Deep Gaussian Process Surrogates for Computer Experiments

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Where are we going?

1. Deep Gaussian Processes
   - Why?
   - What?
   - How?
2. Active Learning
   - Why?
   - What?
   - How?
3. Vecchia Approximation
   - Why?
   - What?
   - How?

Surrogates as statistical models of computer experiments

Surrogates are meta-models of computer experiments.

Surrogates are used to make **predictions** with appropriate **uncertainty quantification (UQ)**.

As simulations become more complex, surrogate models must keep up.

"Shallow" Gaussian process (GP) surrogates

The typical surrogate model is a GP

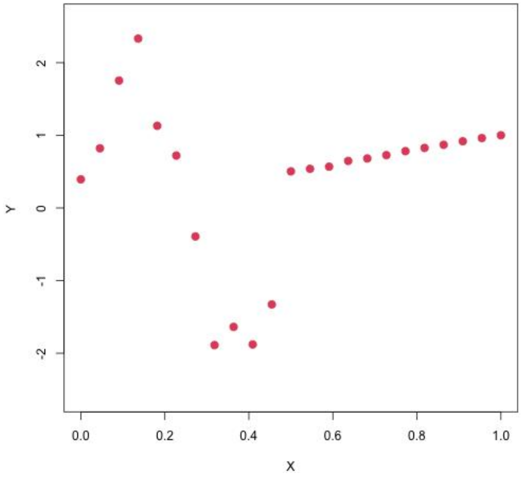
- nonlinear
- nonparametric (mostly)
- adept at uncertainty quantification

A GP assumes a MVN prior

$$Y \sim \mathcal{N}(0, \Sigma(X))$$

All of the "work" is in the covariance

$$\Sigma(X)^{ij} = \tau^2 \left(k \left(\frac{||x_i - x_j||^2}{\theta} \right) + g\mathbb{I}_{i=j} \right)$$



Higdon (2002), Virtual Library of Simulation Experiments (VLSE)

"Shallow" Gaussian process (GP) surrogates

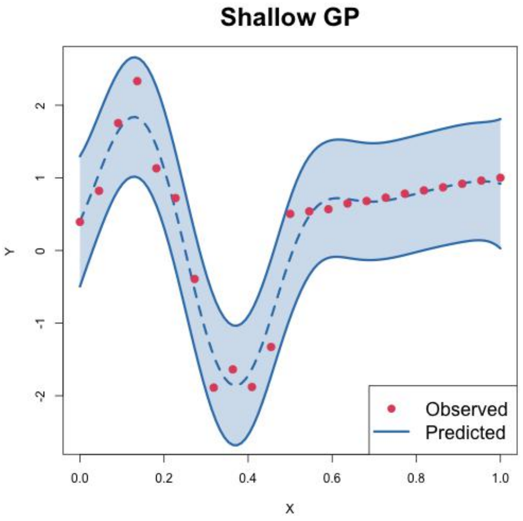
Conditioned on observed data (X, Y) and hyperparameter settings, posterior predictions at locations $\mathcal{X}$ follow

$$Y(\mathcal{X}) \mid X, Y \sim \mathcal{N}(\mu^\star, \Sigma^\star)$$

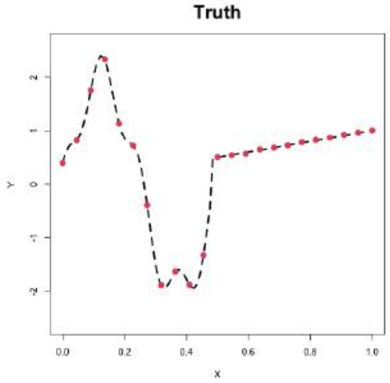
where

$$\mu^\star = \Sigma(\mathcal{X}, X)\Sigma(X)^{-1}Y$$
$$\Sigma^\star = \Sigma(\mathcal{X}) - \Sigma(\mathcal{X}, X)\Sigma(X)^{-1}\Sigma(X, \mathcal{X})$$

Hyperparameters may be estimated through MLE or sampled through MCMC.



"Shallow" GP surrogates are limited by stationarity



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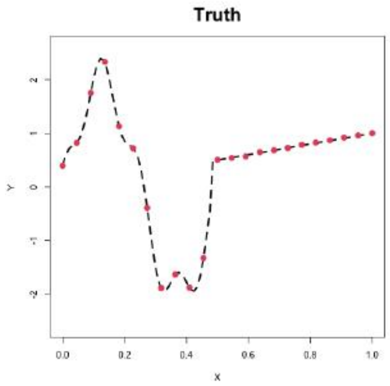

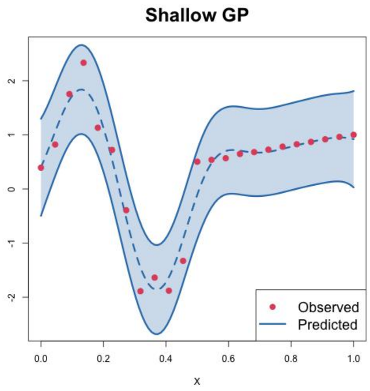

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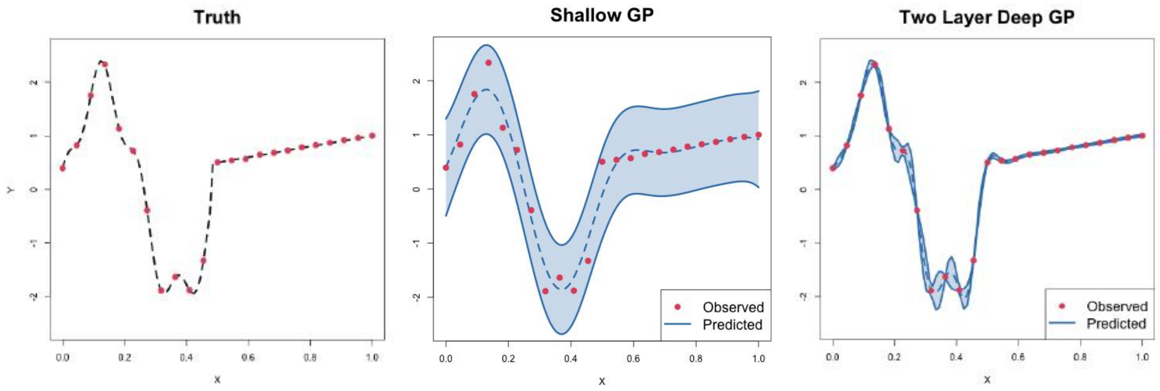

