DIFFERENT VIEWS ON ADDITIONAL RANDOM PARAMETERS IN EXPERIMENT DESIGN FOR THERMOPHYSICAL PARAMETERS ESTIMATION

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Design of experiment to get a "best" estimate of parameters of a stochastic model.

$Y_1, \dots, Y_n$ ... data
$\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)^T$ ... parameters of interest
$\boldsymbol{\xi} = (\xi_1, \dots, \xi_m)^T$ ... design parameters

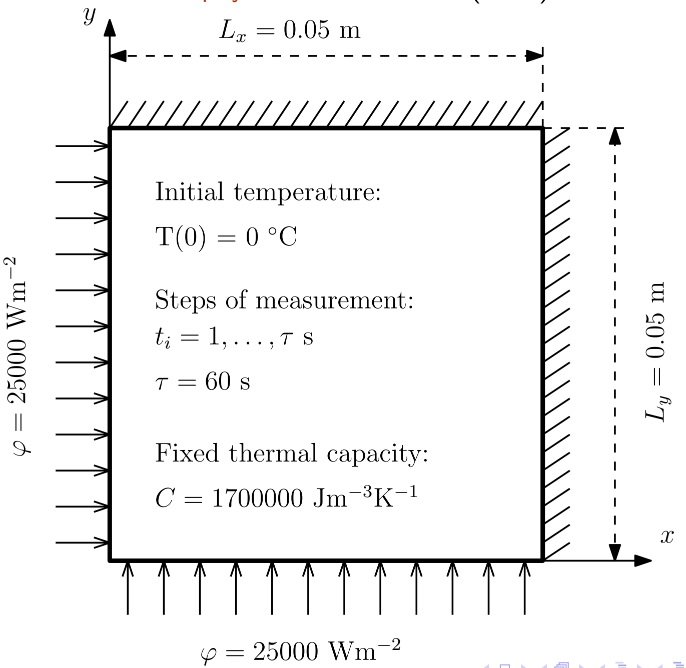
frequency approach
$\widehat{\boldsymbol{\theta}} = \left(\widehat{\theta}_1 = T_1(Y_1, \dots, Y_n), \dots, \widehat{\theta}_p = T_p(Y_1, \dots, Y_n)\right)^T$

$E_{\boldsymbol{\theta}} \widehat{\boldsymbol{\theta}} = \boldsymbol{\theta}$ ... unbiased estimator
$Var_{\boldsymbol{\theta}} \widehat{\boldsymbol{\theta}} = ||cov(\widehat{\theta}_i, \widehat{\theta}_j)||_{i,j=1}^p$.

CRITERIA

$\frac{Var\widehat{\theta}_1}{\theta_1^2} + \dots + \frac{Var\widehat{\theta}_p}{\theta_p^2}$ ... F criterium
$det\left(Var\widehat{\boldsymbol{\theta}}\right)$ ... D criterium

Experiment in thermophysics - Ruffio et al. (2012)



The solution may be approximated by:

$$T(t;\lambda_x,\lambda_y;x,y)=\theta_x(t;\lambda_x;C;\varphi;x)+\theta_y(t;\lambda_y;C;\varphi;y),$$

$$\theta_x(t;\lambda_x;C;\varphi;x)=\frac{2\varphi}{\sqrt{C\lambda_x}}\sqrt{t}F\Big(\frac{\widetilde{x}}{\sqrt{t}}\Big),$$
$$\theta_y(t;\lambda_y;C;\varphi;y)=\frac{2\varphi}{\sqrt{C\lambda_y}}\sqrt{t}F\Big(\frac{\widetilde{y}}{\sqrt{t}}\Big),$$

$$F(z)=\frac{\exp(-z^2)}{\sqrt{\pi}}-z\Big(1-\frac{2}{\sqrt{\pi}}\int_0^z e^{-v^2}\,dv\Big),\quad z\geq 0.$$

with $\widetilde{x}=(x/2)\sqrt{C/\lambda_x}$, $\widetilde{y}=(y/2)\sqrt{C/\lambda_y}$.

It is assumed that temperature is measured at n time points ($n = 60$) by a fixed number of sensors with measurement errors $\{e_i\}$ that are distributed according to $N(0, \sigma_e^2)$ where σ_e^2 is known. The measurement errors corresponding to different time points are independent. For one sensor we may expressed dependence of measured temperatures $\{Y_i\}$ on λ_x, λ_y:

$$Y_i = T(i/n; \lambda_x, \lambda_y; x, y) + e_i,\ i = 1, \ldots, n.$$

Goal is to find an "optimal" position (x, y) to get the "best" estimate of thermal conductivities λ_x, λ_y. (Thermal capacity C and heat flux ϕ are supposed to be known.)

