Optimal Design : Surrogate Models

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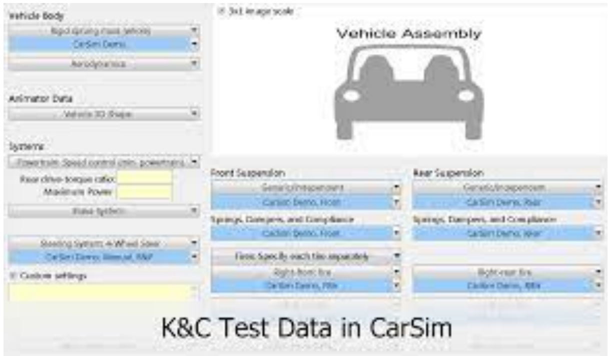
A good model should represent reality in the simplest meaningful manner.

A surrogate model is a simpler analysis model extracted from the more sophisticated ones using a variety of data-handling techniques.

Model forms

- Analytical models in mathematical form : based on fundamental science with proper assumptions. Generally easier to calculate but with limited applications.

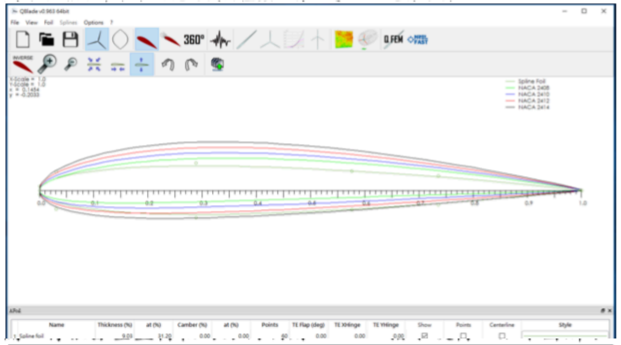
- Computer simulations : most commonly used in engineering practice. These codes are wrapped within a graphical user interface (GUI). One must understand the limitations and assumptions behind these computer logics.

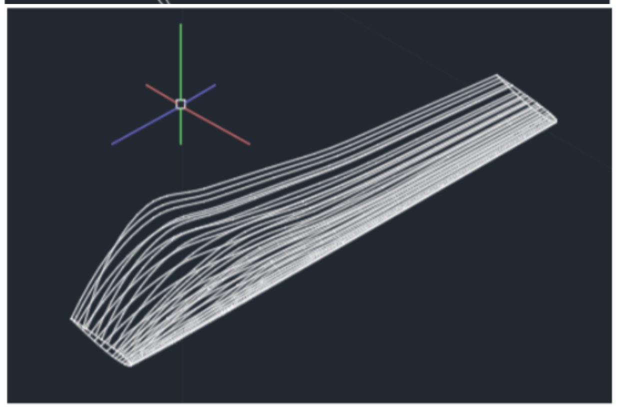


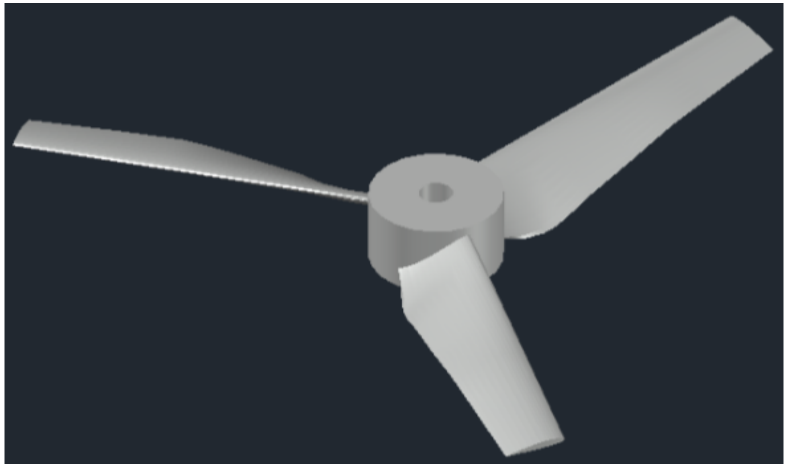
- Experiment data fitting : also one of the most common practice in engineering. Although in math forms, it does not provide basic science and usually limited to interpolations.