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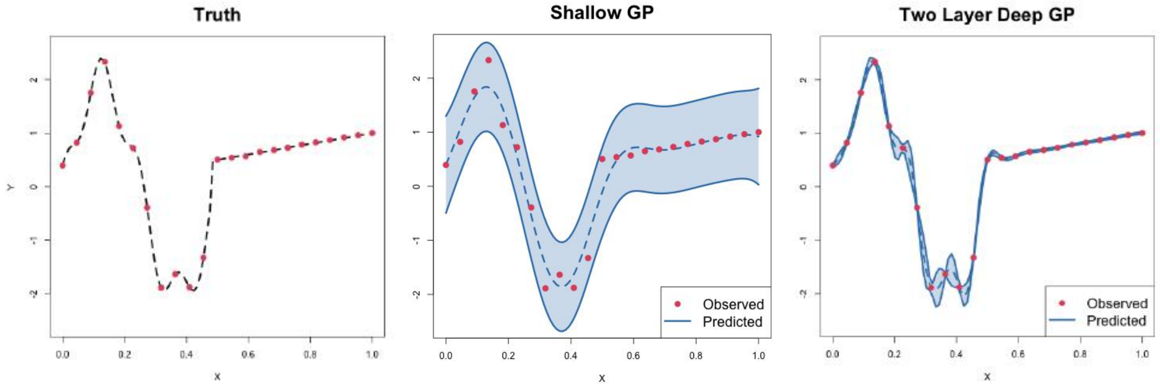
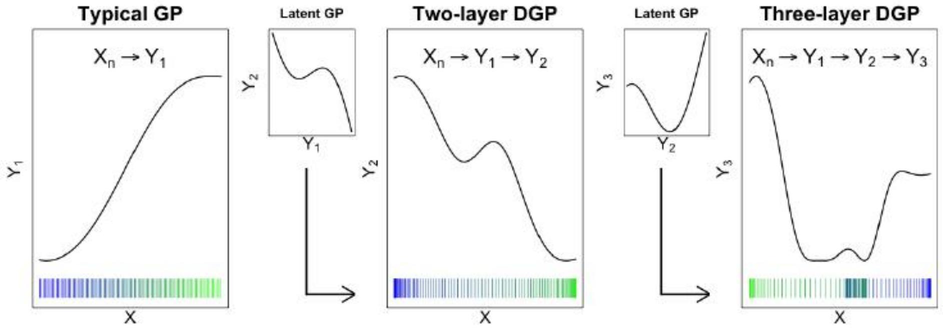


Approaches to modeling non-stationarity

- Non-stationary kernels (Paciorek & Schervish, 2003; Higdon et al., 1999)
- Partition/Local GPs (Gramacy & Lee, 2007; Gramacy & Apley, 2015)
- Deep GPs (Damianou & Lawrence, 2012; Schmidt & O'Hagan, 2003)

DGPs are functional compositions of GPs



$$Y_1 \sim \mathcal{N}(0, \Sigma(X)) \quad \longrightarrow \quad Y_2 \sim \mathcal{N}(0, \Sigma(Y_1)) \quad \longrightarrow \quad Y_3 \sim \mathcal{N}(0, \Sigma(Y_2))$$

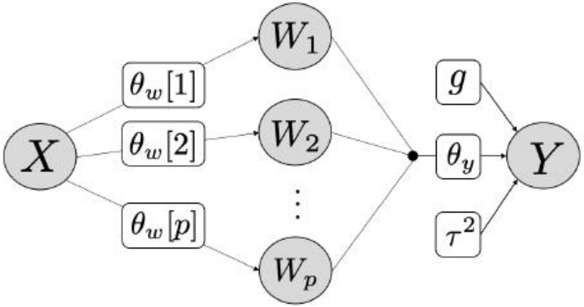
Intermediate Gaussian layers are unobserved/latent

We represent a two-layer DGP prior as

$$Y \mid W \sim \mathcal{N}\left(0, \Sigma(W)\right)$$
$$W_k \overset{\text{ind}}{\sim} \mathcal{N}\left(0, \Sigma(X)\right) \quad \forall \;\; k = 1, \ldots, p.$$

Posterior inference requires

$$\mathcal{L}(Y \mid X) \propto \int \mathcal{L}(Y \mid W)\mathcal{L}(W \mid X)\; dW$$



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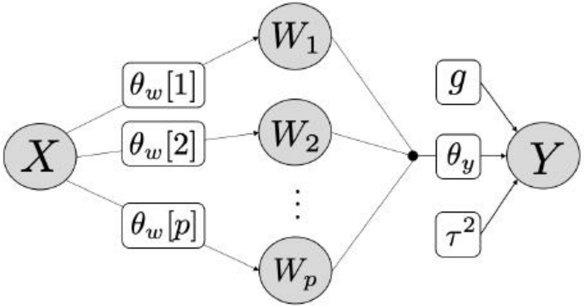

To encourage identifiability and parsimony, we impose

- Unit scale and noise-free latent W
- Conditional independence among nodes of W
- Isotropic length scales (single θ for all dimensions of X and W)

Direct posterior inference for DGPs is intractible

Direct posterior inference is intractible due to the latent layer W.

$$\mathcal{L}(Y \mid X) \propto \int \mathcal{L}(Y \mid W)\mathcal{L}(W \mid X)\, dW$$

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Methods for approximate DGP inference:

- Variational inference (Damianou & Lawrence, 2012; Salimbeni & Deisenroth, 2017; Marmin & Filippone, 2022)
- Expectation propogation (Bui et al., 2016)
- Hamiltonian Monte Carlo sampling (Havasi et al., 2018)