Non-linear regression:

λ_x, λ_y are parameters of interest and x, y are design parameters.

Non-linear regression

$$Y_i = f(i/n; \beta) + e_i, \quad i = 1, \ldots, n.$$

$$\widehat{\beta} = \mathrm{argmin}_{\beta} \sum_{i=1}^{n} \big(Y_i - f(i/n; \beta)\big)^2$$

For n large ($\boldsymbol{\beta}^*$ is a true value of $\boldsymbol{\beta}$):

$\widehat{\boldsymbol{\delta}} =$

$$\underset{\boldsymbol{\delta}}{\operatorname{argmin}} \sum_{i=1}^{n} \left(Y_i - f(i/n; \boldsymbol{\beta}^*) - \frac{\partial f}{\partial \beta_1}(i/n; \boldsymbol{\beta}^*)\delta_1 - \ldots - \frac{\partial f}{\partial \beta_p}(i/n; \boldsymbol{\beta}^*)\delta_p \right)^2$$

$$\mathcal{L}(\sqrt{n}(\widehat{\boldsymbol{\beta}^*} - \boldsymbol{\beta}^*)) \sim \mathcal{L}(\sqrt{n}\,\widehat{\boldsymbol{\delta}}) = N\Big(\mathbf{0}, n\big({\mathbf{F}_n^*}^T\, \mathbf{F}_n^*\big)^{-1} \sigma_e^2\Big)$$

$$\mathbf{F}_n^* = \begin{pmatrix} \frac{\partial f}{\partial \beta_1}(1/n; \boldsymbol{\beta}^*) & \ldots & \frac{\partial f}{\partial \beta_p}(1/n; \boldsymbol{\beta}^*) \\ \vdots & \ldots & \vdots \\ \frac{\partial f}{\partial \beta_1}(1; \boldsymbol{\beta}^*) & \ldots & \frac{\partial f}{\partial \beta_p}(1; \boldsymbol{\beta}^*) \end{pmatrix}$$

$$\frac{1}{n}\mathbf{F}_n^{*T}\mathbf{F}_n^{*} \to \left|\left| \int_0^1 \frac{\partial f}{\partial \beta_i}(t,\boldsymbol{\beta}^*)\frac{\partial f}{\partial \beta_j}(t,\boldsymbol{\beta}^*)\,dt \right|\right|_{i,j=1}^{p}$$

$$n\left(\mathbf{F}_n^{*T}\mathbf{F}_n^{*}\right)^{-1} = ||\sigma_{ij}^{(n)}(\boldsymbol{\beta}^*)||_{i,j=1}^{p} \to \mathbf{\Sigma}^*(\boldsymbol{\beta}^*)$$

We may use the F and D criteria to the matrix $n\left(\mathbf{F}_n^{*T}\mathbf{F}_n^{*}\right)^{-1}$ that depends on the true value of $\boldsymbol{\beta}^*$. The optimal choice od the design parameters depends on the true value of $\boldsymbol{\beta}^*$.

Prior information on $\boldsymbol{\beta}^*$:

a density $\phi(\boldsymbol{\beta}^*)$ with a bounded support $[\beta_1^b, \beta_1^e] \times \cdots \times [\beta_p^b, \beta_p^e]$.

F criterium:

$$\int \cdots \int \left(\frac{\sigma_{11}^{(n)}(\boldsymbol{\beta}^*)}{{\beta_1^*}^2} + \cdots + \frac{\sigma_{pp}^{(n)}(\boldsymbol{\beta}^*)}{{\beta_p^*}^2} \right) \phi(\boldsymbol{\beta}^*) d\boldsymbol{\beta}^*$$

$$\max_{\boldsymbol{\beta}^* \in [\beta_1^b, \beta_1^e] \times \cdots \times [\beta_p^b, \beta_p^e]} \left(\frac{\sigma_{11}^{(n)}(\boldsymbol{\beta}^*)}{{\beta_1^*}^2} + \cdots + \frac{\sigma_{pp}^{(n)}(\boldsymbol{\beta}^*)}{{\beta_p^*}^2} \right)$$

(Non)linear regression with random parameters

Measured temperature may be affected by some other random parameters, e.g. by deviations of the real position of a sensor from the design position denoted here by $\Delta x, \Delta y$. The value of this parameter remains the same in one experiment but varies from an experiment to the other. It is supposed that its fluctuation is known, i.e. its density function is known.