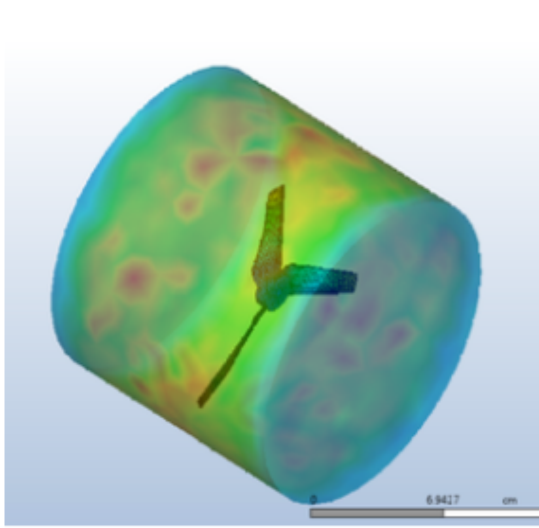
Wind Tunnel with Fluid Dynamics Modeling

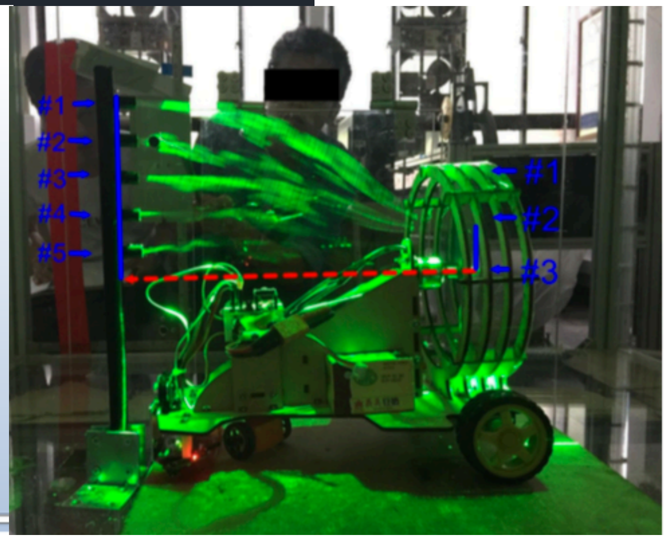
credit to 陳亮宇、沈育儒、柯曼德、楊敦仁、徐征宇



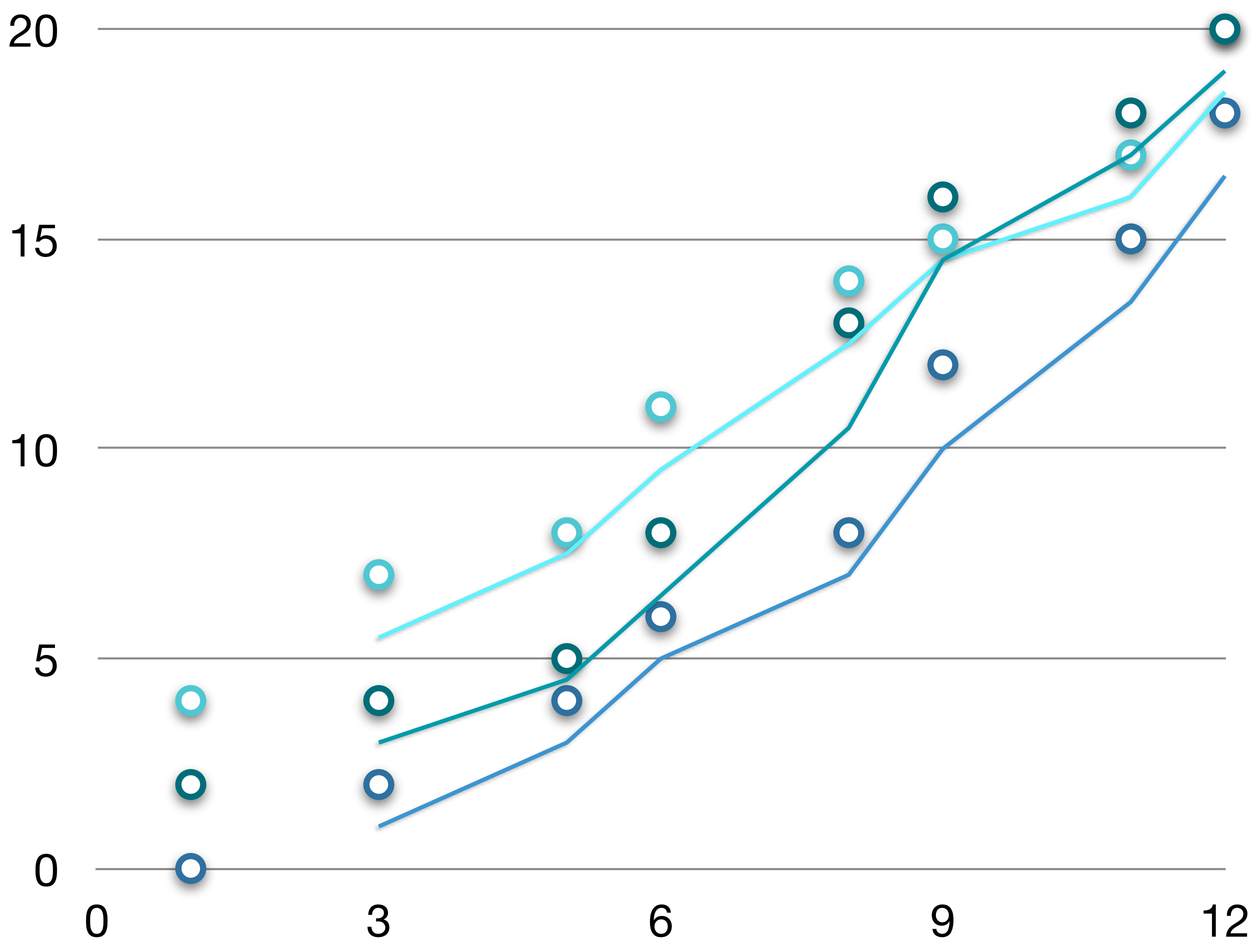




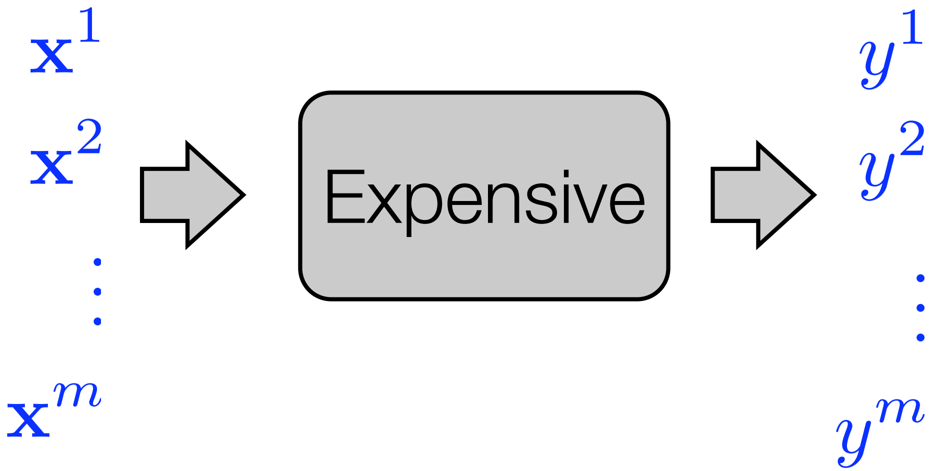




