

Recent Development on Dynamic Computer Experiments

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Design and Analysis of Experiments

Outline

- Large-scale dynamic computer experiments
- Proposed SVD-based Gaussian process models
- Inverse problem
- Concluding remarks

Dynamic Computer Simulators

Computer simulators with time-varying outputs

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Computer simulators with time-varying outputs

- Climate change model (Bhattacharya, 2007)
- Rainfall-runoff model (Conti et al., 2009)
- Marrow stem cell kinetics model (Morris, 2012; Jones et al., 1991)
- **Vehicle suspension system** (Bayrri et al., 2007)
- **Hydrological saturated path model (logSPMs)** (Liu and West, 2007)
- **Sheffield Dynamic Global Vegetation Model** (Conti and O'Hagan, 2010)
- **The Lyon-Fedder-Mobary (LFM) model** (Pratola et al., 2013)
- **Volcanic pyroclastic flow model** (Gu and Berger, 2016)

Dynamic Computer Simulators

- Systems evolving over time

$$Y_t = f(z_t, Y_{t-1}), t = 1, \dots, T \quad (1)$$

where Y_t and Y_{t-1} represent the state vector at time-step t and $t - 1$, respectively, $\mathbf{z}_t = (\mathbf{x}, \mathbf{w}_t)$ denotes the time-independent input \mathbf{x} and the forcing inputs \mathbf{w}_t at time-step t

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- Systems generating time series outputs
 - the training data inputs $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$
 - at time t , the outputs $\mathbf{y}_t = (y(\mathbf{x}_1, t), \dots, y(\mathbf{x}_N, t))^T$

Dynamic Computer Simulators

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- Time-input emulator: include time as an extra input (Kennedy and O'Hagan, 2001)
- Time-varying autoregression (TVAR) models with GP residuals (Liu and West, 2007)

Large-scale Computer Experiments

Computer Experiments with massive outputs

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Computer Experiments with massive outputs

- Mutli-step interpolator (Haaland and Qian, 2011)
- Fixed rank kriging (Cressie and Johannesson, 2008)
- Compactly supported covariance (Kaufman et al., 2011)
- [Local Gaussian process](#) (Gramacy and Apley, 2015; Gramacy et al., 2015; Gramacy and Haaland, 2016)

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- Emery (2009) built a local neighborhood by sequentially including data that make the Kriging variance decrease more.
- Gramacy and Apley (2015) uses a sequential greedy algorithm and an optimality criterion for finding a non-trivial local neighbourhood set.

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- It is not trivial to extend the existing methods for large-scale computer experiments to accommodate the times series outputs
- Thus, it calls for a new method for emulating large-scale dynamic computer simulators

The Proposed Approach

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Model Formulation

- For N training points, let $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]^T$ be the $N \times q$ input matrix, and $\mathbf{Y} = [\mathbf{y}(\mathbf{x}_1), \dots, \mathbf{y}(\mathbf{x}_N)]$ be the $L \times N$ matrix of time series response

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- The SVD on \mathbf{Y} gives

$$\mathbf{Y} = \mathbf{U}\mathbf{D}\mathbf{V}^T = \sum_{i=1}^k d_i \mathbf{u}_i \mathbf{v}_i^T \quad (3)$$

where

- $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_k]$ is an $L \times k$ column orthogonal matrix of left singular vectors, $k = \min\{N, L\}$
- $\mathbf{D} = \text{diag}(d_1, \dots, d_k)$ is a $k \times k$ diagonal matrix of singular values sorted in decreasing order
- \mathbf{V} is an $N \times k$ column-orthogonal matrix of right singular vectors

