Modular Approaches in SAVE

Fei Liu

Duke University

Joint work with M. J. Bayarri, J. Berger, R. Paulo, J. Sacks

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Outline

The Problem

Full Bayes

Modular Approaches

Discussions

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The Problem

- Recall the `SAVE` model for computer model validation,

$$y^F(\cdot) = y^M(\cdot) + b(\cdot) + e(\cdot)$$

- The inputs may include,
  - $\boldsymbol{u}^*$: calibration paramaters (computer model associated).
  - $\boldsymbol{x}_1$: controllable paramters (configuration).
  - $\boldsymbol{x}_2^*$: unknown parameters varying from specimen to specimen.

$$y_i^F(\boldsymbol{x}_1, \boldsymbol{x}_2^*, t) = y^M(\boldsymbol{u}^*, \boldsymbol{x}_1, \boldsymbol{x}_2^*, t) + b(\boldsymbol{x}_1, \boldsymbol{x}_2^*, t) + e_i(t)$$

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The Problem

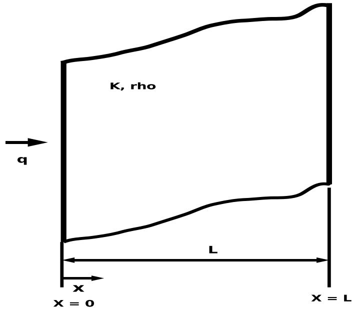
- A simplified SAVE model is,

$$y_i^F(\boldsymbol{x}_1, \boldsymbol{x}_2^*, t) = y^M(\boldsymbol{u}^*, \boldsymbol{x}_1, \boldsymbol{x}_2^*, , t) + b(\boldsymbol{x}_1, t) + e_i^1(t)$$

where $e_i^1(\cdot)$ includes both field measurement error and a nugget to accommodate the simplification in the bias function.

Confounding may still exist between $\boldsymbol{x}_2^*$ and the bias process!

The Sandia Example



- thermal conductivity $\kappa(W/m^oC)$;
- volumetric heat capacity $\rho(J/m^{3o}C)$;
- heat flux $q(W/m^2)$;
- device thickness $L(m)$;
- initial temperature $T_0(^oC)$;
- distance to surface $x(m)$;
- time $t(s)$.

- The Thermal computer model,

$$\begin{aligned} & T^M(\kappa, \rho, T_0, x, L, q; t) \\ = \quad & T_0 + \frac{qL}{\kappa}\left(\frac{\kappa t/\rho}{L^2} + \frac{1}{3} - \frac{x}{L} + \frac{x^2}{2L^2} - \sum_1^6 \frac{2\exp(-\frac{n^2\pi^2\kappa t}{L^2\rho})\cos(n\pi\frac{x}{L})}{\pi^2 n^2}\right) \end{aligned}$$

- Controllable variables for the i'th specimen,

$$\boldsymbol{x}_1^{(i)} = (q_i, L_i, x_i, T_{i0})$$

- Unknown variables for the i'th specimen,

$$\boldsymbol{x}_2^{(i)} = (\kappa_i, \rho_i)$$

- We use $\boldsymbol{x}_2^{(i*)} = \left(\kappa_i^*, \rho_i^*\right)$ represent the associated true values.

The Bayesian Hierarchical Model

- Gaussian stochastic processes,

$$b(\cdot,\cdot) \sim \text{GP}\left(0, \tau^2 c_{x_1}(\cdot,\cdot)\, c_t(\cdot,\cdot)\right), \epsilon(\cdot) \sim \text{GP}\left(0, \sigma^2 c_t(\cdot,\cdot)\right)$$

- Power exponential families for the correlations,

$$c_{x_1}\left(\boldsymbol{x}_1, \boldsymbol{x}_1^{'}\right) = \exp\left(-\sum_1^3 |\beta_k\left(\boldsymbol{x}_{1k} - \boldsymbol{x}_{1k}^{'}\right)|^{\alpha_k}\right)$$

$$c_t(t, t^{'}) = \exp(-|\beta^{(t)}(t - t^{'})|^{\alpha^{(t)}})$$

The unknowns are $\{\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^2, \tau^2, \boldsymbol{b}\}$.