Curve fitting with various models



Linear and Quadratic Fits and Least Squares



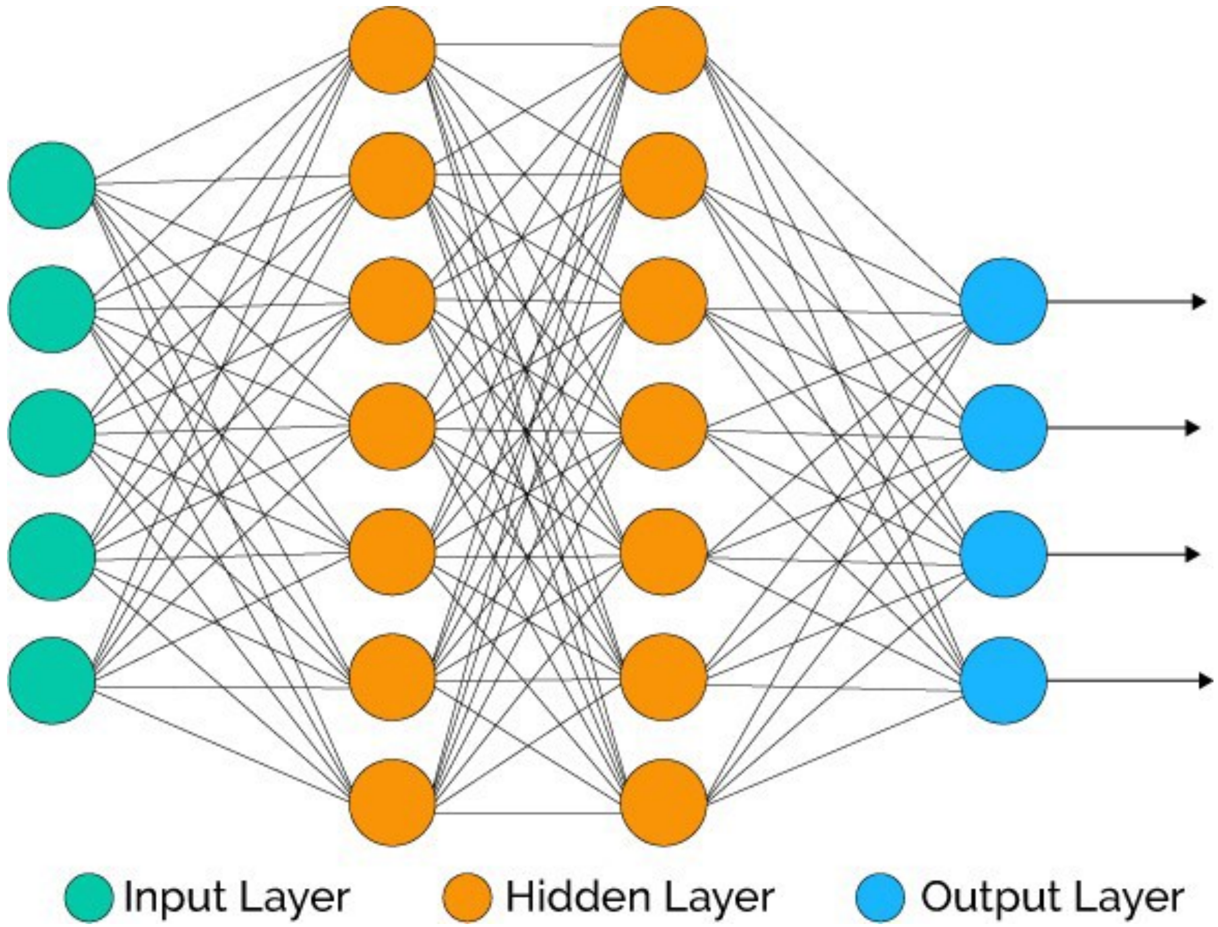
- Let $\hat{y}$ be the approximation function.