Model Formulation

The SVD-based GP model assumes that

$$\mathbf{y}(\mathbf{x}) = \sum_{i=1}^p c_i(\mathbf{x}) \mathbf{b}_i + \varepsilon \quad (4)$$

where $\mathbf{b}_i = d_i \mathbf{u}_i \in \mathcal{R}^L$, $c_i(\mathbf{x}) \sim \text{GP}(0, \sigma_i^2 K_i(\cdot, \cdot; \theta_i))$, for $i = 1, \dots, p$, and $\varepsilon \sim N(0, \sigma^2 \mathbf{I}_L)$. The number of significant singular values, p in (4), is determined empirically by the cumulative percentage criterion

$$p = \min \left\{ m : \frac{\sum_{i=1}^m d_i}{\sum_{i=1}^k d_i} > \gamma \right\},$$

where γ is a prespecified threshold of explained variation ($\gamma \in (0.9, 0.98)$)

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- The formulation reduces the problem of building an emulator that maps from $(0, 1)^q$ to \mathcal{R}^L to building p independent, univariate GP models for each c_i
- Higdon et al. (2008) employ a fully Bayesian analysis via Markov chain Monte Carlo (MCMC), which is computationally intensive in our applications

Empirical Bayesian Inference

- The parameters
 - σ^2 : the error variance
 - σ_i^2 : the process variance, for $i = 1, \dots, p$
 - $\theta_i = (\theta_{i1}, \dots, \theta_{iq})$: the correlation parameters in Gaussian correlation function

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 - $\theta_i = (\theta_{i1}, \dots, \theta_{iq})$: the correlation parameters in Gaussian correlation function
- The priors:
 - $[\sigma^2] \sim \text{IG}\left(\frac{\alpha}{2}, \frac{\beta}{2}\right)$
 - $[\sigma_i^2] \sim \text{IG}\left(\frac{\alpha_i}{2}, \frac{\beta_i}{2}\right), i = 1, \dots, p$
 - $[\frac{1}{\theta_{ij}}] \sim \text{Gamma}(3/2, a)$, for $i = 1, \dots, p$ and $j = 1, \dots, q$, where the scale parameter a is chosen such that maximum squared distance among any two points of the design matrix lies at the position of 95% quantile (Gramacy, 2015)

Empirical Bayesian Inference

The approximate predictive distribution of $\mathbf{y}(\mathbf{x}_0|\mathbf{Y})$:

$$\pi(\mathbf{y}(\mathbf{x}_0)|\mathbf{Y}) \approx \pi(\mathbf{y}(\mathbf{x}_0)|\mathbf{V}^*, \hat{\sigma}^2, \hat{\Theta}) \approx \mathcal{N}(\mathbf{B}\hat{\mathbf{c}}(\mathbf{x}_0|\mathbf{V}^*, \hat{\Theta}), \mathbf{B}\Lambda(\mathbf{V}^*, \hat{\Theta})\mathbf{B}^T + \hat{\sigma}^2\mathbf{I}_L). \quad (5)$$

where

- $\hat{\mathbf{c}}(\mathbf{x}_0|\mathbf{V}^*, \hat{\Theta}) = [\hat{c}_1(\mathbf{x}_0|\mathbf{v}_1, \hat{\theta}_1), \dots, \hat{c}_p(\mathbf{x}_0|\mathbf{v}_p, \hat{\theta}_p)]^T$
- $\Lambda(\mathbf{V}^*, \hat{\Theta}) = \text{diag}(\hat{\sigma}_1^2(\mathbf{x}_0|\mathbf{v}_1, \hat{\theta}_1), \dots, \hat{\sigma}_p^2(\mathbf{x}_0|\mathbf{v}_p, \hat{\theta}_p))$.

- $[\sigma^2 | Y]$ follows the inverse Gamma distribution $IG((NL + \alpha)/2, (r^T r + \beta)/2)$, and

$$\hat{\sigma}^2 = \operatorname{argmax}_{\sigma^2} \pi(\sigma^2 | Y) = \frac{1}{NL + \alpha + 2} (r^T r + \beta). \quad (6)$$

- $\hat{\theta}_i = \operatorname{argmax}_{\theta_i} \pi(\theta_i | \mathbf{v}_i), i = 1, \dots, p.$

$$\pi(\theta_i | \mathbf{v}_i) \propto |K_i|^{-\frac{1}{2}} \left(\frac{\beta_i + \psi_i}{2} \right)^{-(\alpha_i + N)/2} \pi(\theta_i), \quad (7)$$

