

Atmospheric re-entry calibration using a hierarchical generative model with few and incomplete data

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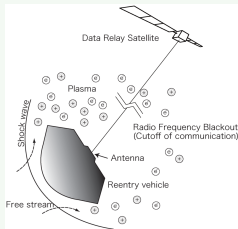
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Context: atmospheric hypersonic reentry vehicle (RV)



ARD, European Space Agency



radio frequency blackout, [TNO16]

■ Phenomenology

- Sharp deceleration/bow shock/high thermal flux/heat transfer.
- Heat shield degradation.

■ Aerodynamic prediction → a major task (e.g. landing zone) [CCL⁺17, JSJB21].

■ Coupled multi-physics simulation (code $\mathcal{T}$)

- Aerothermodynamic: hypersonic flows, turbulence, ablation, material models, ...
- Newtonian flight mechanics.

■ Full-scale experiments $\rightsquigarrow$ information about variability & model error.

■ Incomplete data (e.g. telemetry blackout phenomenon).

Problem formulation: model error calibration ...

- **Ballistic coefficient:** $\beta = S \cdot C_A / \tilde{m}$ (S : reference surface, $\tilde{m}$: mass and C_A : aerodynamic coefficient).
- **RV experiments** ($m = 1 \dots M$)

$$\begin{aligned}\beta(\mathbf{x}_m, h) &= \mathcal{T}(\mathbf{x}_m, h) + \Delta\beta(\mathbf{x}_m, h) && \text{decomposition} \\ \mathbf{y}_m &= \mathbf{S}_m (\mathcal{T}(\mathbf{x}_m) + \Delta\beta_m + \epsilon_m) && \text{observation vector}\end{aligned}$$

with $\mathbf{x}_m$: RV parameters (geometry, materials, ...),
 $\mathbf{S}_m$ a binary selection matrix to manage incomplete data and

$$\Delta\beta_m \triangleq [\Delta\beta(\mathbf{x}_m, h_1) \quad \Delta\beta(\mathbf{x}_m, h_2) \quad \dots \quad \Delta\beta(\mathbf{x}_m, h_K)]^T.$$

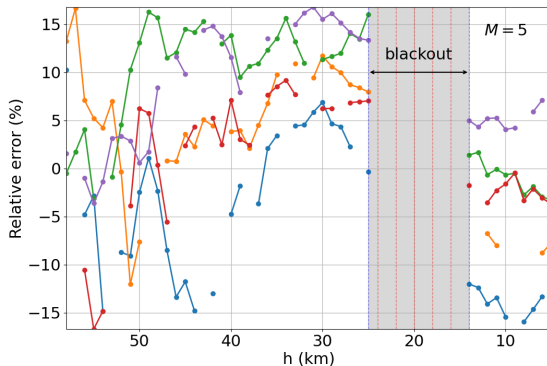
- **Future RV experiment** ($m = \infty$): $\beta(\mathbf{x}_\infty, h) = \mathcal{T}(\mathbf{x}_\infty, h) + \Delta\beta(\mathbf{x}_\infty, h)$

How can we predict $\beta(\mathbf{x}_\infty, h)$, i.e. calibrate the error $\Delta\beta(\mathbf{x}_\infty, h)$?

Problem formulation: ... as a generative problem

Observed relative deviation:

$$100 \cdot [\mathbf{y}_m - \mathcal{T}(\mathbf{x}_m)] / \mathcal{T}(\mathbf{x}_m) \%$$



From the few observed data, how can we generate new representative ones?