- The least square best linear fit is the function such that

$$\min_{a_0, \mathbf{a}_1} \left(\sum_{i=1}^{m} \hat{y}_i - y_i \right)^2$$

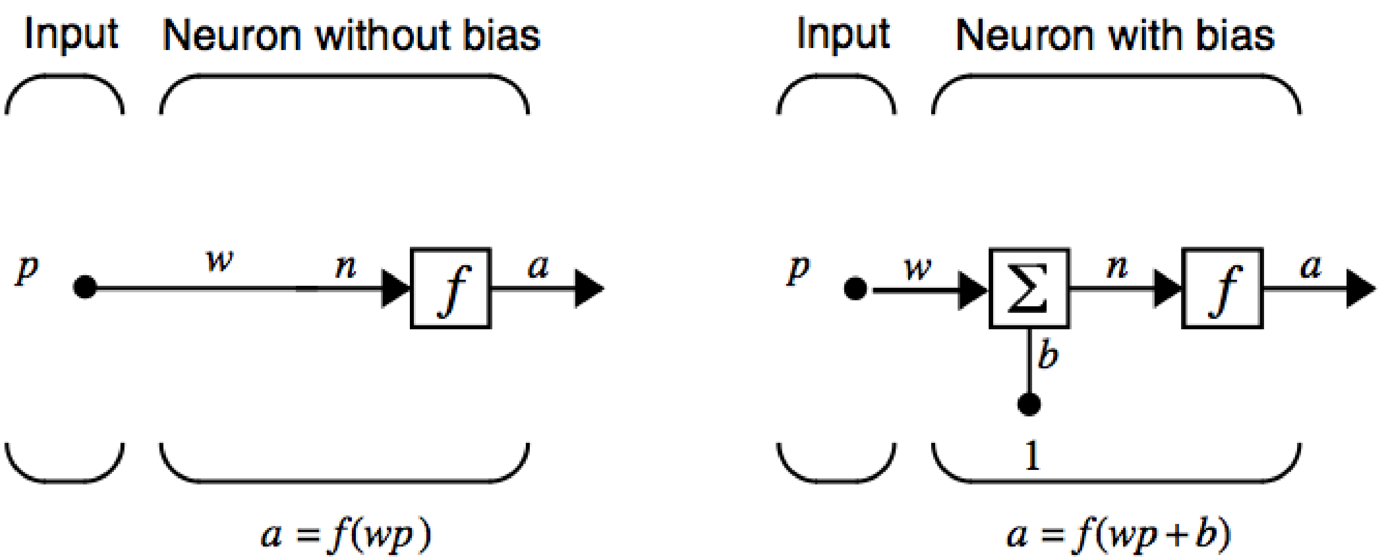
$$\text{subject to} \quad \hat{y}_i = \mathbf{a}_1^T \mathbf{x}_i + a_0$$