Empirical Bayesian Inference

$$\pi(\mathbf{y}(\mathbf{x}_0)|\mathbf{V}^*, \Theta, \sigma^2) \approx \mathcal{N}(\mathbf{B}\hat{\mathbf{c}}(\mathbf{x}_0|\mathbf{V}^*, \Theta), \mathbf{B}\Lambda(\mathbf{V}^*, \Theta)\mathbf{B}^T + \sigma^2\mathbf{I}_L), \quad (8)$$

To compute (8), we make use of

- the distribution of $[\mathbf{y}(\mathbf{x}_0)|\mathbf{V}^*, \Theta, \sigma^2, c_1(\mathbf{x}_0), \dots, c_p(\mathbf{x}_0)]$
- the distribution of $[c_i(\mathbf{x}_0)|\mathbf{v}_i, \theta_i]$

Lemma

(Gelman et al., 2014) Suppose $[\mathbf{y}|\boldsymbol{\beta}, \sigma^2] \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$ and $[\boldsymbol{\beta}] \sim \mathcal{N}(\mathbf{b}, V)$, where $\mathbf{y} \in \mathbb{R}^n$, $\boldsymbol{\beta}, \mathbf{b} \in \mathbb{R}^m$, \mathbf{X} is an $n \times m$ matrix, and V is an $m \times m$ positive definite covariance matrix. Then, $[\mathbf{y}|\sigma^2] \sim \mathcal{N}(\mathbf{X}\mathbf{b}, \mathbf{XVX}^T + \sigma^2 \mathbf{I}_n)$.

- given $[\mathbf{y}(\mathbf{x}_0)|\mathbf{V}^*, \Theta, \sigma^2, c_1(\mathbf{x}_0), \dots, c_p(\mathbf{x}_0)]$
- given $[c_i(\mathbf{x}_0)|\mathbf{v}_i, \theta_i]$
- derive $[\mathbf{y}(\mathbf{x}_0)|\mathbf{V}^*, \Theta, \sigma^2]$

Empirical Bayesian Inference

The conditional distribution of $c_i(\mathbf{x}_0)$ given (\mathbf{v}_i, θ_i) are independent non-central t with $N + \alpha_i$ degrees of freedom, for $i = 1, \dots, p$, i.e.,

$$[c_i(x_0)|\mathbf{v}_i, \theta_i] \sim t_{N+\alpha_i}(\hat{c}_i(\mathbf{x}_0|\mathbf{v}_i, \theta_i), \hat{\sigma}_i^2(\mathbf{x}_0|\mathbf{v}_i, \theta_i)), \quad (9)$$

with the location parameter

$$\hat{c}_i(\mathbf{x}_0|\mathbf{v}_i, \theta_i) = k_i^T(\mathbf{x}_0)K_i^{-1}\mathbf{v}_i, \quad (10)$$

with $k_i(\mathbf{x}_0) = [K(\mathbf{x}_0, \mathbf{x}_1; \theta_i), \dots, K(\mathbf{x}_0, \mathbf{x}_N; \theta_i)]^T$, and the scale parameter

$$\hat{\sigma}_i^2(\mathbf{x}_0|\mathbf{v}_i, \theta_i) = \frac{(\beta_i + \psi_i) \left(1 - k_i^T(\mathbf{x}_0)K_i^{-1}k_i(\mathbf{x}_0)\right)}{\alpha_i + N}. \quad (11)$$

- The posterior distribution of $c_i(\mathbf{x}_0)|\mathbf{v}_i, \theta_i$

$$\pi(c_i(\mathbf{x}_0)|\mathbf{v}_i, \theta_i) \approx \mathcal{N}(\hat{c}_i(\mathbf{x}_0|\mathbf{v}_i, \theta_i), \hat{\sigma}_i^2(\mathbf{x}_0|\mathbf{v}_i, \theta_i)). \quad (12)$$

