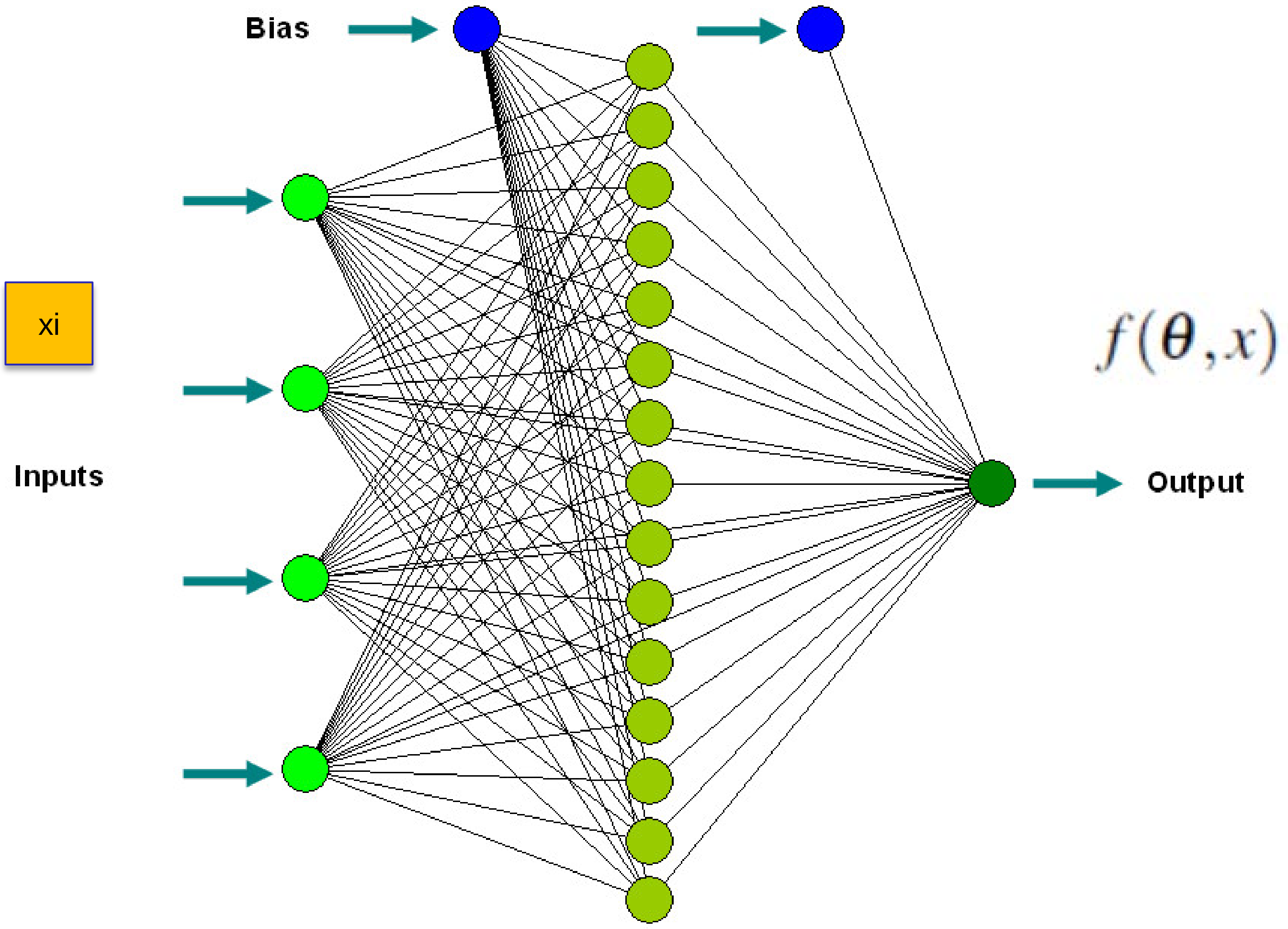
Feed-forward neural networks

«An interesting computational paradigm»