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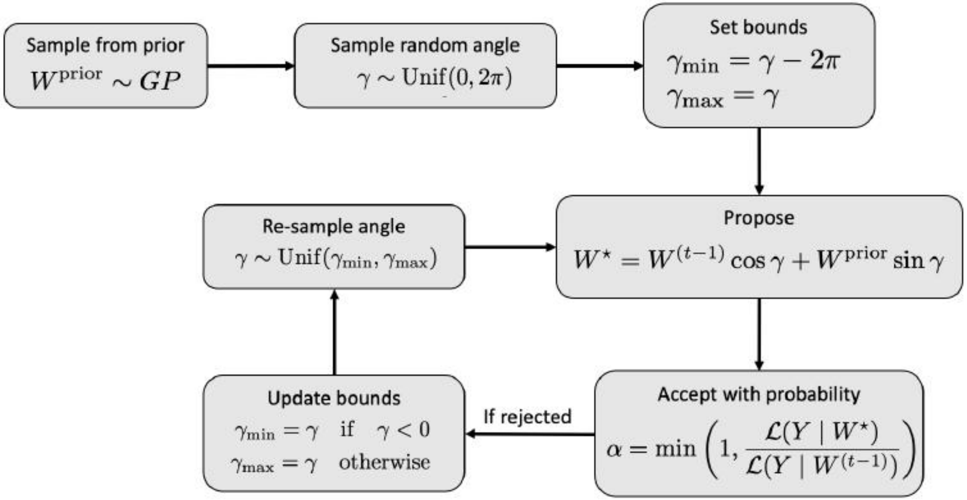
To prioritize UQ, we embrace a fully-Bayesian MCMC inferential scheme.

- Metropolis-Hastings sampling of covariance hyperparameters
- **Elliptical slice sampling of latent Gaussian layers** (Murray et al., 2010)
- Iteration in a Gibbs scheme

Elliptical slice sampling provides efficient mixing


Sample from prior
$W^{\text{prior}} \sim GP$
Sample random angle
$\gamma \sim \text{Unif}(0, 2\pi)$
Set bounds
$\gamma_{\min} = \gamma - 2\pi$
$\gamma_{\max} = \gamma$
Propose
$W^\star = W^{(t-1)} \cos\gamma + W^{\text{prior}} \sin\gamma$
Accept with probability
$\alpha = \min\left(1, \frac{\mathcal{L}(Y \mid W^\star)}{\mathcal{L}(Y \mid W^{(t-1)})}\right)$
If rejected
Update bounds
$\gamma_{\min} = \gamma$ if $\gamma < 0$
$\gamma_{\max} = \gamma$ otherwise
Re-sample angle
$\gamma \sim \text{Unif}(\gamma_{\min}, \gamma_{\max})$

Also used for stochastic imputation (Ming et al., 2021)

Elliptical slice sampling provides efficient mixing

```
R> library(deepgp)
R> fit <- fit_two_layer(x, y, nmcmc = 10000)
R> fit <- trim(fit, 5000, 5)
R> fit <- predict(fit, x_pred)
```

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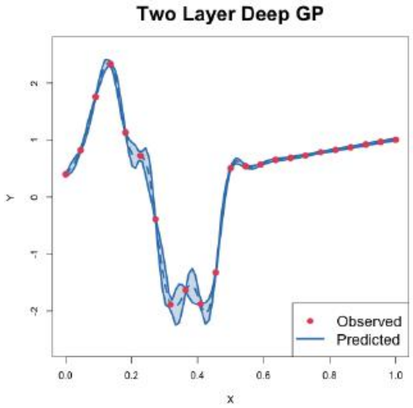
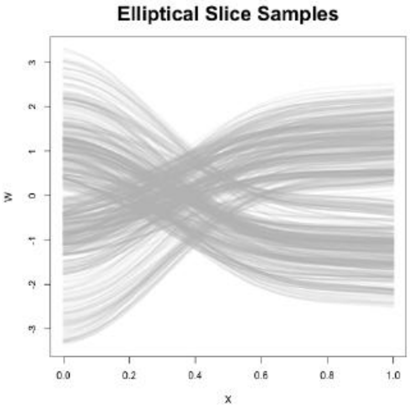
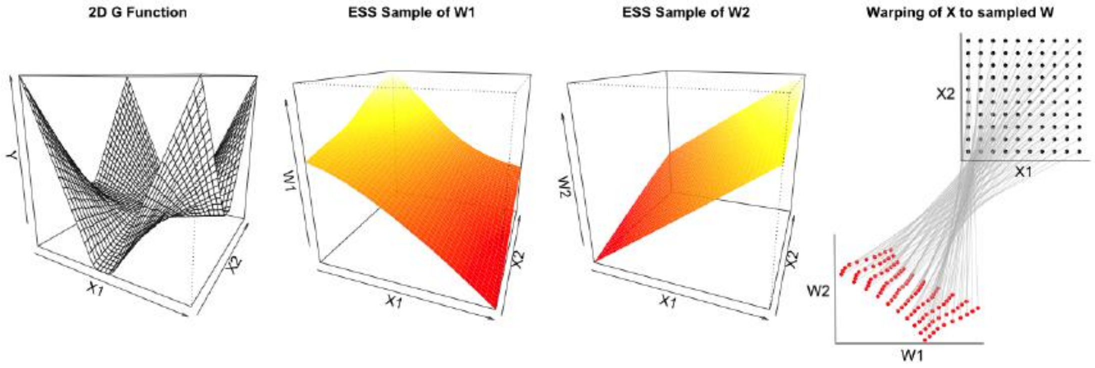




Preview of DGP predictive prowess

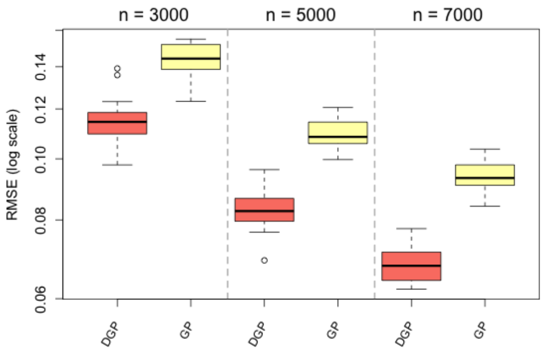
2-dimensional G-function

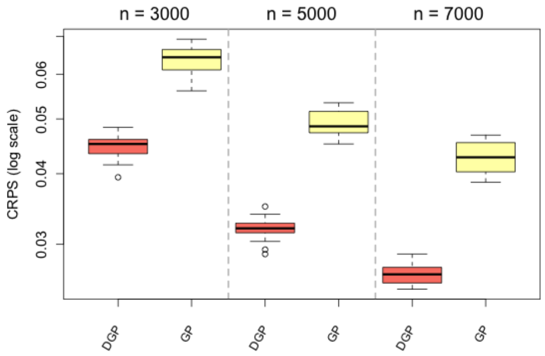


Marrel et al. (2009), VLSE

Preview of DGP predictive prowess

4-dimensional G-function (20 reps)





- RMSE = root mean squared error
- CRPS = continuous rank probability score (Gneiting & Raftery, 2007)

Deep Gaussian processes - Summary

- Why?
  - Non-stationary flexibility while maintaining the predictive prowess and uncertainty quantification of “shallow” GPs
- What?
  - Functional compositions of Gaussian layers
  - Intermediate layers are latent/unobserved
- How?
  - Bayesian MCMC hinging on elliptical slice sampling of latent layers
  - Implementation in the `deepgp` package

Statistical models are only as good as their data

While a DGP has the flexibility to *address* non-stationarity, the data must *reveal* it.