↪ requires a prior knowledge (hierarchical model)

Hierarchical generative model

Gaussian process [WR06] ($\sim$ Kennedy O' Hagan [KO01])

$$\Delta\beta(\mathbf{x}, h) \sim \mathcal{GP}(\mu(\mathbf{x}, h), k(\mathbf{x}, h, \mathbf{x}', h'))$$

- **Stationary among $\mathbf{x}$:** $\Delta\beta(\mathbf{x}, h)$ et $\Delta\beta(\mathbf{x}', h)$ have the same pdf.
- **Non-stationary among h :** Squared Exponential Generalization [HMR⁺16, Gib98, PS03]

$$k_{SEG}(h, h') = \sigma(h)\sigma(h') \sqrt{\frac{2\ell(h)\ell(h')}{\ell(h)^2 + \ell(h')^2}} \exp\left(-\frac{(h - h')^2}{\ell(h)^2 + \ell(h')^2}\right)$$

Likelihood

$$\mathbf{y}_m | \Delta\beta_m \sim \mathcal{N}(\mathbf{S}_m (\mathcal{T}(\mathbf{x}_m) + \Delta\beta_m), \mathbf{S}_m \mathbf{R} \mathbf{S}_m^T)$$

with $\mathbf{R}$: measurement covariance matrix.

Hierarchical generative model

Discretization (discrete-height random process)

$$\Delta\beta_m \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{P}_{\sigma,\ell}^{SEG}), \quad \Delta\beta_\infty \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{P}_{\sigma,\ell}^{SEG})$$

- $\boldsymbol{\mu} \triangleq [\mu(h_1) \quad \mu(h_2) \quad \cdots \quad \mu(h_K)]^T$: mean vector.
- $\mathbf{P}_{\sigma,\ell}^{SEG} \triangleq [k_{SEG}(h_i, h_j)]_{i=1 \dots K, j=1 \dots K}$: covariance matrix

$$[\mathbf{P}_{\sigma,\ell}^{SEG}]_{ij} = \sigma_i \sigma_j \sqrt{\frac{2\ell_i \ell_j}{\ell_i^2 + \ell_j^2}} \exp\left(-\frac{(h_i - h_j)^2}{\ell_i^2 + \ell_j^2}\right)$$

- $\boldsymbol{\sigma} \triangleq [\sigma(h_1) \quad \sigma(h_2) \quad \cdots \quad \sigma(h_K)]^T$: standard deviation vector.
- $\boldsymbol{\ell} \triangleq [\ell(h_1) \quad \ell(h_2) \quad \cdots \quad \ell(h_K)]^T$: correlation length vector.

Hierarchical generative model

Prior law $\theta \triangleq (\mu, \tilde{\sigma}, \tilde{\ell})$

$$\mu \sim \mathcal{N}(0, \mathbf{P}_{\beta_\mu, \gamma_\mu}^{SE})$$

$$\tilde{\sigma} \triangleq \log \sigma \sim \mathcal{N}(\alpha_\sigma \cdot \mathbf{1}_K, \mathbf{P}_{\beta_\sigma, \gamma_\sigma}^{SE})$$

$$\tilde{\ell} \triangleq \log \ell \sim \mathcal{N}(\alpha_\ell \cdot \mathbf{1}_K, \mathbf{P}_{\beta_\ell, \gamma_\ell}^{SE})$$

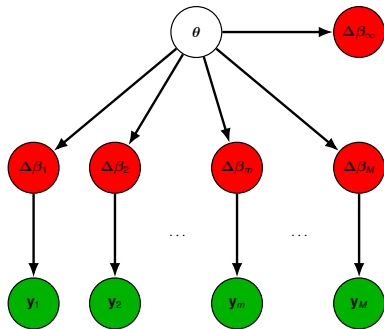
with $\dim(\theta) = 3 \cdot \dim(K) = a \text{ few hundreds.}$

Conditional laws ($m = 1 \dots M$)

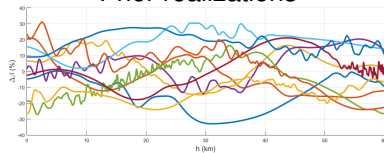
$$\Delta\beta_m | \mu, \tilde{\sigma}, \tilde{\ell} \sim \mathcal{N}(\mu, \mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG})$$

$$\mathbf{y}_m | \Delta\beta_m \sim \mathcal{N}(\mathbf{S}_m(\mathcal{T}(\mathbf{x}_m) + \Delta\beta_m), \mathbf{S}_m \mathbf{R} \mathbf{S}_m^T)$$

$$\Delta\beta_\infty | \mu, \tilde{\sigma}, \tilde{\ell} \sim \mathcal{N}(\mu, \mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG})$$