$$
\begin{aligned}
\pi(\tau^2) &\propto \exp(-0.001\tau^2) \\
\pi(\sigma^2) &\propto 1/\sigma^2 \\
\pi(\alpha) &\propto \mathrm{U}(\alpha \mid 1, 2) \\
\pi(\beta) &\sim \exp(\lambda\beta) \\
\pi(\kappa^*) & \\
\pi(\rho^*) &
\end{aligned}
$$

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Full Bayes Approach

We can use MCMC algorithm to draw posterior samples for the parameters.

- Sample $\left(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^* \mid \text{Data}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^2, \tau^2\right)$ by Metropolis-Hastings algorithm.
- Sample $\left(\boldsymbol{\alpha} \mid \text{Data}, \boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\beta}, \sigma^2, \tau^2\right)$ by Metropolis-Hastings algorithm.
- Sample $\left(\boldsymbol{\beta} \mid \text{Data}, \boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\alpha}, \sigma^2, \tau^2\right)$ by Metropolis-Hastings algorithm.
- Sample $\left(\boldsymbol{b} \mid \text{Data}, \boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^2, \tau^2\right)$.
- Sample $\left(\tau^2 \mid \text{Data}, \boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\alpha}, \boldsymbol{\beta}, \tau^2, \boldsymbol{b}\right)$.
- Sample $\left(\sigma^2 \mid \text{Data}, \boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^2, \boldsymbol{b}\right)$.

Results from Full Bayes Approach

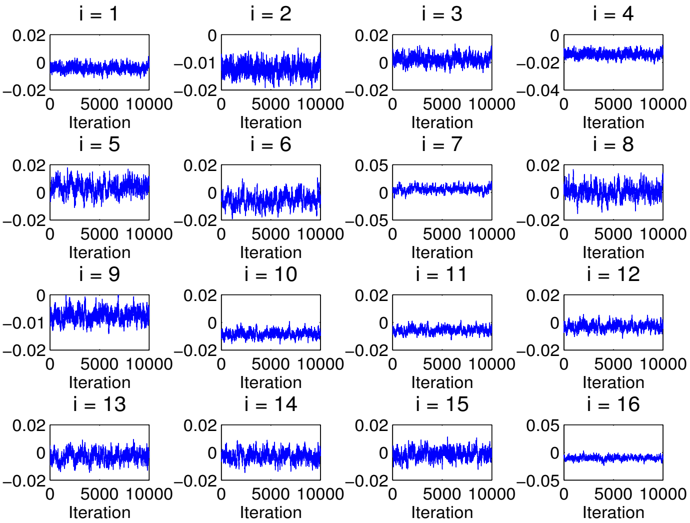

Figure: Trace plots for $\boldsymbol{\kappa}^*$

Results from Full Bayes Approach

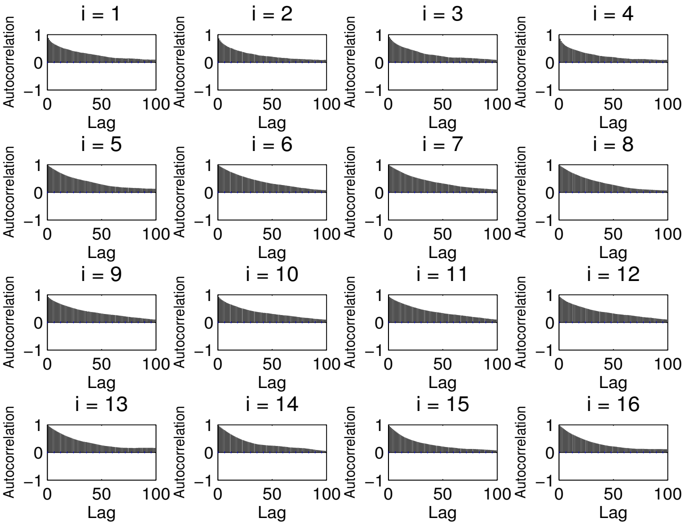

Figure: Acf plots for $\boldsymbol{\kappa}^*$

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Modular Approach 1

- Unlike the full Bayes approach, modular approaches first try to fix $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ in the bias process.
- Modular Approach 1:
  - Get samples of α, β by first approximating the `SAVE` model by,