- Strategically choose input configurations to maximize learning from a limited budget (Sauer, Gramacy & Higdon, 2022; Gramacy, Sauer, & Wycoff, 2022).

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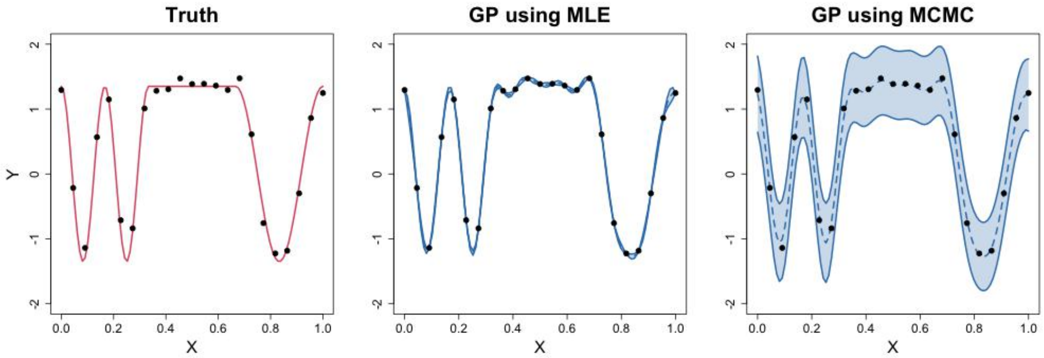
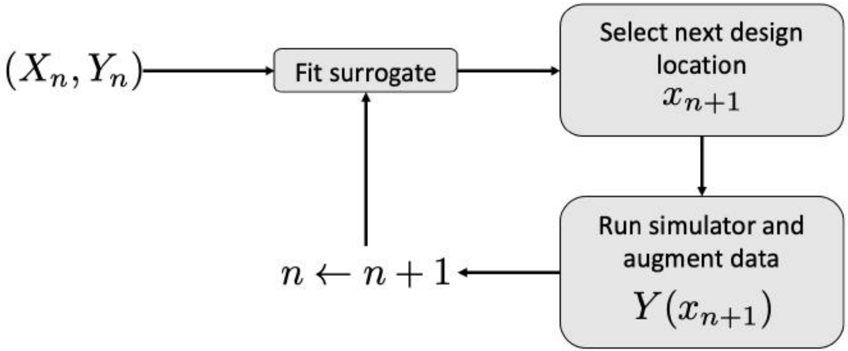


Active Learning/Sequential Design through greedy acquisitions

When computational costs are high, we may make the most of a stringent simulation budget through greedy acquisition: sequential design.


(X_n, Y_n)
Fit surrogate
Select next design location x_{n+1}
Run simulator and augment data $Y(x_{n+1})$
$n \leftarrow n+1$

Active Learning/Sequential Design through greedy acquisitions

$$Y(x) \mid X_n, Y_n \sim \mathcal{N}\left(\mu(x), \sigma^2(x)\right) \quad \text{for} \quad \begin{aligned} \mu(x) &= \Sigma(x, X_n)\Sigma(X_n)^{-1} Y_n \\ \sigma^2(x) &= \Sigma(x) - \Sigma(x, X_n)\Sigma(X_n)^{-1}\Sigma(X_n, x) \end{aligned}$$

Given augmented inputs $X_{n+1} = \{X_n, x_{n+1}\}$, the variance becomes

$$\sigma^2_{n+1}(x) = \Sigma(x) - \Sigma(x, X_{n+1})\Sigma(X_{n+1})^{-1}\Sigma(X_{n+1}, x)$$

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$$\sigma^2_{n+1}(x) = \Sigma(x) - \Sigma(x, X_{n+1})\Sigma(X_{n+1})^{-1}\Sigma(X_{n+1}, x)$$

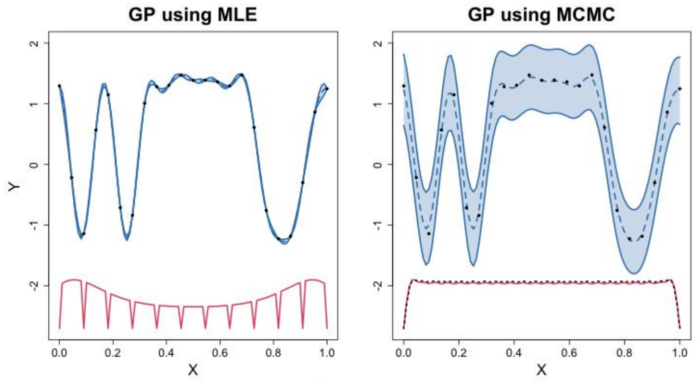
We choose acquisitions to minimize the posterior predictive variance.

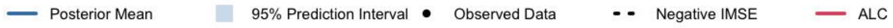
$$x_{n+1} = \underset{x_{n+1}}{\text{argmin}}\ \mathrm{IMSE}(x_{n+1}) \quad \text{where} \quad \mathrm{IMSE}(x_{n+1}) = \int \sigma^2_{n+1}(x)dx$$

For faster computation, we also utilize the sum approximation (Cohn, 1994).