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- The local SVD-based GP model uses n ($\ll N$) points for approximating the predicted response at an arbitrary \mathbf{x}_0
- The *naive local SVD-based GP model* uses n nearest neighbour points based on the Euclidean distance
- The proposed *greedy local SVD-based GP model* sequentially finds the n neighbour points with the aim of reducing the prediction error

Greedy Local SVD-based GP Model

- Let k denote the current number of points in the neighbourhood set, $\mathbf{X}^{(k)}$ and $\mathbf{X} \setminus \mathbf{X}^{(k)}$ be the sets of selected and unselected (remaining) training points, respectively, and $\hat{\Theta}^{(k)} = \{\hat{\theta}_1^{(k)}, \dots, \hat{\theta}_p^{(k)}\}$ be the estimated correlation parameters.

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- The next follow-up point is chosen as

$$x_{k+1}^* = \operatorname{argmin}_{x \in \mathbf{X} \setminus \mathbf{X}^{(k)}} J(\mathbf{x}_0, \mathbf{x}),$$

J-Criterion

$$J(\mathbf{x}_0, \mathbf{x}) = E \left\{ E \left[\left\| \mathbf{y}(\mathbf{x}_0) - \hat{\mathbf{y}}(\mathbf{x}_0 | \mathbf{c}(\mathbf{x}), \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}) \right\|^2 \middle| \mathbf{c}(\mathbf{x}), \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}, (\hat{\sigma}^{(k)})^2 \right] \middle| \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}, (\hat{\sigma}^{(k)})^2 \right\}, \quad (13)$$

with

$$\begin{aligned} \hat{\mathbf{y}}(\mathbf{x}_0 | \mathbf{c}(\mathbf{x}), \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}) &= E \left[y(x_0) \middle| \mathbf{c}(\mathbf{x}), \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}, (\hat{\sigma}^{(k)})^2 \right] \\ &= \mathbf{B}^{(k)} \hat{\mathbf{c}}(\mathbf{x}_0 | \mathbf{c}(\mathbf{x}), \mathbf{V}^{*(k)}, \hat{\Theta}^{(k)}), \end{aligned}$$

Proposition

Suppose the expectations in (13) and (14) are taken with respect to the approximate predictive distribution (8). Then, for any $\mathbf{x} \in \mathbf{X} \setminus \mathbf{X}^{(k)}$

$$J(\mathbf{x}_0, \mathbf{x}) = (\hat{\sigma}^{(k)})^2 L + \sum_{i=1}^{p_k} (d_i^{(k)})^2 \hat{\sigma}_i^2(x_0 | \mathbf{x}, \mathbf{v}_i^{(k)}, \hat{\theta}_i^{(k)}), \quad (14)$$

where $d_i^{(k)}$ is the i -th largest singular value of $\mathbf{Y}^{(k)}$,

$$\hat{\sigma}_i^2(\mathbf{x}_0 | \mathbf{x}, \mathbf{v}_i^{(k)}, \hat{\theta}_i^{(k)}) = \frac{\rho_i^{(k)}(\mathbf{x}_0, \mathbf{x})}{\alpha_i + k} \left(\beta_i + \frac{\alpha_i + k}{\alpha_i + k - 1} \psi_i^{(k)} \right),$$

$$\begin{aligned} \rho_i^{(k)}(\mathbf{x}_0, \mathbf{x}) &= 1 - \tilde{\mathbf{k}}_i(\mathbf{x}_0, \mathbf{x})^T \tilde{\mathbf{K}}_i^{-1}(\mathbf{x}) \tilde{\mathbf{k}}_i(\mathbf{x}_0, \mathbf{x}), \\ \boldsymbol{\psi}_i^{(k)} &= (\mathbf{v}_i^{(k)})^T (\mathbf{K}_i^{(k)})^{-1} \mathbf{v}_i^{(k)}, \\ \tilde{\mathbf{k}}_i(\mathbf{x}_0, \mathbf{x}) &= [K(\mathbf{x}_0, \mathbf{x}_1^{(k)}; \hat{\boldsymbol{\theta}}_i^{(k)}), \dots, K(\mathbf{x}_0, \mathbf{x}_k^{(k)}; \hat{\boldsymbol{\theta}}_i^{(k)}), K(\mathbf{x}_0, \mathbf{x}; \hat{\boldsymbol{\theta}}_i^{(k)})]^T, \\ \tilde{\mathbf{K}}_i(\mathbf{x}) &= \begin{bmatrix} \mathbf{K}_i^{(k)} & \mathbf{k}_i^{(k)}(\mathbf{x}) \\ \mathbf{k}_i^{(k)}(\mathbf{x})^T & 1 \end{bmatrix}, \end{aligned}$$