    $$y_i^F(\kappa_i^*, \rho_i^*, x_i, L_i, q_i; t) \approx y^M(\hat{\kappa}, \hat{\rho}, x_i, L_i, q_i; t) + b(x_i, L_i, q_i; t) + \epsilon_i^{(2)}(t)$$

    where $(\hat{\kappa}, \hat{\rho})$ are the prior means of $\boldsymbol{\kappa}^*$ and ρ^*.
  - Fix α, β at posterior means $\hat{\alpha}, \hat{\beta}$, and draw samples for $\left(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \sigma^2, \tau^2, \boldsymbol{b} \mid \text{Data}, \hat{\alpha}, \hat{\beta}\right)$.

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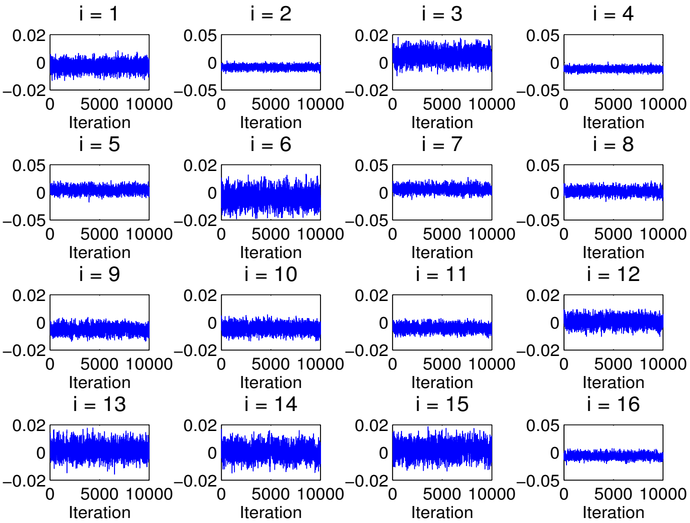
    where $(\hat{\kappa}, \hat{\rho})$ are the prior means of $\boldsymbol{\kappa}^*$ and ρ^*.
  - Fix $\boldsymbol{\alpha}, \boldsymbol{\beta}$ at posterior means $\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}$, and draw samples for $\left(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \sigma^2, \tau^2, \boldsymbol{b} \mid \text{Data}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}\right)$.

Results from Modular Approach 1



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Results from Modular Approach 1

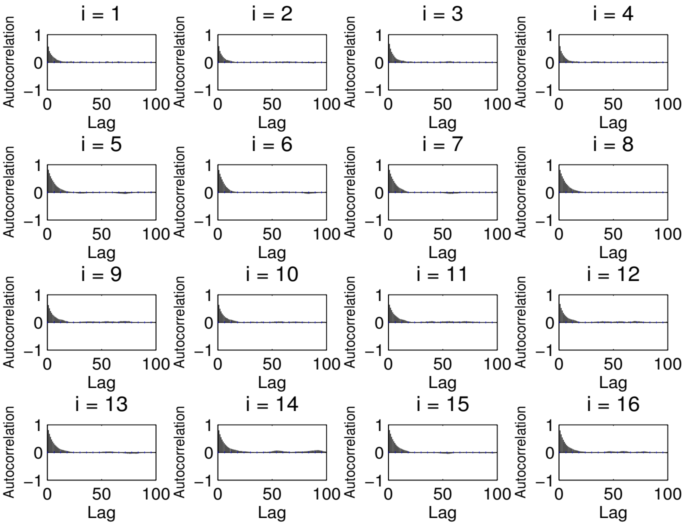

Figure: Acf plots for $\boldsymbol{\kappa}^*$

Modular Approach 2

Modular Approach 2:

- Draw samples for $\boldsymbol{\alpha}, \boldsymbol{\beta}$ by first approximating the SAVE model by,

$$\begin{aligned} y_i^F(\kappa_i^*, \rho_i^*, x_i, L_i, q_i; t) &\approx \mathbb{E}\left(y^M(\kappa_i^*, \rho_i^*, x_i, L_i, q_i; t)\right) \\ &\quad + b(x_i, L_i, q_i; t) + \epsilon_i^{(3)}(t) \end{aligned}$$

  This can be done by sampling $\kappa_i^* \sim \pi\left(\kappa_i^*\right), \rho_i^* \sim \pi\left(\rho_i^*\right)$.
- Fix $\boldsymbol{\alpha}, \boldsymbol{\beta}$ at the posterior means $\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}$, and draw samples for $\left(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \sigma^2, \tau^2, \boldsymbol{b} \mid \text{Data}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}\right)$.

Results from Modular Approach 2

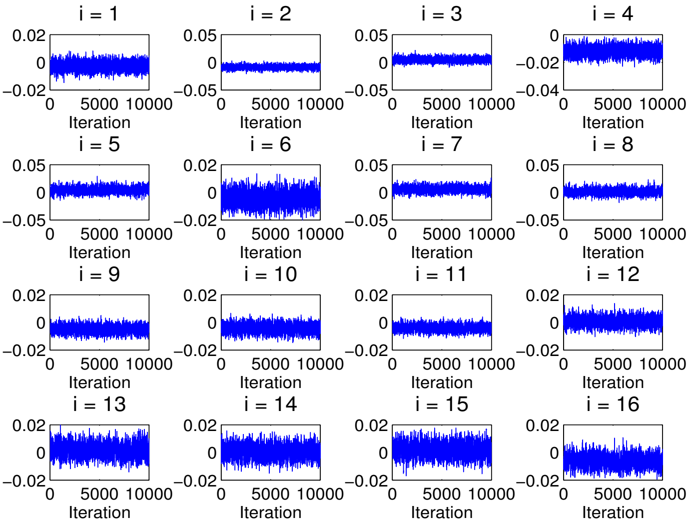

Figure: Trace plots for $\boldsymbol{\kappa}^*$

Results from Modular Approach 2

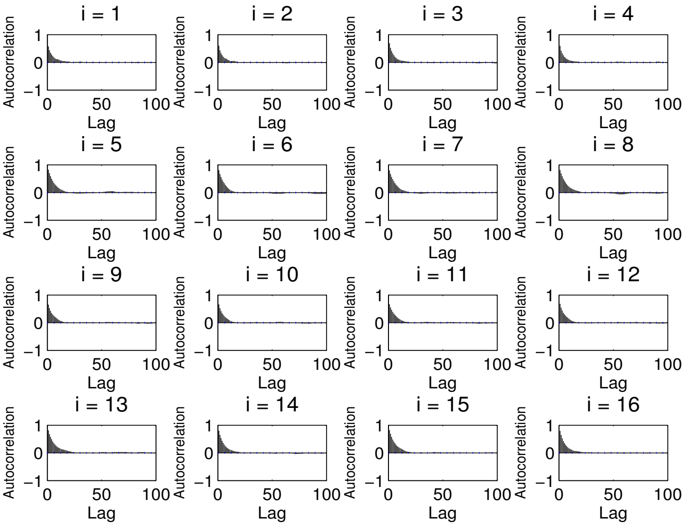

Figure: Acf plots for $\boldsymbol{\kappa}^*$

Modular Approach 3

Modular Approach 3:

- Draw samples for $(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*)$ by first assuming $\boldsymbol{b} = 0$ in the $\texttt{SAVE}$ model, i.e.,

$$y_i^F(\kappa_i^*, \rho_i^*, x_i, L_i, q_i; t) = y^M(\kappa_i^*, \rho_i^*, x_i, L_i, q_i; t) + \epsilon_i^{(4)}(t)$$

- Fix $\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*$ at posterior means $\hat{\boldsymbol{\kappa}^*}, \hat{\boldsymbol{\rho}^*}$, and draw samples for $\left(\boldsymbol{\alpha}, \boldsymbol{\beta}, \sigma^2, \tau^2, \boldsymbol{b} \mid \text{Data}, \hat{\boldsymbol{\kappa}^*}, \hat{\boldsymbol{\rho}^*}\right)$.
- Fix $\boldsymbol{\alpha}, \boldsymbol{\beta}$ at the posterior means $\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}$, and draw samples for $\left(\boldsymbol{\kappa}^*, \boldsymbol{\rho}^*, \sigma^2, \tau^2, \boldsymbol{b} \mid \text{Data}, \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}\right)$.