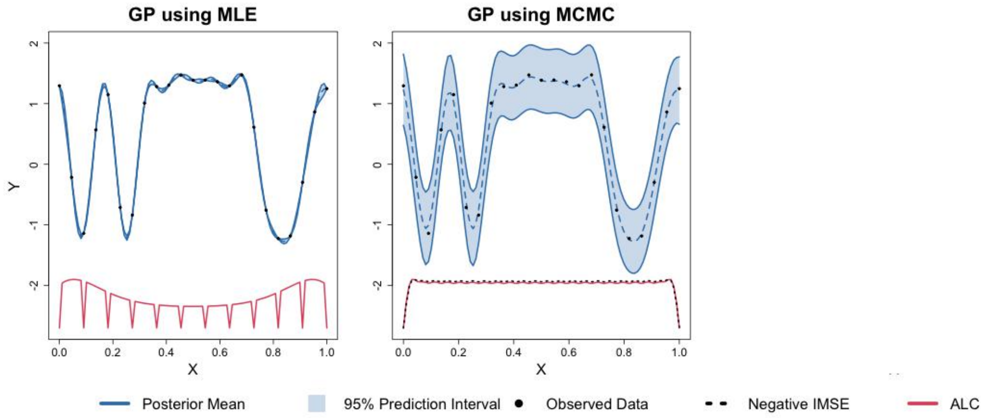
$$x_{n+1} = \underset{x_{n+1}}{\text{argmax}}\ \mathrm{ALC}(x_{n+1}) \quad \text{where} \quad \mathrm{ALC}(x_{n+1}) \propto -\sum_{x \in X_{ref}} \sigma^2_{n+1}(x)$$

Active Learning/Sequential Design through greedy acquisitions





Active Learning/Sequential Design through greedy acquisitions

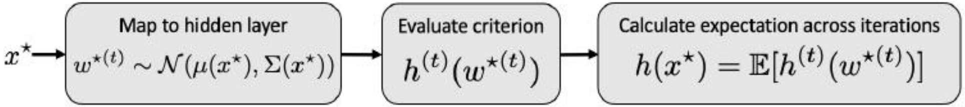


If the surrogate is stationary, sequential designs will end up "space-filling."

Active Learning for DGPs

Novel inputs $x^\star$ are mapped to hidden layer $w^{\star(t)}$ using typical GP prediction.

Criteria (IMSE/ALC) are calculated for $w^{\star(t)}$ and averaged across iterations.


$x^\star$
Map to hidden layer
$w^{\star(t)} \sim \mathcal{N}(\mu(x^\star), \Sigma(x^\star))$
Evaluate criterion
$h^{(t)}(w^{\star(t)})$
Calculate expectation across iterations
$h(x^\star) = \mathbb{E}[h^{(t)}(w^{\star(t)})]$

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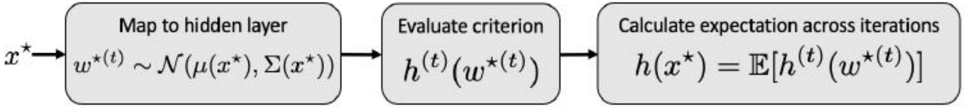
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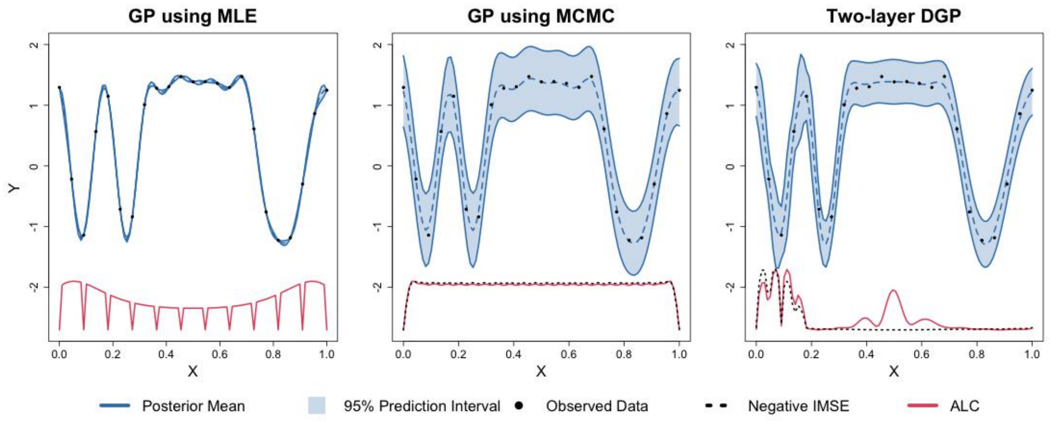
$x^\star$

```
R> fit <- fit_two_layer(x, y)
R> imse <- IMSE(fit, x_candidates)
R> alc <- ALC(fit, x_candidates)
```

DGPs depart from space filling and outperform on RMSE/SCORE



▸ plot of ESS samples

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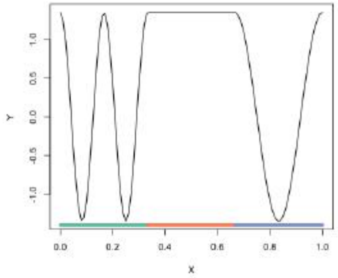
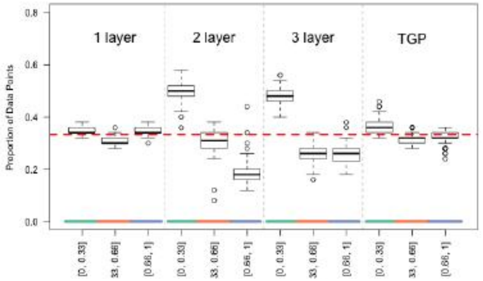
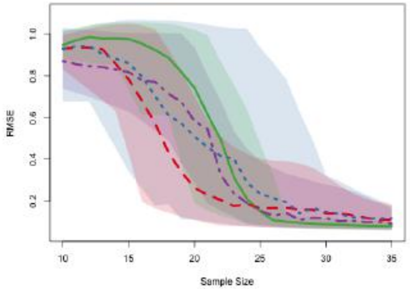
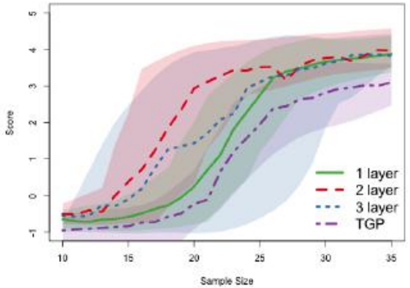