with $\mathbf{v}_i^{(k)}$ being the i -th column of $\mathbf{V}^{*(k)}$, for $i = 1, \dots, p_k$, $\mathbf{x}_j^{(k)}$ being the j -th point of $\mathbf{X}^{(k)}$ for $j = 1, \dots, k$, $\mathbf{K}_i^{(k)}$ being a $k \times k$ matrix with $K(\mathbf{x}_j^{(k)}, \mathbf{x}_l^{(k)}; \hat{\boldsymbol{\theta}}_i^{(k)})$, as the (j, l) -th entry, and $\mathbf{k}_i^{(k)}(\mathbf{x}) = [K(\mathbf{x}, \mathbf{x}_1^{(k)}; \hat{\boldsymbol{\theta}}_i^{(k)}), \dots, K(\mathbf{x}, \mathbf{x}_k^{(k)}; \hat{\boldsymbol{\theta}}_i^{(k)})]^T$.

J -Criterion

- Finding x_{k+1}^* by minimizing the J -criterion in Proposition 1 is equivalent to obtaining

$$x_{k+1}^* = \operatorname{argmin}_{x \in X \setminus \mathbf{x}^{(k)}} \left[\sum_{i=1}^{p_k} (d_i^{(k)})^2 \hat{\sigma}_i^2(x_0 | \mathbf{x}, \mathbf{v}_i^{(k)}, \hat{\theta}_i^{(k)}) \right]. \quad (15)$$

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- This J -criterion is a generalization of the active learning Cohn (ALC) criterion (Cohn et al., 1996)

$$\int_{\mathbf{x}} \left[\int_y (\hat{y}(\mathbf{x}) - y(\mathbf{x}))^2 dP(y|\mathbf{x}) \right] dP(\mathbf{x}),$$

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- We use L_2 norm discrepancy instead of the squared error.

Simulations

- We compare the performance of the three methods *full svdGP*, *naive local svdGP*, and *greedy local svdGP*

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- We compare the performance of the three methods *full svdGP*, *naive local svdGP*, and *greedy local svdGP*
- The performance is evaluated by comparing

$$\text{NMSPE}(x) = \frac{\sum_{t=1}^L (y_t(x) - \hat{y}_t(x))^2}{\sum_{t=1}^L (y_t(x) - \bar{y}(x))^2}, \quad (16)$$

where $y_t(x)$ is the real (scalar) response for input x at time t , $t = 1, \dots, L$, $\hat{y}_t(x)$ is the corresponding model prediction, and $\bar{y}(x) = \sum_{t=1}^L y_t(x)/L$.

Example 1 (Forrester et al., 2008)

$$f(x, t) = (x_1 t - 2)^2 \sin(x_2 t - x_3), \quad (17)$$

where $x = (x_1, x_2, x_3)^T \in [4, 10] \times [4, 20] \times [1, 7]$, and $t \in [1, 2]$ is on a 200-point equidistant time-grid.