Prior realizations



Computational statistics

Predictive distribution

$$p(\Delta\beta_\infty|\mathbf{y}_{1:M}) = \int p(\Delta\beta_\infty|\theta, \mathbf{y}_{1:M})p(\theta|\mathbf{y}_{1:M})d\theta \approx \frac{1}{N} \sum_{n=1}^N p(\Delta\beta_\infty|\theta^{(n)}, \mathbf{y}_{1:M})$$

Sample $\theta^{(n)} \sim p(\theta|\mathbf{y}_{1:M})$

- **Dynamic Hamiltonian Monte Carlo (HMC): No U-Turn Sampler [HG⁺14].**
 - Fast gradient-based MCMC appropriate for high dimensional space.
 - Mimics Hamiltonian dynamics/Strömer-Verlet integration.
 - Automatic tuning of control parameters (adaptive integration length).

Sample $\Delta\beta_\infty^{(n)} \sim p(\Delta\beta_\infty|\theta^{(n)}, \mathbf{y}_{1:M}) = \mathcal{N}(\Delta\beta_\infty, \mu^{(n)}, \mathbf{P}_{\tilde{\sigma}^{(n)}, \tilde{\ell}^{(n)}}^{SEG})$

- **Gaussian Mixture Model (GMM).**

Analytical expressions

Log posterior $\log p(\theta|\mathbf{y}_{1:M})$

$$\begin{aligned} \log p(\theta|\mathbf{y}_{1:M}) \quad \# \quad & -\frac{1}{2} \sum_{m=1}^M \left[\tilde{\mathbf{y}}_m^T [\mathbf{S}_m(\mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} + \mathbf{R})\mathbf{S}_m^T]^{-1} \tilde{\mathbf{y}}_m + \log \det[\mathbf{S}_m(\mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} + \mathbf{R})\mathbf{S}_m^T] \right] + \log p(\boldsymbol{\mu}|\beta_\mu, \gamma_\mu) \\ & + \log p(\tilde{\sigma}|\alpha_\sigma, \beta_\sigma, \gamma_\sigma) + \log p(\tilde{\ell}|\alpha_\ell, \beta_\ell, \gamma_\ell) \quad \text{with: } \tilde{\mathbf{y}}_m \triangleq \mathbf{y}_m - \mathbf{S}_m(\mathcal{T}(\mathbf{x}_m) + \boldsymbol{\mu}) \end{aligned}$$

Log posterior gradient $\nabla_\theta \log p(\theta|\mathbf{y}_{1:M})$

$$\begin{aligned} \frac{\partial \log p(\theta|\mathbf{y}_{1:M})}{\partial \boldsymbol{\mu}} &= \sum_{m=1}^M \mathbf{S}_m^T \tilde{\mathbf{y}}_m - (\mathbf{P}_{\beta_\mu, \gamma_\mu}^{SE})^{-1} \boldsymbol{\mu} \quad \text{with: } \tilde{\mathbf{y}}_m \triangleq [\mathbf{S}_m(\mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} + \mathbf{R})\mathbf{S}_m^T]^{-1} \tilde{\mathbf{y}}_m \\ \frac{\partial \log p(\theta|\mathbf{y}_{1:M})}{\partial \tilde{\sigma}} &= \text{diag} \left(\sum_{m=1}^M \mathbf{S}_m^T \left(\tilde{\mathbf{y}}_m \tilde{\mathbf{y}}_m^T - [\mathbf{S}_m(\mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} + \mathbf{R})\mathbf{S}_m^T]^{-1} \right) \mathbf{S}_m \mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} \right) - (\mathbf{P}_{\beta_\sigma, \gamma_\sigma}^{SE})^{-1} (\tilde{\sigma} - \alpha_\sigma \cdot \mathbf{1}_K) \\ \frac{\partial \log p(\theta|\mathbf{y}_{1:M})}{\partial \tilde{\ell}_i} &= \frac{1}{2} \text{tr} \left(\sum_{m=1}^M \mathbf{S}_m^T \left(\tilde{\mathbf{y}}_m \tilde{\mathbf{y}}_m^T - [\mathbf{S}_m(\mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG} + \mathbf{R})\mathbf{S}_m^T]^{-1} \right) \mathbf{S}_m \frac{\partial \mathbf{P}_{\tilde{\sigma}, \tilde{\ell}}^{SEG}}{\partial \tilde{\ell}_i} \right) - [(\mathbf{P}_{\beta_\ell, \gamma_\ell}^{SE})^{-1} (\tilde{\ell} - \alpha_\ell \cdot \mathbf{1}_K)]_i \end{aligned}$$