Results from Modular Approach 3

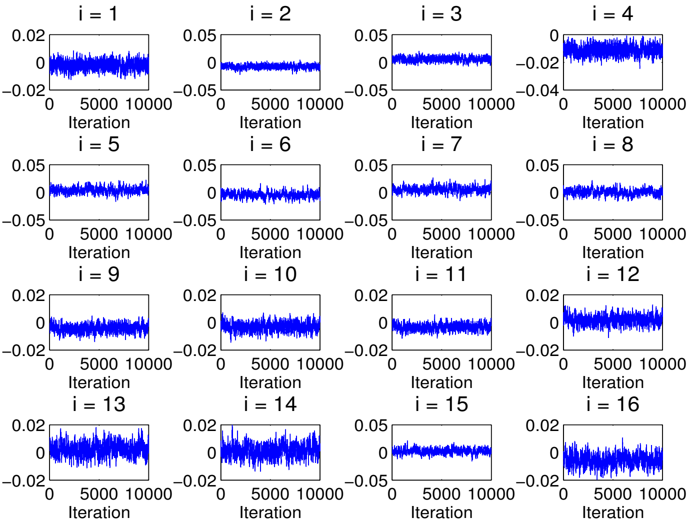

Figure: Trace plots for $\boldsymbol{\kappa}^*$

Results from Modular Approach 3

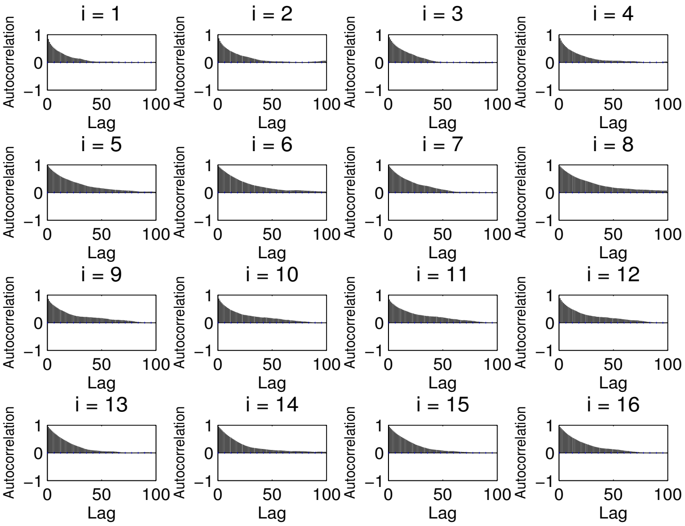

Figure: Acf plots for $\boldsymbol{\kappa}^*$

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Posterior Summaries

	FB	MA 1	MA 2	MA 3
β_2	5.40	10.75	14.62	38.71
	(1.56, 17.56)	(1.29, 36.86)	(1.20, 115.49)	(7.85, 120.44)
$\beta_3 \times 10^6$	1.08	1.12	1.07	1.10
	(0.56, 2.82)	(0.55, 2.91)	(0.51, 2.91)	(0.56, 2.79)
$\alpha^{(t)}$	1.941	1.998	1.998	1.9985
	(1.898, 1.966)	(1.997, 1.999)	(1.997, 1.999)	(1.9975, 1.9991)
$\beta^{(t)} \times 10^3$	1.20	1.06	1.05	0.94
	(0.93, 1.54)	(0.94, 1.19)	(0.94, 1.19)	(0.82, 1.06)
τ^2	2079	23307	22843	30055
	(1209, 3755)	(14940, 37647)	(14658, 36737)	(18889, 48386)
σ^2	1.55	41.55	43.25	65.74
	(0.98, 2.57)	(32.37, 54.39)	(33.77, 57.27)	(50.95, 86.40)

