Modern Family Sample Code

Scalar Version

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Informatik 12:
Software and Tools for Computational Engineering

RWTH Aachen University

Contents

Outline

Objective

- Introduction to scalar Modern Family sample problem and code

Learning Outcomes

- You will understand
  - motivation for the sample problem;
  - mathematical formulation of the sample problem.
- You will be able to
  - build and run the sample code.

Outline

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Cover Story

Relevance ...

Software and Tools for Computational Engineering

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LEBEN UND LERNEN Schlagzeilen | Wetter | DAX 12.142,64 | TV-Programm | Abo

Nachrichten > Leben und Lernen > Uni > Studienabbrecher > Alkohol im Studium: Studie - wer Bier trinkt, bricht seltener ab

Verblüffender Effekt

Wer Bier trinkt, bricht seltener das Studium ab

Wissenschaftler haben einen Zusammenhang zwischen dem Genuss von Alkohol und einem erfolgreichen Studienabschluss gefunden. Doch die Promille sind gar nicht entscheidend.

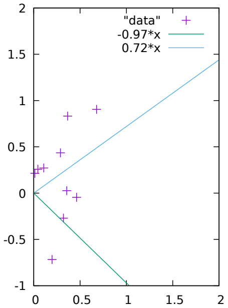
DPA

Männer mit Bierkasten

Gender Equality …

©dex1.info: Dinge, die Männer an Frauen unattraktiv finden

We aim to understand / reproduce / predict reality (of a given target system, e.g, the Modern Family scenario) based on observed / measured data



$$(x, y) \in \boldsymbol{R}^m \times \boldsymbol{R}^m$$

(e.g, positions visited by the guys) through determination of a mathematical model

$$y = f(p, x) : \boldsymbol{R} \times \boldsymbol{R} \rightarrow \boldsymbol{R}$$

with x describing the state of the system (e.g, sets of x-coordinates in between pub and home) and with

a (free) model parameters p to be determined such that the results obtained from the model match the data in the best possible way.

Our discussion will be restricted to scalar models ($y \in \boldsymbol{R}$).

Outline

- An exact match with the m data points can be constructed by interpolation, e.g. linear, cubic splines, polynomial of degree m.
- While unknown values in between known data points ("inside" the data) may be predicted adequately this approach typically yields poor extrapolation properties, that is, prediction of values "outside" of the data becomes difficult.
- Moreover, an exact match may not even be desirable due to errors and uncertainty in the given data.
- We chose to select a parameterized mathematical model to reflect the qualitative behavior of the underlying problem. This model is calibrated against the given data to improve the accuracy of its quantitative results.
- Calibration amounts to modification of the values of the (free) model parameters with the objective to minimize some "average" error between the prediction of the model and the given data.

For observed / measured positions (x_i, y_i), $i = 0, \ldots, m-1$, visited by the guys in reality we search for a model

$$y = f(p, x) : \boldsymbol{R} \times \boldsymbol{R} \rightarrow \boldsymbol{R}$$

with parameter p to be determined such that the "average distance" between m observations $\mathrm{y} = (y_i)_{i=0}^{m-1} \in \boldsymbol{R}^m$ at positions $\mathrm{x} = (x_i)_{i=0}^{m-1} \in \boldsymbol{R}^m$ and the corresponding simulated results produced by the model $(f(p, x_i))_{i=0}^{m-1} \in \boldsymbol{R}^m$ becomes minimal, e.g,

$$0 \leq \quad E = E(p, \mathrm{x}, \mathrm{y}) \equiv \sum_{i=0}^{m-1} (f(p, x_i) - y_i)^2 \quad \rightarrow \min$$

We aim for minimization of this least-squares objective.

Minima of unconstrained nonlinear convex objectives such as

$$E = E(p, \mathrm{x}, \mathrm{y}) = \sum_{i=0}^{m-1} (f(p, x_i) - y_i)^2 ,$$

where $p \in \boldsymbol{R}$, $\mathrm{x}, \mathrm{y} \in \boldsymbol{R}^m$, are characterized by the following

- necessary (first order) optimality condition:

$$E' \equiv \frac{dE}{dp}(p, \mathrm{x}, \mathrm{y}) = 0$$

  (stationary point)

- sufficient (second order) optimality condition:

$$E'' \equiv \frac{d^2E}{dp^2}(p, \mathrm{x}, \mathrm{y}) > 0$$

  (strict convexity in a neighborhood of the stationary point).

