Uncertainty quantification and calibration of a photovoltaic plant model: warranty of performance and robust estimation of the long-term production

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Context

Industrial context

A certain amount of experimental data is gathered on the field.

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Industrial issues

How to trust the numerical code which, supposedly reproduces the experimental data?

Mathieu Carmassi (EDF-AgroParisTech)





























Contents



Calibration in theory

- Mathematical definition of the numerical code
- Different statistical models
- Stimation methods



Application Case: Code for the prediction of power from a PV plant (Python code)

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Application Case: Code for the prediction of power from a PV plant (Python code)

Calibration Physical system and the code



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Calibration First statistical model

The measurement error

$$\forall t \in \{1, \dots, T\} \quad Y_{exp_t} = \zeta(\boldsymbol{X}_t) + \epsilon_t, \tag{1}$$

where $\epsilon_t \stackrel{iid}{\sim} \mathcal{N}(\mathbf{0}, \sigma_{err}^2)$.

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The first model

$$\mathcal{M}_1 : \forall t \in \{1, \dots, T\} \quad Y_{exp_t} = f_c(\boldsymbol{x}_t, \boldsymbol{\theta}) + \epsilon_t.$$
(2)

Context



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Calibration Second statistical model

In the case of a time consuming code

In Maximum Likelihood Estimation (MLE) or in a Bayesian estimation (which recourse to many MCMC iteration) $\downarrow\downarrow$ intractable to work with a time consuming f_c (Sacks et al., 1989)

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The second model (Cox et al., 2001)

$$\mathcal{M}_2 : \forall t \in \{1, \dots, T\} \quad Y_{exp_t} = \mathbf{F}(\mathbf{x}_t, \theta) + \epsilon_t, \tag{3}$$

where $F(\bullet, \bullet) \sim \mathcal{GP}(m_c(\bullet, \bullet), c_c(\{\bullet, \bullet\}, \{\bullet, \bullet\})).$

Calibration The Gaussian process

Mean

$$m_c(\bullet,\bullet) = \beta_{c_0} + \sum_{j=1}^M \beta_{c_j} h_{c_j}(\bullet,\bullet),$$

where $\beta_c = (\beta_{c_1}, \dots, \beta_{c_M})$ is the coefficient vector to be estimated, and $h_c(\bullet, \bullet) = (h_{c_0}(\bullet, \bullet), \dots, h_{c_M}(\bullet, \bullet))$ is the design matrix of regression.

Covariance

$$c_{c}(\{\bullet,\bullet\},\{\bullet,\bullet\}) = \sigma_{c}^{2} r_{c_{\psi_{c}}}(\{\bullet,\bullet\},\{\bullet,\bullet\}),$$

where σ_c^2 stands for the variance, and $r_{c_{\psi_c}}$ for the correlation function with a vector parameter ψ_c which is the scale and the regularity of the kernel.

The third model

The discrepancy

Some papers as Bayarri et al. (2007),Kennedy and O'Hagan (2001),Higdon et al. (2004) advocate adding another error term:

 $\delta(\boldsymbol{x}_t) = \zeta(\boldsymbol{x}_t) - f_c(\boldsymbol{x}_t, \boldsymbol{\theta}^*).$

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The third model

 $\mathcal{M}_{3} : \forall t \in \{1, \dots, T\} \quad Y_{exp_{t}} = f_{c}(\boldsymbol{x}_{t}, \boldsymbol{\theta}) + \delta(\boldsymbol{x}_{t}) + \epsilon_{t}, \qquad (4)$ where $\delta(\boldsymbol{x}_{t}) \sim \mathcal{GP}(m_{\delta}(\bullet), c_{\delta}(\bullet, \bullet))$.

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Identifiability problem

An infinity of (θ, δ) is possible.

