Bayesian inference for expensive computer models in chemical engineering

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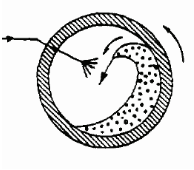
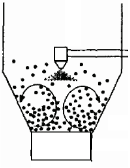
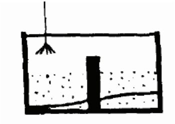
Granulation

- Products

- Devices

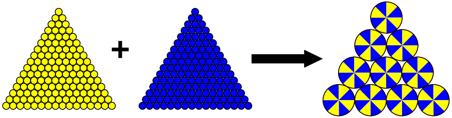




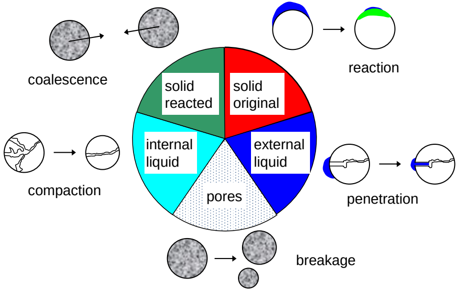


Granulation

- Lump small particles into bigger entities
  - Improve handling (storage, transport, safety,...)
  - Creation of micro mixtures (segregation, distribution of active components)
- Desire knowledge about:
  - Influences of precursors, process design and conditions on final product



Granulation model



transformation	unknown parameter
coalescence	k_{coag}
compaction	k_{compact}
breakage	k_{break}
penetration	k_{pen}
reaction	k_{reac}

Regression I

Aim: Regress for some data points $\boldsymbol{y}_{\text{obs}}$ over input space $\mathcal{Z}$

- Assume

$$y_{\text{obs}}(z) = y(z) + \epsilon \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, \tau^2) \tag{1}$$

- Underlying $y(z)$ is *unknown*, so endow with prior distribution :
  - $y(.) \sim \text{GP}(\,\mu(.), \sigma^2\Sigma(.,.)\,)$
  - mean function $\mu(z)$
  - correlation function $\Sigma(z_1, z_2)$

Regression II

- Make observations $\boldsymbol{y}_{\text{obs}} := y(\boldsymbol{z}) + \boldsymbol{\epsilon}$ at $\boldsymbol{z} = (z_1, \ldots, z_n)^\top$
- Want predictions at $\widetilde{\boldsymbol{z}}$

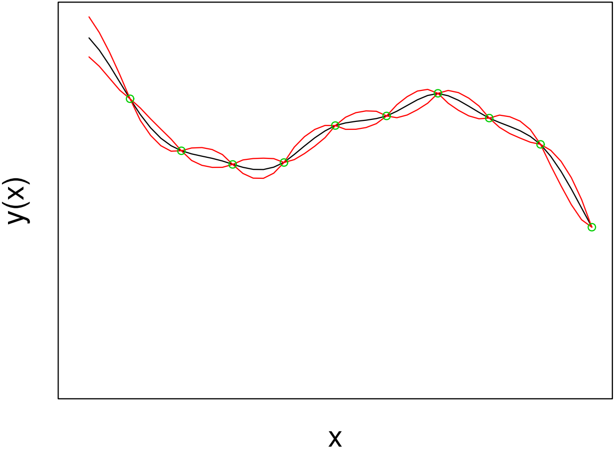
Posterior of $y(\widetilde{\boldsymbol{z}}) \,|\, \boldsymbol{y}_{\text{obs}}$:

- $y(\widetilde{\boldsymbol{z}}) \,|\, \boldsymbol{y}_{\text{obs}}$ has a multivariate normal distribution with

$$\mathbb{E}\left[y(\widetilde{\boldsymbol{z}}) \,|\, \boldsymbol{y}_{\text{obs}}\right] = \mu(\widetilde{\boldsymbol{z}}) + \sigma^2\Sigma(\widetilde{\boldsymbol{z}}, \boldsymbol{z}) \left[\sigma^2\Sigma(\boldsymbol{z}, \boldsymbol{z}) + \tau^2 I\right]^{-1} (\boldsymbol{y}_{\text{obs}} - \mu(\boldsymbol{z})) \quad (2)$$

$$\text{Var}\left(y(\widetilde{\boldsymbol{z}}) \,|\, \boldsymbol{y}_{\text{obs}}\right) = \sigma^2\Sigma(\widetilde{\boldsymbol{z}}, \widetilde{\boldsymbol{z}}) - \sigma^4\Sigma(\widetilde{\boldsymbol{z}}, \boldsymbol{z}) \left[\sigma^2\Sigma(\boldsymbol{z}, \boldsymbol{z}) + \tau^2 I\right]^{-1} \Sigma(\widetilde{\boldsymbol{z}}, \boldsymbol{z})^\top \quad (3)$$