Table: Posterior medians with 95% predictive intervals

The Bias functions

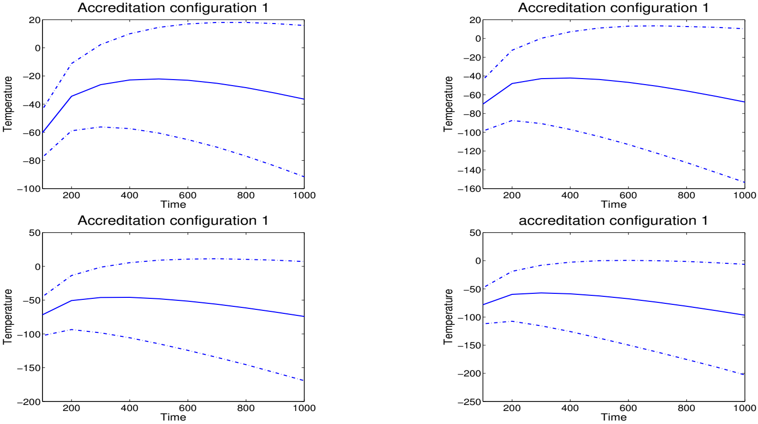

Figure: The bias functions for: upper-left: full Bayes approach; upper-right: approach 1; lower-left: approach 2; lower-right: approach 3

Pure Model predictions

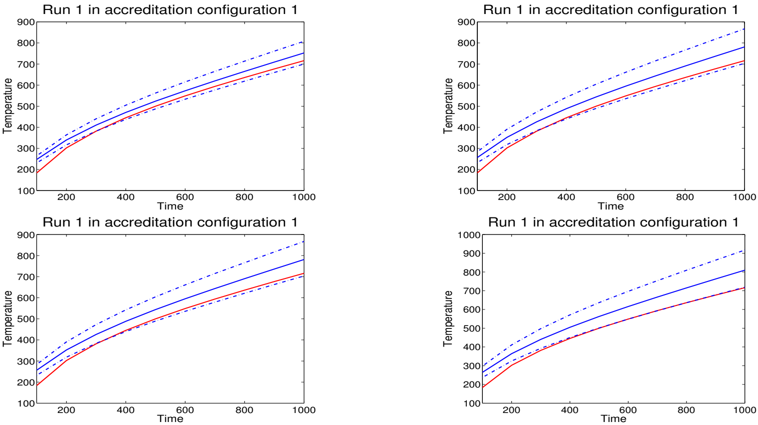

Figure: The pure model predictions for upper-left: full Bayes approach; upper-right: approach 1; lower-left: approach 2; lower-right: approach 3

Predictions for the reality

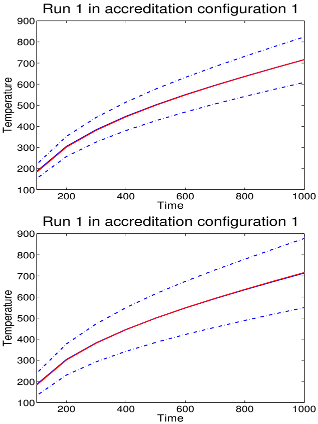

Figure: The predictions for the reality — upper-left: full Bayes approach; upper-right: approach 1; lower-left: approach 2; lower-right: approach 3

Conclusion

- The range and roughness parameters are similar in all the approaches.
- The Full Bayes approach has smaller variances both for the bias processes and the nuggets. But the auto-correlation functions of $\boldsymbol{\kappa}^*$ is suggesting that it does not converge.
- The modular approach 1 and 2 have bigger variances both for the bias processes and the nuggets. But the auto-correlation functions shows that the samples of $\boldsymbol{\kappa}^*$ are less correlated.
- Modular approach 1 allows fast computation (use of `MLE`).
- The modular approach 3 does not solve the confounding problem. Acf decays slowly.

Thank you!