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- The training data is generated using a 10000-point random Latin hypercube design (LHD)
- The test data is generated using a 2000-point random LHD
- For local svdGP, use $n = 20, 40$, and $n_0 = \lceil n/4 \rceil, \lceil n/2 \rceil$

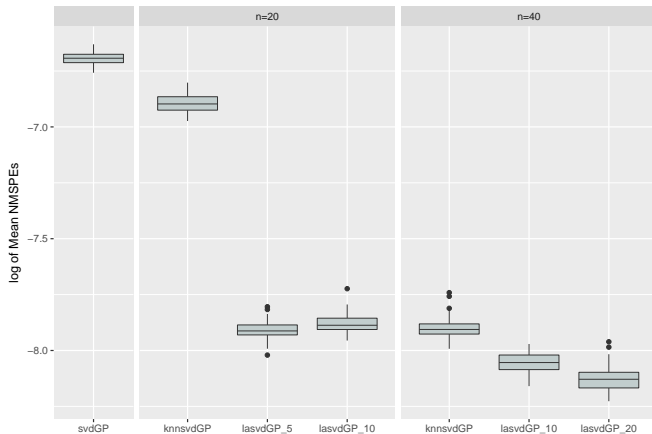


Figure: Boxplots of the log of mean NMSPE computed from 2,000 test points over 50 simulations for the computer simulator (17).

Example 2 (Bliznyuk et al.,2008)

$$f(x, t) = \frac{M}{\sqrt{Dt}} \exp\left(\frac{-s^2}{4Dt}\right) + \frac{M}{\sqrt{D(t-\tau)}} \exp\left(-\frac{(s-L)^2}{4D(t-\tau)}\right) I(\tau < t),$$

(18)

where $x = (M, D, L, \tau, s)^T$, M denotes the mass of pollutant spilled at each location, D is diffusion rate in the channel, L is location of the second spill, and τ is time of the second spill, $t \in [0.3, 60]$ is on a regular 200-point equidistant time grid,
 $x \in [7, 13] \times [0.02, 0.12] \times [0.01, 3] \times [30.01, 30.295] \times [0, 3], .$

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- For local svdGP, use $n = 30, 50$, and $n_0 = \lceil n/4 \rceil, \lceil n/2 \rceil$

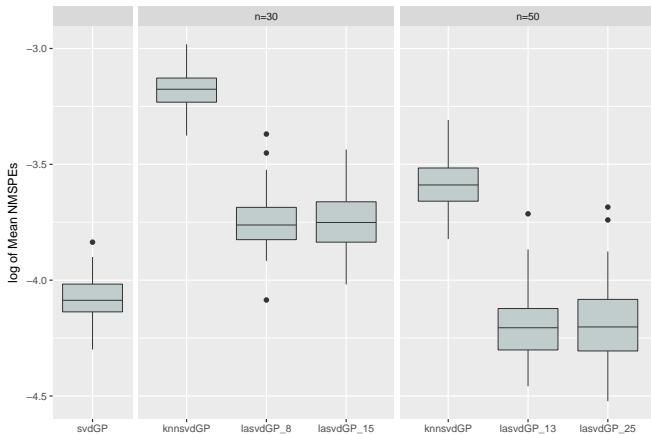


Figure: Boxplots of the log of mean NMSPE computed from 2,000 test points over 50 simulations for the computer simulator (19).

Example 3 (TDB simulator)

- The two-delay blowfly (TDB) model (Teismann et al., 2009) simulates European red mites (ERM) population dynamics under predator-prey interactions in apple orchards via numerically solving the Nicholson's blowfly differential equation (Gurney et al., 1980).

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- $N = 20,000$ training and $M = 10,000$ test points are generated using random LHDs for the emulation of this process.