Regression IV



Correlation function

Choices of $\Sigma(z_1, z_2)$:

- Exponential :

$$\Sigma(z_1, z_2) = \prod_{k=1}^{\dim(\mathcal{Z})} \exp\left(-\phi_k \cdot |z_{1k} - z_{2k}|^{\phi_0}\right) \quad (4)$$

- Matérn :

$$\Sigma(z_1, z_2) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{2\nu^{\frac{1}{2}}||z_1 - z_2||}{\rho}\right)^{\nu} \mathcal{K}_{\nu}\left(\frac{2\nu^{\frac{1}{2}}||z_1 - z_2||}{\rho}\right) \quad (5)$$

where $\mathcal{K}$ is modified Bessel function of 2^{nd} kind.

Notation

- $\mathcal{X}$ is space of *process conditions* or covariates
- Θ is space of unknown parameters of a model
- $\mathcal{Z} := \mathcal{X} \times \Theta$

Regression Models

- Underlying **Simulator** function $\eta_s(z)$:
  - $\eta_s(z) \sim \text{GP}\left(\mu_s(.), \sigma_s^2 \Sigma_s(.,.)\right)$
- Underlying **Experimental** function $\eta_e(x)$:
  - Fix calibrated value of $\theta = \theta_c$ (unknown)
  - $\eta_e(x) := \eta_s(x, \theta_c) + \delta(x)$
  - $\delta(x) \sim \text{GP}\left(\mu_e(.), \sigma_e^2 \Sigma_e(.,.)\right)$
- $\implies \eta_e \sim \text{GP}\left(\mu_s(.,.) + \mu_e(.)\,,\, \sigma_s^2 \Sigma_s(.,.) + \sigma_e^2 \Sigma_e(.,.)\right)$

Available data

- Observed **Experimental** data :
  - Have $\boldsymbol{y}_{\mathsf{e}} := (\eta_e(x_1), \ldots, \eta_e(x_{n_e}))^\top + \boldsymbol{\epsilon}_e$
- Observed **Simulator** data :
  - Have $\boldsymbol{y}_{\mathsf{s}} := \left(\eta_s(x_1^*, \theta_1^*), \ldots, \eta_s(x_{n_e}^*, \theta_{n_e}^*)\right)^\top + \boldsymbol{\epsilon}_s$
- Full data $\boldsymbol{d} := (\boldsymbol{y}_s^\top, \boldsymbol{y}_e^\top)^\top$
- Observation errors ϵ_e, ϵ_s for simplicity:
  - $\boldsymbol{\epsilon}_e \sim \mathcal{N}(0, \tau_e^2\, I)$ and $\boldsymbol{\epsilon}_s \sim \mathcal{N}(0, \tau_s^2\, I)$

Priors

- GP Priors
  - GP Matérn parameters ϕ_e, ϕ_s—$U[0, \phi_{\text{upper}}]$
  - GP mean linear parameters β_e, β_s—constant prior
  - GP variance parameters σ_e^2, σ_s^2—inverse gamma
- Observation error priors
  - τ_e^2, τ_s^2—inverse gamma
- Prior for θ is given by user
- All unknown values — represent as $(\theta, \beta_s, \beta_e, \boldsymbol{\xi})$

θ-estimation

- Posterior for $(\theta, \beta_s, \beta_e, \boldsymbol{\xi})$:

$$\pi(\theta, \beta_s, \beta_e, \boldsymbol{\xi} \,|\, \boldsymbol{d}) \propto \underbrace{f(\boldsymbol{d} \,|\, \theta, \beta_s, \beta_e, \boldsymbol{\xi})}_{\text{gaussian likelihood}} \times \underbrace{\pi(\theta)\pi(\beta_s)\pi(\beta_e)\pi(\boldsymbol{\xi})}_{\text{prior}} \tag{6}$$

- Integrate out β_s and β_e *analytically*
- Integrating out $\boldsymbol{\xi}$ is harder - do this via Wang-Laudau sampling
- Do similar for prediction of $\eta_e(x)$ and $\eta_s(x, \theta)$.