Results: posterior distribution $p(\Delta\beta_\infty|\mathbf{y}_{1:M})$

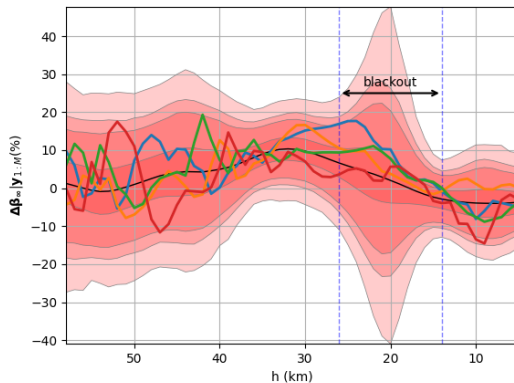


Figure 1: 4 realizations from $p(\Delta\beta_\infty|\mathbf{y}_{1:M})$ (color); the posterior mean (black), the pointwise equal-tailed 50%, 90%, 95% and 99% credible bands.

HMC convergence analysis

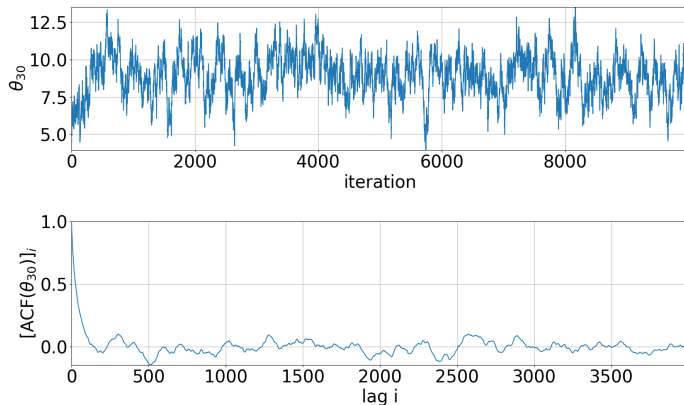


Figure 2: MCMC convergence and autocorrelation of θ_{30} .



Landing conclusion

- **Hierarchical generative model from a small number of incomplete data** ($\sim$ *non-stationary Gaussian process regression* [HMR⁺16]).
- **Numerical workhorse: dynamic HMC** for sampling the posterior distribution of the aerodynamic model error conditionnally to the data.

Perspectives

- Integration of a **dynamic model** to **take into account the non-stationarity among the RV parameters x** .
- HMC improvment (Riemannian, WALNUTS, CHEESE-HMC, ...).

Thanks! Any questions?

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Scatter plot matrix

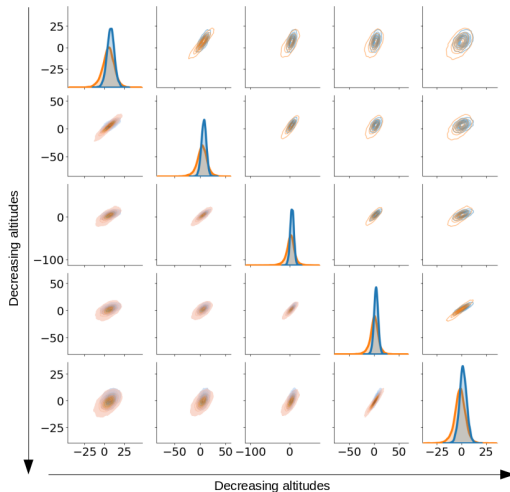


Figure 3: Pairwise KDE plot matrix of $p(\Delta\beta_\infty | \mathbf{y}_{1:M})$: complete data (blue) vs incomplete