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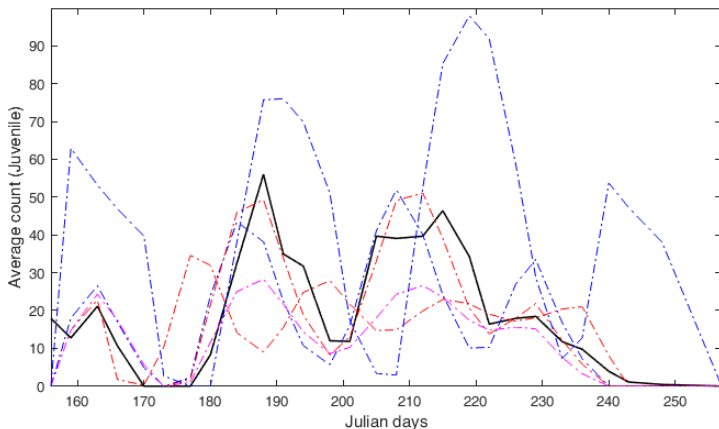
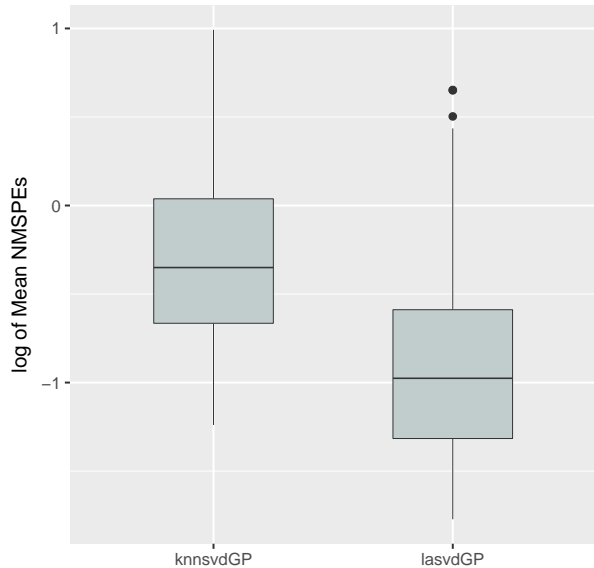


Figure: Juvenile ERM population dynamics as outputs of the TDB model at five different inputs. Black solid curve shows the field data and the other curves show the TDB outputs.

Example 3 (TDB simulator)



Inverse Problem

- Take a q -dimensional input \mathbf{x} and return a time series response $\mathbf{y}(\mathbf{x}) = \{y(\mathbf{x}, t), t = 1, \dots, L\}$ and consider a target field observation \mathbf{z}_0

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- The inverse problem refers to searching the input \mathbf{x} such that the computer simulator $y(\mathbf{x}, t) \approx z_0(t)$ for all $t = 1, \dots, L$.
- Consider the following model, for $t = 0.5, 0.52, \dots, 2.5$ and $x \in [0, 1]$,

$$y(x, t) = \frac{\sin(10\pi t)}{2t} + |t - 1|^{(2+4x)}, \quad (19)$$

and let the true field data correspond to $x_0 = 0.5$.

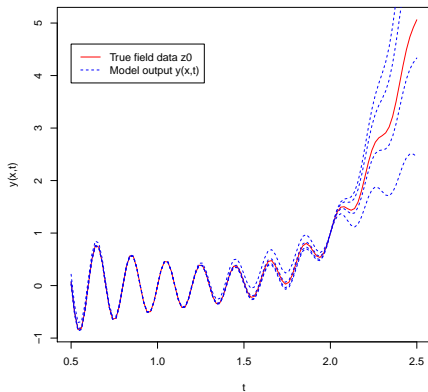


Figure: A few computer model outputs and the true field data for the computer simulator (19).

Existing Methods

- Scalarization by likelihood ratio statistic (Pratola et al., 2013)

$$\Delta(\mathbf{t}_i) = -2\log\left(\frac{L_r^*(\delta(\mathbf{t}_i))}{L_u^*(\delta(\mathbf{t}_i))}\right), \quad (20)$$

where $\delta(\mathbf{t}_i) = \mathbf{Y}^f - \mathbf{Y}_i^c$, $\mathbf{Y}^f = \eta(\theta) + \varepsilon$, and $\mathbf{Y}_i^c = \eta(\mathbf{t}_i)$, \mathbf{t}_i is the i th input setting of calibration parameters.

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- Scalarization by L_2 discrepancy (Ranjan et al., 2016).

$$w(\mathbf{x}) = \|\mathbf{y}(\mathbf{x}) - \mathbf{z}_0\| = \sqrt{\frac{1}{L} \sum_{t=1}^L |\mathbf{y}(\mathbf{x}, t) - \mathbf{z}_0(t)|^2} \quad (21)$$

and find the minimum of $w(\mathbf{x})$.