Example - simulator function $\eta_s(x, \theta)$

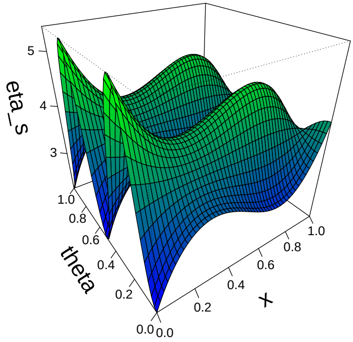
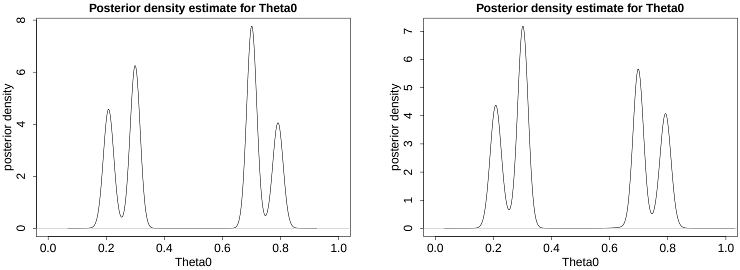


Figure: True $\eta_s(x, \theta)$

$$\mu_s(x, \theta) := \frac{1}{4}\left[6(x - 0.15)(x - 0.5)(x - 0.85) - 0.27\right]\left[10 \cos(4\pi\theta) + 0.3\right] + \text{const}$$

$$\theta_c = 0.2$$

Example - θ-posterior

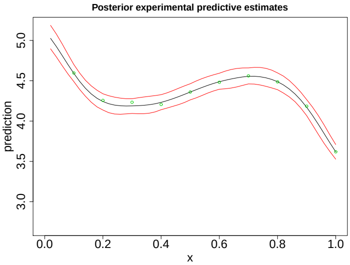


(a) assuming $\tau_s^2 = 0$, τ_e^2 unknown, $\delta(x) \equiv 0$

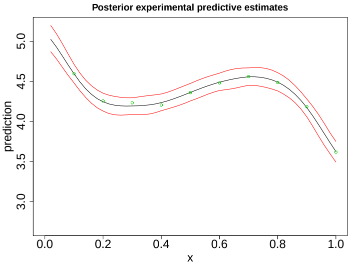
(b) assuming $\tau_s^2 = 0$, τ_e^2 and $\delta(x)$ unknown

Figure: θ posterior plots making different assumptions

Example - $y_e(x)$-posterior prediction + noise



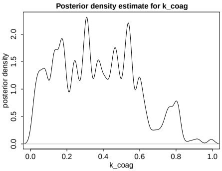
(a) assuming $\tau_s^2 = 0$, τ_e^2 unknown, $\delta(x) \equiv 0$



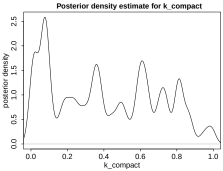
(b) assuming $\tau_s^2 = 0$, τ_e^2 and $\delta(x)$ unknown

Figure: $y_e(x)$ (+noise) posterior plots making different assumptions

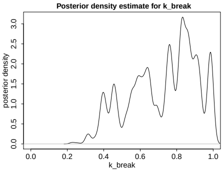
Granulation - $(k_{\text{coag}}, k_{\text{compact}}, k_{\text{break}}, k_{\text{pen}}, k_{\text{reac}})$-posteriors



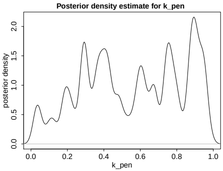
(a) k_{coag} posterior



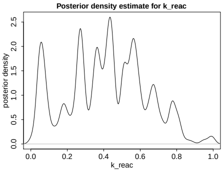
(b) k_{compact} posterior



(c) k_{break} posterior



(d) k_{pen} posterior



(e) k_{reac} posterior

Figure: Assuming $\tau_s^2 = 0$, $\tau_e^2, \delta(x)$ unknown