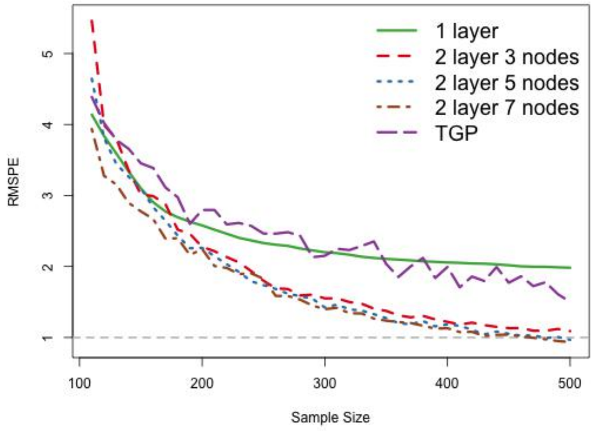


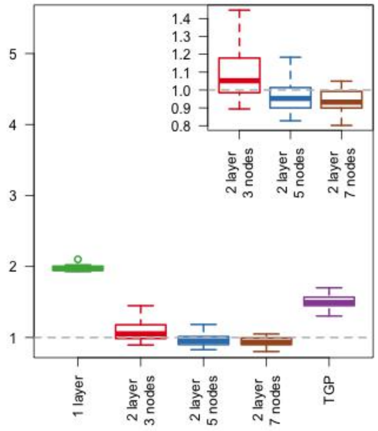




Satellite drag computer simulation

- *Test Particle Monte Carlo (TPM)* simulator developed at LANL (Sun et al., 2019)
- Inputs: 7 configuration variables, satellite mesh, atmospheric composition
- Goal: RMSPE below 1% **starting on a restricted domain**





Active Learning for DGPs - Summary

- Why?
  - When computer simulations are expensive, the "budget" of evaluations is limited
- What?
  - Sequential selection of inputs using greedy acquisition criteria
  - IMSE or ALC (see Gramacy, Sauer, & Wycoff, 2022 for Expected Improvement)
- How?
  - Map inputs through hidden layers and evaluate criterion on mapped values
  - Sequential selections depart from space-filling and focus on regions of interest

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- Deploy a space filling design that is large enough to pick up on changes in the response surface (Sauer, Cooper & Gramacy, 2022).

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Large datasets present computational bottlenecks for GP inference ($\mathcal{O}(n^3)$).

$$\mathcal{L}(Y \mid X) \propto |\Sigma(X)|^{-1/2} \exp\left(-\frac{1}{2} Y^\top \Sigma(X)^{-1} Y\right)$$

These are compounded in a Bayesian DGP setting.

Inducing points are popular, but not effective

Competing implementations for DGP inference ...

- Variational inference (Damianou & Lawrence, 2012; Salimbeni & Deisenroth, 2017; Marmin & Filippone, 2022)
- Expectation propogation (Bui et al., 2016)
- Hamiltonian Monte Carlo sampling (Havasi et al., 2018)

All (but one) use **inducing point** approximations to handle large data sizes (Snelson & Ghahramani, 2006; Banerjee et al., 2008):

- observe covariance through fixed set of "knots" which are tricky to place and result in blurry predictions (Garton et al., 2020; Wu et al., 2022).

Marmin & Filippone (2022) utilize **random feature expansions**.

Vecchia approximation from conditional distributions

Any joint distribution may be represented as a product of conditional distributions, i.e.

$$f(y_3, y_2, y_1) = f(y_3 \mid y_2, y_1) f(y_2 \mid y_1) f(y_1).$$

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In general,

$$\mathcal{L}(Y) = \prod_{i=1}^{n} \mathcal{L}\left(y_i \mid Y_{c(i)}\right) \quad \text{for} \quad c_0 = \emptyset \quad \text{and} \quad c_i = \{1, 2, \ldots, i-1\} \;\; \forall \;\; i = 2, \ldots, n.$$

The Vecchia approximation (Vecchia, 1988) instead takes the subset

$$c_i \subset \{1, 2, \ldots, i-1\} \quad \text{of size} \quad |c_i| = \min(m, i-1).$$

Vecchia approximation of GPs

In a typical "shallow" GP setting we have

$$\mathcal{L}(Y) = \prod_{i=1}^{n} \mathcal{L}\left(y_i \mid Y_{c(i)}\right),$$

where

$$\mathcal{L}(y_i \mid Y_{c(i)}) \sim \mathcal{N}_1(\mu_i(X), \sigma_i^2(X)) \quad \text{for} \quad \begin{aligned} B_i(X) &= \Sigma(x_i, X_{c(i)})\Sigma(X_{c(i)})^{-1} \\ \mu_i(X) &= B_i(X)Y_{c(i)} \\ \sigma_i^2(X) &= \Sigma(x_i) - B_i(X)\Sigma(X_{c(i)}, x_i). \end{aligned}$$

This converts an $\mathcal{O}(n^3)$ computation into n-many $\mathcal{O}(m^3)$ computations.

Stein et al., 2004; Datta et al., 2016; Stroud et al., 2017; Finley et al., 2019; Katzfuss & Guinness 2020, 2021

Vecchia approximation induces sparsity in precision matrix

The Cholesky decomposition of the precision matrix is **sparse**.

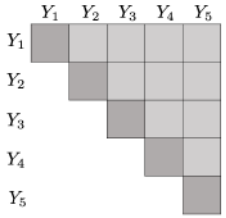
$$Y \sim \mathcal{N}\left(0, \Sigma = Q^{-1} = (UU^\top)^{-1}\right)$$

The upper triangular U matrix has closed-form

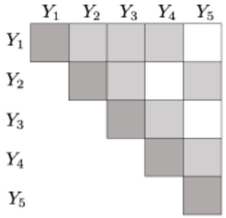
$$U^{ji} = \begin{cases} \frac{1}{\sigma_i(X)} & i = j \\ -\frac{1}{\sigma_i(X)} B_i(X)[\#j \in c(i)] & j \in c(i) \\ 0 & \text{otherwise} \end{cases}$$

whose entries may be populated **in parallel**.