The fourth model (Kennedy and O'Hagan, 2001)

$$\mathcal{M}_4 : \forall t \in \{1, \dots, T\} \quad Y_{exp_t} = F(\mathbf{x}_t, \boldsymbol{\theta}) + \delta(\mathbf{x}_t) + \epsilon_t.$$
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Calibration The fourth model

The fourth model (Kennedy and O'Hagan, 2001)

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Summary

the model	$\zeta(oldsymbol{X})$
\mathcal{M}_1	$f_c(\boldsymbol{X}, \boldsymbol{\theta})$
\mathcal{M}_2	$m{F}(m{X},m{ heta})$
\mathcal{M}_3	$f_c(\boldsymbol{X}, \boldsymbol{\theta}) + \delta(\boldsymbol{X})$
\mathcal{M}_4	$F(X, \theta) + \delta(X)$

Context



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II

Application Case: Code for the prediction of power from a PV plant (Python code)

Likelihoods

Notations

• let us consider D a N sized DOE chosen in the space $\mathcal{H} \times \mathcal{Q}$ such that $\mathbf{y}_{\mathbf{c}} = f_{\mathbf{c}}(D)$,

- notations for the surrogate
 - *H_c* the design matrix,
 - $\Phi_c = \{\beta_c, \psi_c, \sigma_c^2\}$ the coefficient vector, the regularity of the kerne and the variance,
 - r_c the correlation function,
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$$\mathbf{y} = (\mathbf{y}_{exp}, \mathbf{y}_c)^T$$
 of size $T + N$.

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$$\mathbf{y} = (\mathbf{y}_{exp}, \mathbf{y}_{c})^{T}$$
 of size $T + N$.

Not time consuming code \rightarrow the full likelihood

$$\boldsymbol{y}_{exp}, \boldsymbol{X} | \boldsymbol{\theta}, \sigma_{err}^2 \sim \mathcal{N}_{\boldsymbol{T}}(\boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{V}(\boldsymbol{X})).$$

$$\mathcal{L}^{F}(\boldsymbol{\theta};\boldsymbol{y}_{exp},\boldsymbol{X}) = \frac{1}{(2\pi)^{T/2}|\boldsymbol{V}(\boldsymbol{X})|^{1/2}} \exp\left\{-\frac{1}{2}\left(\boldsymbol{y}_{exp} - \boldsymbol{m}(\boldsymbol{X},\boldsymbol{\theta})\right)^{T}\boldsymbol{V}(\boldsymbol{X})^{-1}\left(\boldsymbol{y}_{exp} - \boldsymbol{m}(\boldsymbol{X},\boldsymbol{\theta})\right)\right\}.$$

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$$\mathcal{M}_1 \qquad \qquad \mathcal{M}_3$$

$$\mathbf{V}(\mathbf{X}) = \sigma_{err}^2 I_T + \mathbf{\Sigma}_{\delta}(\mathbf{X})$$

 $\boldsymbol{m}(\boldsymbol{X},\boldsymbol{\theta}) = f_c(\boldsymbol{X},\boldsymbol{\theta}) \qquad \qquad \boldsymbol{m}(\boldsymbol{X},\boldsymbol{\theta}) = f_c(\boldsymbol{X},\boldsymbol{\theta}) + \boldsymbol{H}_{\delta}(\boldsymbol{X})\boldsymbol{\beta}_{\delta}$

Not time consuming code \rightarrow the full likelihood

$$\boldsymbol{y}_{exp}, \boldsymbol{X} | \boldsymbol{\theta}, \sigma_{err}^2, \boldsymbol{\Phi}_{\boldsymbol{\delta}} \sim \mathcal{N}_{\boldsymbol{T}}(\boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{V}(\boldsymbol{X})).$$

$$\mathcal{L}^{\mathcal{F}}(\boldsymbol{\theta}, \boldsymbol{\Phi}_{\boldsymbol{\delta}}; \boldsymbol{y}_{exp}, \boldsymbol{X}) = \frac{1}{(2\pi)^{T/2} |\boldsymbol{V}(\boldsymbol{X})|^{1/2}} \exp\left\{-\frac{1}{2} \left(\boldsymbol{y}_{exp} - \boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta})\right)^{T} \boldsymbol{V}(\boldsymbol{X})^{-1} \left(\boldsymbol{y}_{exp} - \boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta})\right)\right\}$$

\mathcal{M}_1	\mathcal{M}_3
-----------------	-----------------

$\boldsymbol{V}(X) = \sigma_{err}^2 \boldsymbol{I}_T \qquad \qquad \boldsymbol{V}(X) = \sigma_{err}^2 \boldsymbol{I}_T$	$+ \Sigma_{\delta}(\mathbf{X})$
---	---------------------------------