Feedforward Neural Networks

Not rarely $f(\theta, x)$ is chosen as

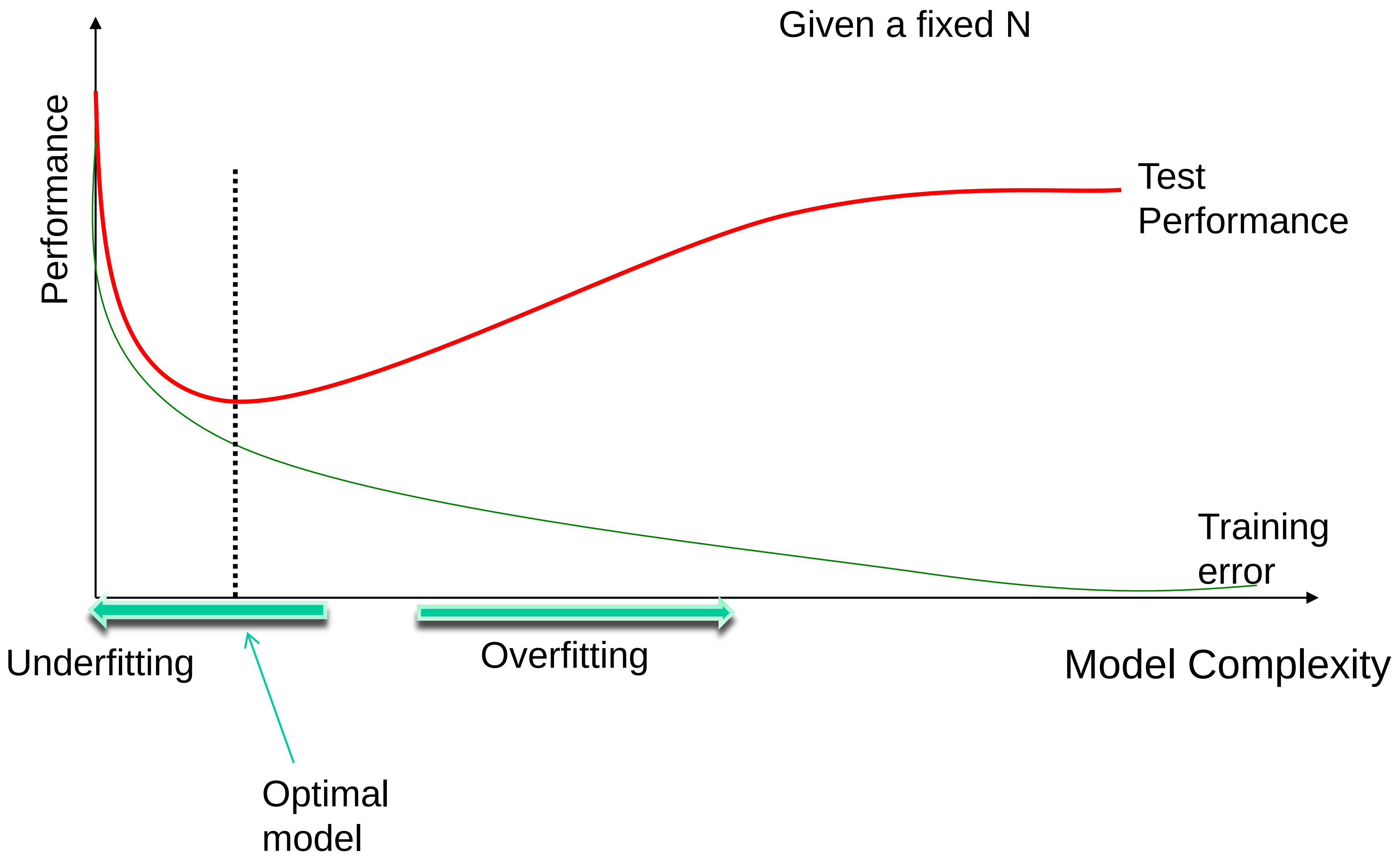


Universal approximation theorem

A feedforward network with a single hidden layer containing a finite number of neurons and a linear output neuron approximates any continuous function defined on compact subsets

K. Hornik, "Approximation Capabilities of Multilayer Feedforward Networks", *Neural Networks*, No.4 Vol. 2, 251–257, 1991

Approximation performance vs. Model complexity



Controlling the model complexity

- Trial & error
- Early stopping
- Dropout
- Tikhonov regularization