In Ruffio et al. Δx and Δy were independent normally distributed $N(0, \sigma_\gamma^2)$:

$$Y_i = T(i/n; \lambda_x, \lambda_y; \Delta x, \Delta y; x, y) + e_i, \ i = 1, \ldots, n.$$

There are at least two approaches how to deal with the design problem (how to find "optimal" values for x and y).

(Non)linear regression with random parameters

To explain a difference between two approaches we start with a linear regression problem with one-dimensional parameter of interest β, one-dimensional random parameter γ and a design parameter ξ:

$$Y_i = \beta\, b(i/n;\xi) + \gamma\, h(i/n,\xi) + e_i, \quad i = 1, \ldots, n.$$

$\{e_i\}$ are i.i.d. distributed according to a known normal distribution $N(0, \sigma_e^2)$ and γ is distributed according to a known normal distribution $N(0, \sigma_\gamma^2)$. The true value of β is β^*.

Designer $\times$ experimenter-statisticien

Approach A

In one single experiment the value of random parameter is γ.
The experimenter-statisticien thinks that $\gamma = 0$ so that he/she estimates β by minimizing

$$\widehat{\beta} = \mathrm{argmin}_{\beta} \sum_{i=1}^{n} \left(Y_i - \beta\, b(i/n;\xi) \right)^2$$

$$\widehat{\beta} = \frac{\sum b(i/n,\xi) Y_i}{\sum b^2(i/n;\xi)} = \beta^* + C_1(n)\,\gamma + \frac{1}{\sqrt{n}} C_2(n)\varepsilon_n$$

where $\varepsilon_n \sim N(0, \sigma_e^2)$.

$$C_1(n) = \frac{\sum b(i/n;\xi) g(i/n;\xi)}{\sum b^2(i/n;\xi)} \to \frac{\int_0^1 b(t,\xi) g(t,\xi)\, dt}{\int_0^1 b^2(t,\xi)\, dt},$$

$$C_2(n) = \frac{1}{\sqrt{(1/n)\sum b^2(i/n;\xi)}} \to \frac{1}{\sqrt{\int_0^1 b^2(t;\xi)\, dt}}.$$

For n large the variability of $\widehat{\beta}$ is given by fluctuation of γ.

For n large:

$E\widehat{\beta} = \beta^*$.

$Var\widehat{\beta}$ expresses how much fluctuates values of $\widehat{\beta}$ around β^* in repeated experiments. Repetitions are made under different conditions, i.e. in repeated experiments values of the random parameters fluctuate (according to a known distribution). Minimizing $Var\widehat{\beta}$ with respect to ξ by a designer means that he/she desires that the difference in estimating β in repeated experiments is as small as possible.

$$Var\widehat{\beta} \approx \left(\frac{\sum b(i/n;\xi) g(i/n;\xi)}{\sum b^2(i/n;\xi)} \right)^2 \sigma_\gamma^2 \approx \left(\frac{\int_0^1 b(t,\xi) g(t,\xi)\, dt}{\int_0^1 b^2(t;\xi)\, dt} \right)^2 \sigma_\gamma^2$$

Approach B

The experimenter-statisticien knows that the random parameter might be different from zero. In one single experiment he/she estimates together with a parameter of interest. Let the value of the random parameter in one single experiment be γ. The experimenter-statisticien considers the model:

$$Y_i = \beta\, b(i/n;\xi) + \gamma\, g(i/n;\xi) + e_i, \quad i = 1, \ldots, n.$$

$$\begin{pmatrix} \widetilde{\beta} \\ \widetilde{\gamma} \end{pmatrix} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{Y},$$

$$\mathbf{X} = \begin{pmatrix} b(1/n;\xi) & g(1/n;\xi) \\ \vdots & \vdots \\ b(1;\xi) & g(1;\xi) \end{pmatrix}$$

$E\widetilde{\beta} = \beta^*$

A variance (conditional variance) $Var\widetilde{\beta}$ says how accurate is the estimate in one single experiment. In the other words how much $\widetilde{\beta}$ varies if we repeatedly perform the experiment under the assumption that the random parameter attains the same value in all repetitions.