 $m(\mathbf{X}, \theta) = f_c(\mathbf{X}, \theta) \qquad m(\mathbf{X}, \theta) = f_c(\mathbf{X}, \theta) + \mathbf{H}_{\delta}(\mathbf{X}) \boldsymbol{\beta}_{\delta}$

Time consuming code \rightarrow the full likelihood

$$\boldsymbol{y}, \boldsymbol{X} | \boldsymbol{\theta}, \boldsymbol{\Phi}, \sigma_{err}^2 \sim \mathcal{N}_{\boldsymbol{T}+\boldsymbol{N}}(\boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{V}(\boldsymbol{X}, \boldsymbol{\theta})).$$

Time consuming code \rightarrow the full likelihood

$$\boldsymbol{y}, \boldsymbol{X} | \boldsymbol{\theta}, \boldsymbol{\Phi}, \sigma_{err}^2 \sim \mathcal{N}_{\boldsymbol{T+N}}(\boldsymbol{m}(\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{V}(\boldsymbol{X}, \boldsymbol{\theta})).$$

 \mathcal{M}_2

$$V(\mathbf{X}, \theta) = \begin{pmatrix} \mathbf{\Sigma}_{exp,exp}(\mathbf{X}, \theta) + \sigma_{err}^2 \mathbf{I}_T & \mathbf{\Sigma}_{exp,c}((\mathbf{X}, \theta), \mathbf{D}) \\ \mathbf{\Sigma}_{exp,c}((\mathbf{X}, \theta), \mathbf{D})^T & \mathbf{\Sigma}_{c,c}(\mathbf{D}) \end{pmatrix} \quad V(\mathbf{X}, \theta) = \begin{pmatrix} \mathbf{\Sigma}_{exp,exp}(\mathbf{X}, \theta) + \sigma_{err}^2 \mathbf{I}_T + \mathbf{\Sigma}_{\delta}(\mathbf{X}) & \mathbf{\Sigma}_{exp,c}((\mathbf{X}, \theta), \mathbf{D}) \\ \mathbf{\Sigma}_{exp,c}((\mathbf{X}, \theta), \mathbf{D})^T & \mathbf{\Sigma}_{c,c}(\mathbf{D}) \end{pmatrix}$$
$$m(\mathbf{X}, \theta) = H(\mathbf{X}, \theta)\beta_c = \begin{pmatrix} H_c(\mathbf{X}, \theta) \\ H_c(\mathbf{D}) \end{pmatrix} \beta_c \qquad m(\mathbf{X}, \theta) = H(\mathbf{X}, \theta)\beta_c = \begin{pmatrix} H_c(\mathbf{X}, \theta) \\ H_c(\mathbf{D}) \end{pmatrix} \begin{pmatrix} \beta_c \\ \beta_{\delta} \end{pmatrix}$$

Time consuming code \rightarrow the full likelihood

$$m{y}, m{X} | m{ heta}, \Phi, \sigma_{err}^2 \sim \mathcal{N}_{T+N}(m{m}(m{X}, m{ heta}), m{V}(m{X}, m{ heta})).$$

$$\mathcal{M}_2$$
 \mathcal{M}_4

$$V(X, \theta) = \begin{pmatrix} \Sigma_{exp,exp}(X, \theta) + \sigma_{err}^2 I_T & \Sigma_{exp,c}((X, \theta), D) \\ \Sigma_{exp,c}((X, \theta), D) T & \Sigma_{c,c}(D) \end{pmatrix} V(X, \theta) = \begin{pmatrix} \Sigma_{exp,exp}(X, \theta) + \sigma_{err}^2 I_T + \Sigma_{\delta}(X) & \Sigma_{exp,c}((X, \theta), D) \\ \Sigma_{exp,c}((X, \theta), D) T & \Sigma_{c,c}(D) \end{pmatrix}$$
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Calibration Partial likelihood

Time consuming code \rightarrow the partial likelihood

 $\boldsymbol{y}_{c}|\Phi_{c}\sim\mathcal{N}_{N}(\boldsymbol{m}_{c},\boldsymbol{V}_{c}).$