$m = n - 1$



$m = 2$



Katzfuss & Guinness (2021, Proposition 1)

GP tasks hinge on the sparse U matrix

Likelihood Evaluation

$$\log \mathcal{L}(Y) \propto \sum_{i=1}^{n} \log(U^{ii}) - \frac{1}{2} Y^\top U U^\top Y$$

Prior Samples

$$Y^\star = (U^\top)^{-1} z$$
$$z \sim \mathcal{N}(0, \mathbb{I})$$

Posterior Predictions

$$\mathcal{Y} \mid Y, X \sim \mathcal{N}(\mu^\star, \Sigma^\star)$$
$$\mu^\star = -(U_{\mathcal{X}}^\top)^{-1} U_{x,\mathcal{X}}^\top Y$$
$$\Sigma^\star = \left(U_{\mathcal{X}} U_{\mathcal{X}}^\top\right)^{-1}$$

Vecchia-approximated DGPs

Recall our “un-approximated” DGP model

$$Y \mid W \sim \mathcal{N}(0, \Sigma(W)) \qquad W_k \overset{\text{ind}}{\sim} \mathcal{N}(0, \Sigma(X)) \;\; \forall \;\; k = 1, \ldots, p.$$

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In our DGP-Vecchia model, we impose a Vecchia approximation at each GP

$$Y \mid W \sim \mathcal{N}\left(0, (U_w U_w^\top)^{-1}\right) \qquad W_k \overset{\text{ind}}{\sim} \mathcal{N}_n\left(0, \left((U_x^{(k)})(U_x^{(k)})^\top\right)^{-1}\right) \;\; \forall \;\; k = 1, \ldots, p.$$

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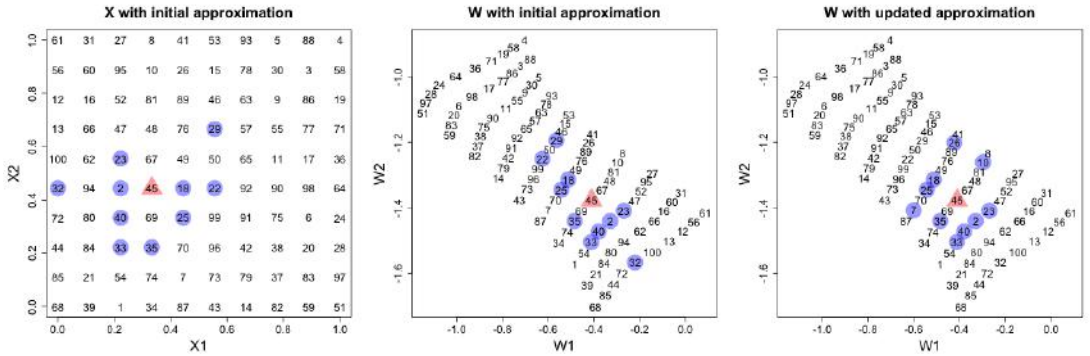
Within our DGP MCMC algorithm, we replace every (i) likelihood evaluation, (ii) prior sample, and (iii) GP prediction with its Vecchia-approximated counterpart.

```
R> fit <- fit_two_layer(x, y, vecchia = TRUE)
R> fit <- predict(fit, x_pred)
```

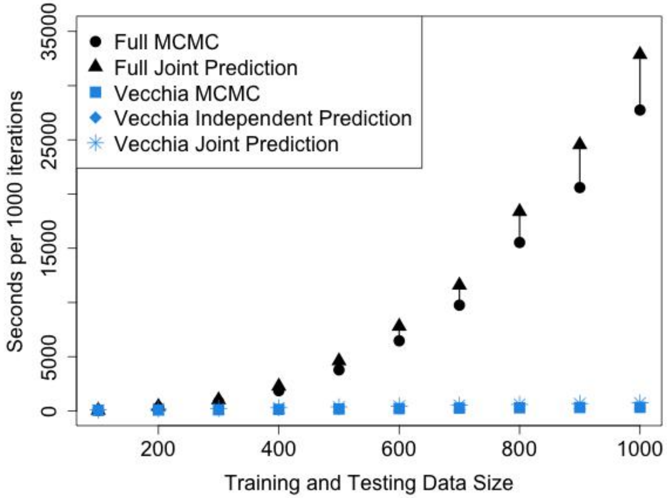
Ordering/conditioning specifications

We utilize

- Random orderings at each Gaussian layer (Guinness, 2018; Wu et al., 2022)
- Nearest-neighbor conditioning sets (Datta et al., 2016)
- Updating of conditioning sets based on learned latent layer warpings



Computation scales linearly

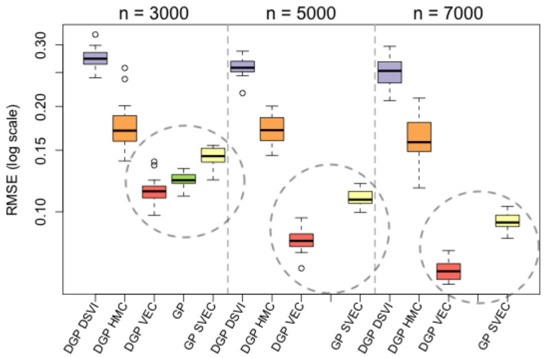


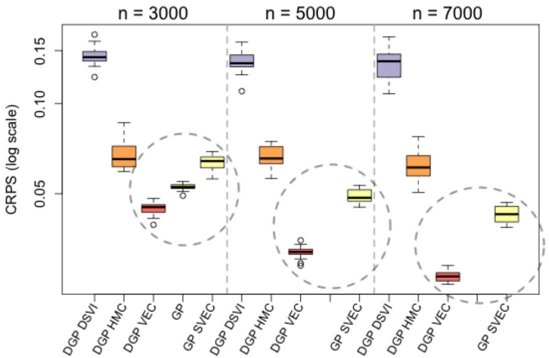
Deep and shallow competitors

- DGP DSVI: "doubly stochastic" VI (Salimbeni & Deisenroth, 2017)
  - utilizes inducing points
- DGP HMC: Hamiltonian Monte Carlo (Havasi et al., 2018)
  - utilizes inducing points
- DGP VEC: our Vecchia-approximated ESS (Sauer, Cooper, & Gramacy, 2022)
- GP: full un-approximated GP (when feasible)
- GP SVEC: Scaled Vecchia "shallow" GP (Katzfuss et al., 2020)

DGP-Vecchia outperforms both deep and shallow competitors

4-dimensional G-function (20 reps)