Neural Network Modeling

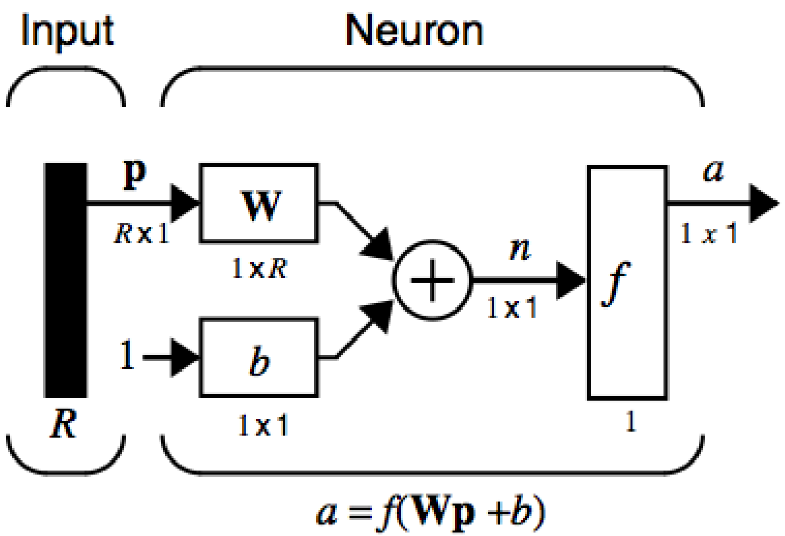


Basic Neuron

- Basic neuron without bias
- Basic neuron with bias



General Neural Network Model



Where...

R = number of elements in input vector

weights

$$\hat{y}(\mathbf{x}) = \varphi\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

activation function

Kriging Modeling

The Origins of Kriging[1]

Noel Cressie[2]

In this article, kriging is equated with spatial optimal linear prediction, where the unknown random-process mean is estimated with the best linear unbiased estimator. This allows early appearances of (spatial) prediction techniques to be assessed in terms of how close they came to kriging.

KEY WORDS: blue, blup, covariance function, geodesy, homogeneous structure function, meteorology, mining, optimum interpolation, spatial blup, statistics, variogram.

Kriging Model

is in the form

$$\hat{y}(\mathbf{x}) = f(\mathbf{x}) + z(\mathbf{x})$$

where

$$\mathbf{R}(\mathbf{x}^i, \mathbf{x}^j) = e^{-\sum_{k=1}^{n} \theta_k |x_k^i - x_k^j|^2}$$

$$f(\mathbf{x}) = \beta = (\mathbf{I}^T \mathbf{R}^{-1} \mathbf{I})^{-1} \mathbf{I}^T \mathbf{R}^{-1} \mathbf{y}$$

with

$$\theta = \mathrm{argmin} \left[|\mathbf{R}|^{\frac{1}{m}} \sigma^2 \right]$$

$$\sigma^2 = \frac{1}{m} (\mathbf{y} - \beta \mathbf{I}) \mathbf{R}^{-1} (\mathbf{y} - \beta \mathbf{I})$$

Matlab Functions

- NEWFF
- TRAIN
- kriging demo.zip
- kriging-ych.zip