$$
\begin{aligned}
Var\widetilde{\beta} &= \frac{\sum g^2(i/n;\xi)}{\left(\sum b^2(i/n;\xi)\right)\left(\sum g^2(i/n;\xi)\right) - \left(\sum b(i/n;\xi)g(i/n;\xi)\right)^2}\,\sigma_e^2 \\
&\approx \frac{\int_0^1 g^2(t,\xi)\,dt}{\left(\int_0^1 b^2(t,\xi)\,dt\right)\left(g^2(t;\xi)\,dt\right) - \left(\int_0^1 b(t;\xi)g(t;\xi)\,dt\right)^2}\,\frac{\sigma_e^2}{n}
\end{aligned}
$$

Minimizing $Var\widetilde{\beta}$ designer desires that the estimate in one single experiment is as much accurate as possible. In the other words he/she desires that the estimates of the parameter of interest in repeated experiments under the same conditions (the same value of random parameters) vary as less as possible.

Nonlinear regression

We consider one-dimensional parameter of interest β and one-dimensional random parameter γ.

$$Y_i = f(i/n; \beta; \gamma; \xi) + e_i, \quad i = 1, \dots, n.$$

$$f(i/n; \beta; \gamma; \xi) \approx$$

$$\approx f(i/n; \beta^*; 0; \xi) + \frac{\partial f}{\partial \beta}(i/n; \beta^*; 0; \xi)(\beta - \beta^*) + \frac{\partial f}{\partial \gamma}(i/n; \beta^*; 0; \xi)\,\gamma.$$

Approach A

$$\widehat{\beta} = \text{argmin}_{\beta} \sum_{i=1}^{n} \left(Y_i - f(i/n; \beta, 0, \xi) \right)^2$$

$$Var\widehat{\beta} \approx \left(\frac{\sum \frac{\partial f}{\partial \beta}(i/n; \beta^*, 0, \xi) \frac{\partial f}{\partial \gamma}(i/n; \beta^*; 0; \xi)}{\sum \left(\frac{\partial f}{\partial \beta}(i/n; \beta^*; 0; \xi) \right)^2} \right)^2 \sigma_\gamma^2.$$

Approach B

$$(\widetilde{\beta}, \widetilde{\gamma}) = \text{argmin}_{(\beta,\gamma)} \sum_{i=1}^{n} \left(Y_i - f(i/n; \beta; \gamma; \xi)\right)^2.$$

$Var(\widetilde{\beta}) \approx$

$$\frac{\sigma_e^2 \sum \left(\frac{\partial f}{\partial \beta}(\frac{i}{n}; \beta^*, \gamma)\right)^2}{\sum \left(\frac{\partial f}{\partial \beta}(\frac{i}{n}; \beta^*, \gamma)\right)^2 \sum \left(\frac{\partial f}{\partial \gamma}(\frac{i}{n}; \beta^*, \gamma)\right)^2 - \left(\sum \frac{\partial f}{\partial \beta}(\frac{i}{n}; \beta^*, \gamma)\frac{\partial f}{\partial \gamma}(\frac{i}{n}; \beta^*, \gamma)\right)^2}$$

$Var\widetilde{\beta}$ depends on β^* and γ.

1. We may minimize

$$\int\int \left(Var\widetilde{\beta}(\beta^*,\gamma)\right) \varphi_{\beta^*}(\beta^*)\varphi_\gamma(\gamma)\, d\beta^*\, d\gamma.$$

2. We may consider a minmax criterium, i. e. to minimize the "worst situation" with respect to both parameters.

3. We combine the both approaches.

$L = 0.05\ [m]$, $C = 1\,700\,000\ [Jm^{-3}K^{-1}]$, $\phi = 25\,000\ [Wm^{-2}]$, $\sigma_e = 0.1\ [^0C]$, $\sigma_x = \sigma_y = 0.0005\ [m]$.

$\lambda_x^* = 0.6$, $\lambda_y^* = 4.7$

F criterium (one sensor):

Approach	optimal coordinates of sensor	value of F
exact position	$x_{op} = 0.0024$, $y_{op} = 0$	0.0016
A	$x_{op} = 0.0165$, $y_{op} = 0.0158$	0.04
B	$x_{op} = 0.0057$, $y_{op} = 0$	0.0131

Problems

1. Linearization is not justified by an asymptotic theory. Is it possible to apply a linear approximation in Approach A? Would it be better to use simulations and numerical optimization?
Jarušková and Kučerová (2017).
2. Problem with the distribution of a random parameters: distribution of Δx and Δy cannot be normal - optimal solution is on the border.

References:

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