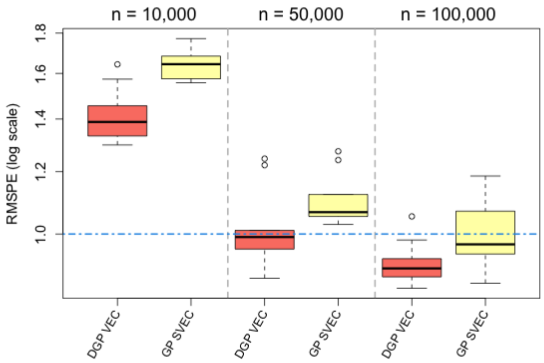


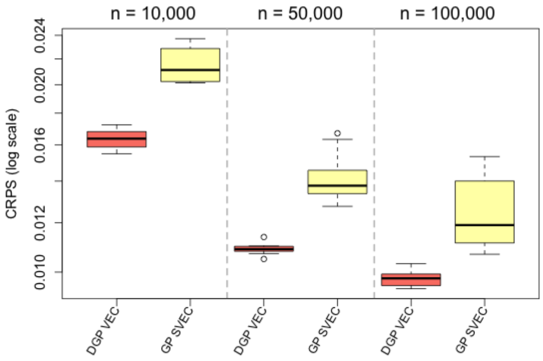


▸ simulation with noise ▸ larger scale simulation

Satellite drag computer simulation

- Same TPM simulator, **bigger data set/domain**
- Same Goal: RMSPE below 1%





DGP DSVI and DGP HMC omitted from figure with RMSPE's 30-35%

Vecchia approximation for DGPs - Summary

- Why?
  - Cubic computational bottlenecks, compounded in DGP MCMC
- What?
  - Imposing sparsity in the precision matrix (and its Cholesky decomposition)
  - Maintaining global scale
- How?
  - Same DGP MCMC scheme with Vecchia-approximation for each GP component
  - Random ordering at each layer
  - Nearest-neighbor conditioning, optionally adjusted based on learned latent layer

Thanks!

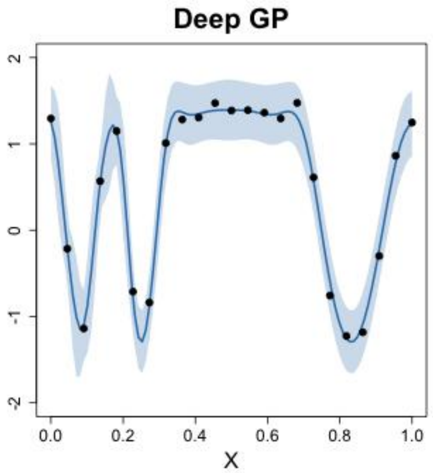
Everything you saw today is supported by

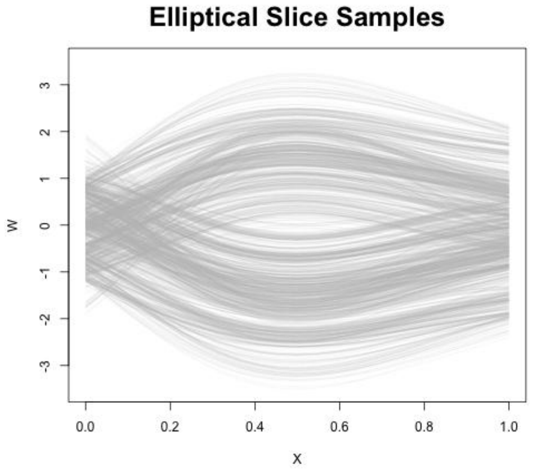
- deepgp for R on CRAN (Sauer, 2022)
- and a git repo of examples:

`https://bitbucket.org/gramacylab/deepgp-ex/`

Many thanks for your attention!

Elliptical slice samples for 1d piecewise function





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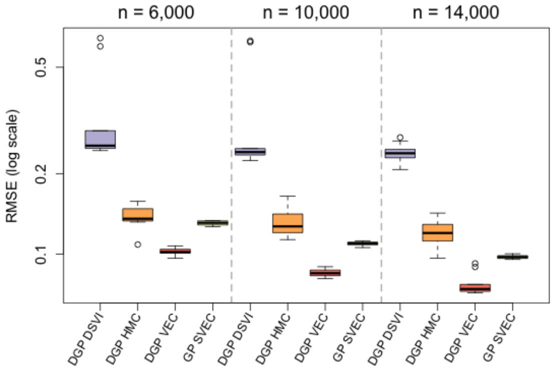
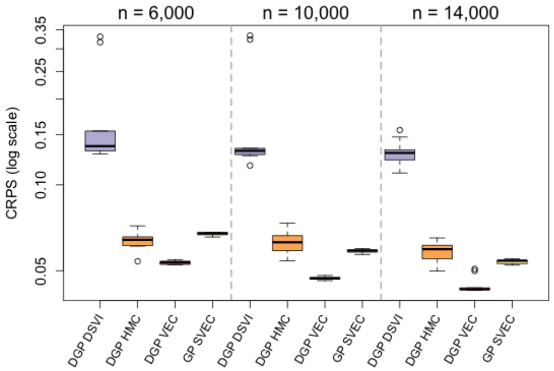
Simulation with noise

4-dimensional G-function with white noise





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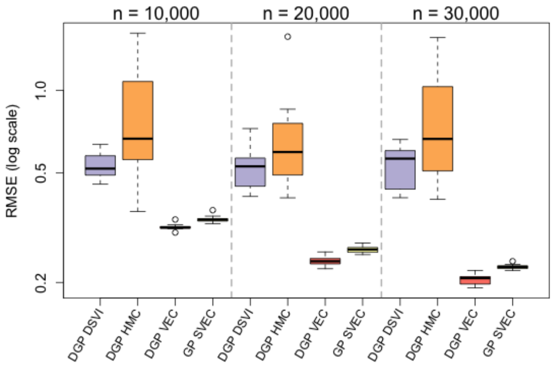
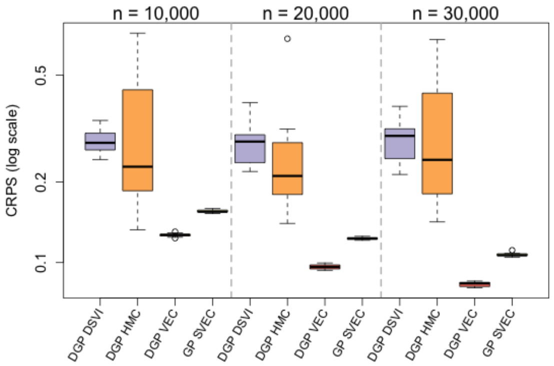
Larger scale simulation

6-dimensional G-function





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