Time consuming code \rightarrow the partial likelihood

 $\boldsymbol{y}_{c}|\Phi_{c}\sim\mathcal{N}_{N}(\boldsymbol{m}_{c},\boldsymbol{V}_{c}).$



 \mathcal{M}_4

 $V_c = \Sigma_{c,c}(D)$

 $m_c = H_c(D)\beta_c$

Time consuming code \rightarrow the conditional distribution $[m{y}_{exp}|m{y}_{c}]$

$$\begin{pmatrix} \mathbf{y}_{exp} \\ \mathbf{y}_{c} \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \boldsymbol{m}_{exp}(\boldsymbol{X}, \boldsymbol{\theta}) \\ \boldsymbol{m}_{c} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{exp, exp}(\boldsymbol{X}, \boldsymbol{\theta}) & \boldsymbol{\Sigma}_{exp, c}((\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{D}) \\ \boldsymbol{\Sigma}_{exp, c}((\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{D})^{T} & \boldsymbol{\Sigma}_{c, c}(\boldsymbol{D}) \end{pmatrix} \right)$$

Time consuming code \rightarrow the conditional distribution $[\mathbf{y}_{exp} | \mathbf{y}_{c}]$

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Then,

 $oldsymbol{y}_{exp} | oldsymbol{y}_{c} \sim \mathcal{N}(oldsymbol{\mu}_{exp|c}((oldsymbol{X},oldsymbol{ heta}),oldsymbol{D}), oldsymbol{\Sigma}_{exp|c}((oldsymbol{X},oldsymbol{ heta}),oldsymbol{D})),$

Time consuming code \rightarrow the conditional distribution $[\mathbf{y}_{exp} | \mathbf{y}_{c}]$

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with:

 $\mu_{exp|c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D}) = \boldsymbol{m}_{exp}(\boldsymbol{X},\boldsymbol{\theta}) + \boldsymbol{\Sigma}_{exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})\boldsymbol{\Sigma}_{c,c}(\boldsymbol{D})^{-1}(\boldsymbol{y}_{c} - \boldsymbol{m}_{c}(\boldsymbol{D})),$

Time consuming code \rightarrow the conditional distribution $[\mathbf{y}_{exp}|\mathbf{y}_{c}]$

$$\begin{pmatrix} \mathbf{y}_{exp} \\ \mathbf{y}_{c} \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \boldsymbol{m}_{exp}(\boldsymbol{X}, \boldsymbol{\theta}) \\ \boldsymbol{m}_{c} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{exp, exp}(\boldsymbol{X}, \boldsymbol{\theta}) & \boldsymbol{\Sigma}_{exp, c}((\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{D}) \\ \boldsymbol{\Sigma}_{exp, c}((\boldsymbol{X}, \boldsymbol{\theta}), \boldsymbol{D})^{T} & \boldsymbol{\Sigma}_{c, c}(\boldsymbol{D}) \end{pmatrix} \right)$$

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 $\boldsymbol{\Sigma}_{exp|c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D}) = \boldsymbol{\Sigma}_{exp,exp}(\boldsymbol{X},\boldsymbol{\theta}) - \boldsymbol{\Sigma}_{exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})\boldsymbol{\Sigma}_{c,c}(\boldsymbol{D})^{-1}\boldsymbol{\Sigma}_{exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})^{T}.$

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with:

$$\mu_{\exp|c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D}) = \boldsymbol{m}_{\exp}(\boldsymbol{X},\boldsymbol{\theta}) + \boldsymbol{\Sigma}_{\exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})\boldsymbol{\Sigma}_{c,c}(\boldsymbol{D})^{-1}(\boldsymbol{y}_{c} - \boldsymbol{m}_{c}(\boldsymbol{D})),$$

 $\boldsymbol{\Sigma}_{exp|c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D}) = \boldsymbol{\Sigma}_{exp,exp}(\boldsymbol{X},\boldsymbol{\theta}) - \boldsymbol{\Sigma}_{exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})\boldsymbol{\Sigma}_{c,c}(\boldsymbol{D})^{-1}\boldsymbol{\Sigma}_{exp,c}((\boldsymbol{X},\boldsymbol{\theta}),\boldsymbol{D})^{T}.$