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- The first term represents the L_2 distance between the posterior mean of the simulator response at \mathbf{x} and the projection of \mathbf{z}_0 on $\mathcal{M}(\mathbf{B})$ with $\mathbf{B} = \mathbf{U}^* \mathbf{D}^*$; the second term represents the model uncertainty at \mathbf{x} .

Sequential Designs

Choose the follow-up design points by sequentially maximizing the criterion

$$\begin{aligned}\mathbf{x}_{new} &= \operatorname{argmax}_{\mathbf{x}} J_I(\mathbf{x}) \\ &= \operatorname{argmax}_{\mathbf{x}} \sum_{i=1}^p d_i^2 [\xi \hat{\sigma}_i^2(\mathbf{x}|\mathbf{v}_i, \hat{\theta}_i) - (\hat{c}_i(\mathbf{x}|\mathbf{v}_i, \hat{\theta}_i) - \hat{c}_{\mathbf{z}_0, i})^2]\end{aligned}$$

where ξ is a tuning parameter which controls the emphasis on reducing the model uncertainty.

Simulation Study

- Consider the inverse problem using one-shot designs and sequential designs

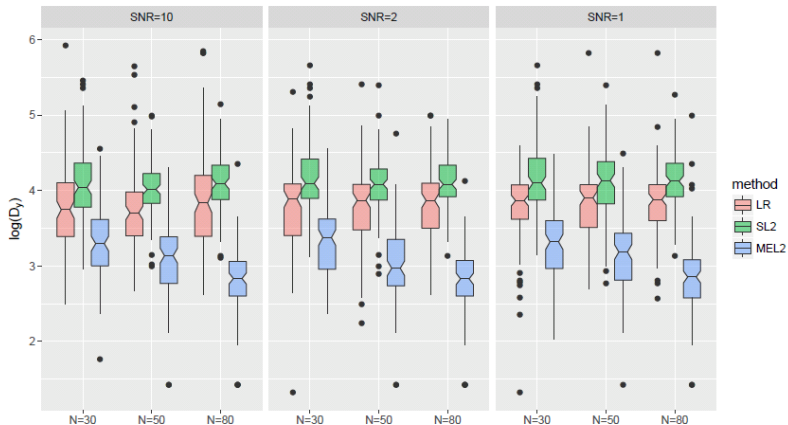
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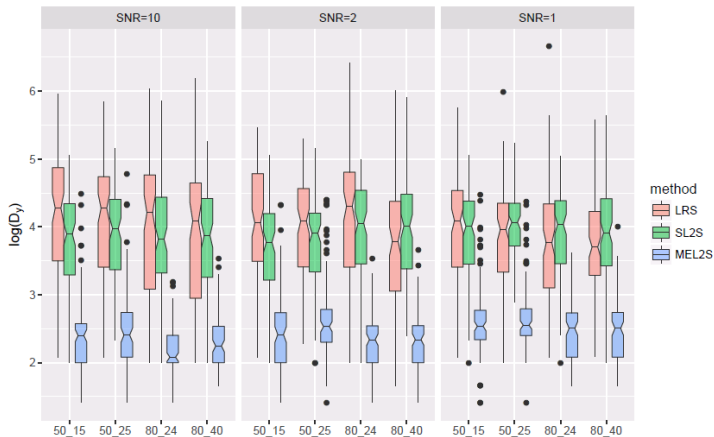
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- Consider the inverse problem using one-shot designs and sequential designs
- Compare LR (Pratola et al.,2013), SL2 (Ranjan et al., 2016), and MEL2 (the proposed approach)
- For a pre-specified \mathbf{x}^* , compare using $D_{\mathbf{y}} = \|\mathbf{y}(\hat{\mathbf{x}}^*) - \mathbf{y}(\mathbf{x}^*)\|_2$.

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Concluding Remarks

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- Proposed a new design criterion to determine local neighbour sequentially
- Introduced a new design criterion to solve the inverse problem in dynamic computer experiments

Thank you! Q&A.