Objective $\rightarrow \min\limits_{p \in R}$

$$E = E(p, x, y) = \sum_{i=0}^{m-1} (f(p, x_i) - y_i)^2$$

Residual $\rightarrow 0$

$$E' = \frac{dE}{dp}(p, x, y) = 2 \cdot \sum_{i=0}^{m-1} \left((f(p, x_i) - y_i) \cdot \frac{df}{dp}(p, x_i) \right)$$

Derivative of Residual > 0

$$E'' = \frac{d^2E}{dp^2}(p, x, y) = 2 \cdot \sum_{i=0}^{m-1} \left(\left(\frac{df}{dp}(p, x_i) \right)^2 + (f(p, x_i) - y_i) \cdot \frac{d^2f}{dp^2}(p, x_i) \right)$$

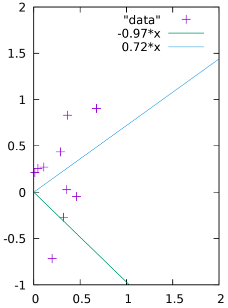
Let the model f be linear in p satisfying the constraint $f(p,0)=0$, e.g,

$$f = f(p,x) = p \cdot x \quad \Rightarrow \quad E = \sum_{i=0}^{m-1} (p \cdot x_i - y_i)^2 = p^2 \cdot \mathrm{x}^T \cdot \mathrm{x} - 2 \cdot p \cdot \mathrm{y}^T \cdot \mathrm{x} + \mathrm{y}^T \cdot \mathrm{y}$$

First and second derivatives of the objective E are formulated in terms of first and second derivatives of the model f:

$$f' = \frac{df}{dp}(p,x) = x \quad \Rightarrow \quad E' = 2 \cdot \sum_{i=0}^{m-1} (p \cdot x_i - y_i) \cdot x_i = 2 \cdot (p \cdot \mathrm{x}^T \cdot \mathrm{x} - \mathrm{y}^T \cdot \mathrm{x})$$

$$f'' = \frac{d^2 f}{dp^2}(p,x) = 0 \quad \Rightarrow \quad E'' = 2 \cdot \sum_{i=0}^{m-1} x_i^2 = 2 \cdot \mathrm{x}^T \cdot \mathrm{x} \,.$$



Our sample implementation generates $m = 10$ pseudo-random observations plotted as “data” and computes the optimal $p = 0.721618$ starting from an initial guess of $p = -0.967399$.

At the solution we find

$$\begin{aligned} E &= 1.8645 \\ E' &= -7.72029e-08 \\ E'' &= 2.34613\ . \end{aligned}$$

See sample code.

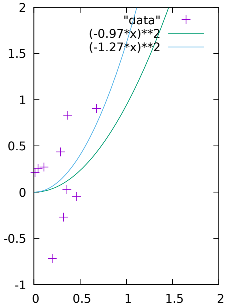
Let the model f be nonlinear in p satisfying the constraint $f(p,0)=0$, e.g,

$$f(p,x)=(p\cdot x)^2 \quad \Rightarrow \quad E=\sum_{i=0}^{m-1}((p\cdot x_i)^2-y_i)^2=\sum_{i=0}^{m-1}(p\cdot x_i)^4-2\cdot(p\cdot x_i)^2\cdot y_i+y_i^2$$

First and second derivatives of the objective E are formulated in terms of first and second derivatives of the model f:

$$f'=\frac{df}{dp}(p,x)=2\cdot p\cdot x^2 \quad \Rightarrow \quad E'=\sum_{i=0}^{m-1}4\cdot p^3\cdot x_i^4-4\cdot p\cdot x_i^2\cdot y_i$$

$$f''=\frac{d^2f}{dp^2}(p,x)=2\cdot x^2 \quad \Rightarrow \quad E''=\sum_{i=0}^{m-1}12\cdot p^2\cdot x_i^4-4\cdot x_i^2\cdot y_i\ .$$



Our sample implementation generates $m = 10$ pseudo-random observations plotted as "data" and computes the optimal $p = -1.27568$ starting from an initial guess of $p = -0.967399$.

At the solution we find

$$
\begin{aligned}
E &= 1.65408 \\
E' &= -2.30582e - 07 \\
E'' &= 4.03737 \; .
\end{aligned}
$$

See sample code.

Outline

Summary

- Calibration problem and sample code were introduced.
- Linear and nonlinear models were considered.

Next Steps

- Download the sample code.
- Inspect the sample code
- "Play" with the sample code
- Continue the course to find out more ...