Conditional likelihood

 $\mathbf{y}_{exp}|\mathbf{y}_{c}, \mathbf{X}, \mathbf{D}, \boldsymbol{\theta}, \boldsymbol{\Phi}, \sigma_{err}^{2} \sim \mathcal{N}_{\mathsf{T}}(\boldsymbol{\mu}_{exp|c}((\mathbf{X}, \boldsymbol{\theta}), \mathbf{D}), \boldsymbol{\Sigma}_{exp|c}((\mathbf{X}, \boldsymbol{\theta}), \mathbf{D}))).$

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Different kind of estimations

- Maximum likelihood estimator (SMLE) (Cox et al., 2001; Wong et al., 2017),
- Bayesian framework (Bayarri et al., 2007; Kennedy and O'Hagan, 2001; Higdon et al., 2004).

Estimation

main methods

• **joint estimation** (Higdon et al., 2004): all the parameters in Φ and σ_{err}^2 are jointly estimated by maximizing the full likelihood $\mathcal{L}^F(\theta, \Phi_{\delta}; \mathbf{y}, \mathbf{X})$ (after integration over β with a weak prior),

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- modularization (Liu et al., 2009) : Stepwise method
 - $\circ \ (\hat{\Phi}_c) = argmax \quad \mathcal{L}^P(\Phi_c | \boldsymbol{y}_c) \ (Maximum \ likelihood \ estimates),$
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Context



- Mathematical definition of the numerical code
- Different statistical models
- Estimation methods



Application Case: Code for the prediction of power from a PV plant (Python code)

Recorded data



Recorded data















Python code

- $m_{\delta}=0$,
- r_{δ} as Gaussian,
- D is a LHS maximin of 50 points,
- $h_c(\bullet, \bullet)$ composed of linear functions,
- r_c as Matérn 5/2,
- Prior densities :
 - $\eta \sim \mathcal{N}(0.143, 2.5.10^{-3}),$ • $\mu_t \sim \mathcal{N}(-0.4, 1.10^{-2}),$ • $a_t \sim \mathcal{N}(0.17, 3.6.10^{-3}),$ • $\sigma_{err}^2 \sim \Gamma(2, 169),$ • $\sigma_{\delta}^2 \sim \Gamma(3, 1),$

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• $\psi_{\delta} \sim \mathcal{U}(0, 1).$
Application case Results 1/3



Application case Results 2/3



$(\mathcal{M}_1 \text{ to } \mathcal{M}_3: \text{ Add of the discrepancy})$

Bar





 $(\mathcal{M}_3 \text{ to } \mathcal{M}_4: \text{ Emulation of the code})$



 \mathcal{M}_4



-0.50 -0.25 0.00

 μ_t

40

30

20

10





Application case Results 3/3



 σ_{δ}^2



Sequential design

Sequential design

- Aim: add selected points in the original design to improve calibration,
- some improvements can be performed on the GPE such as the Efficient Global Optimization algorithm (EGO (Jones et al., 1998)),
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Bayesian calibration Sequential design

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Improvement of the GPE

Choice: add 10 points in original design according to Damblin et al. (2018).

Results with sequential design



$(\mathcal{M}_2 \text{ before sequential design})$

Bur

-0.25 0.00

-1.00







 $(\mathcal{M}_2 \text{ after sequential design})$





 μ_t





Results with sequential design



 \mathcal{M}_4

 $\mathcal{M}_{4}sd$

$(\mathcal{M}_4 \text{ before sequential design})$

8----







0.00





-0.50

 μ_t





Conclusion

Conclusion

- Bayesian calibration better assessed the uncertainty on the parameters regarding experimental data,
- in the case of performance monitoring, Bayesian calibration works well,
- the article Carmassi et al. (2018), submitted available at arXiv:1801.01810, presents a review of main calibration methods,
- the package CaliCo (Carmassi, 2018) available on CRAN and at arXiv:1808.01932,
- a shiny application is built to help EDF employees apply Bayesian calibration on their different industrial cases.

Perspectives

Perspective

- Be placed in a case where the design of the project has to be done,
- use a real time consuming code on real sized PV plant,
- extend calibration on time series code outputs,
- use Bayesian Model Selection / Averaging to elect a better model, regarding the data (Damblin, 2015; Kamary, 2016).

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