

# Computer Model Emulation in Agriculture

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# Iowa Agricultural Production

<https://www.iadg.com/iowa-advantages/target-industries/>

*Iowa is the largest producer of corn, pork and eggs in the United States and second in soybeans and red meat production.*



<https://www.britannica.com/plant/corn-plant>

<https://www.nationalhogfarmer.com/marketing/total-pork-production-2014-down-slightly>

<https://www.medicalnewstoday.com/articles/283659>

<https://www.midwestfarmreport.com/2019/12/11/state-soybean-yield-contest-entries-announced/>

<https://www.scientificamerican.com/article/meat-and-environment/>

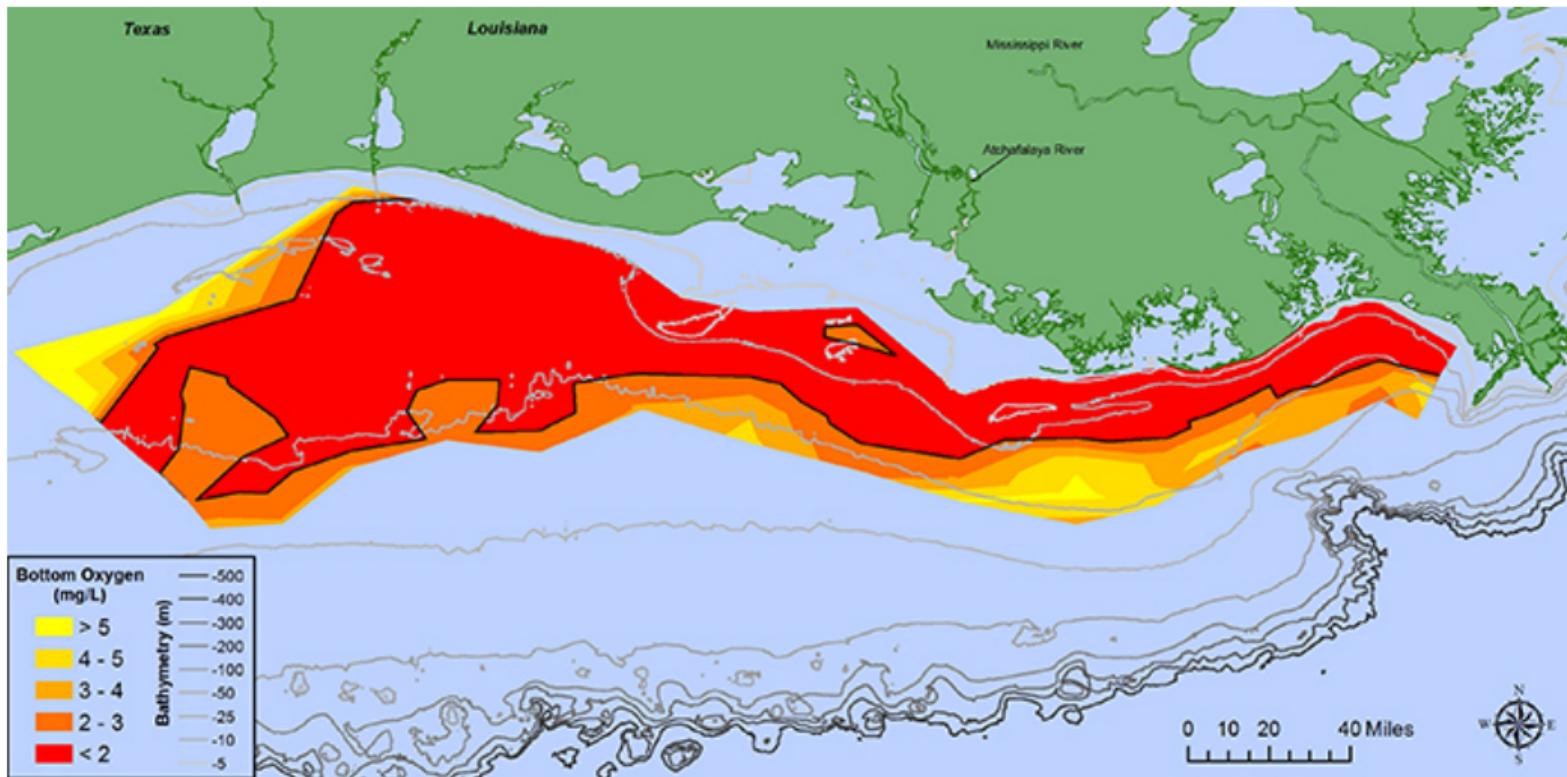
# Soil loss

Iowa loses \$1,000,000,000/year in soil



<https://www.desmoinesregister.com/story/money/agriculture/2014/05/03/erosion-estimated-cost-iowa-billion-yield/8682651/>

# Gulf of Mexico Dead Zone



<https://www.noaa.gov/media-release/gulf-of-mexico-dead-zone-is-largest-ever-measured>

# Des Moines Water Works Lawsuit



<https://www.lwvumrr.org/blog/des-moines-water-works-lawsuit-update>

# C-CHANGE: Science for a changing agriculture



# C-CHANGE

<http://agchange.org>



<http://prairiestrips.org>

# USDA NIFA - Biogas production from manure and herbaceous biomass



## USDA Scientific Research Program Funds Sustainable Agricultural Systems Projects

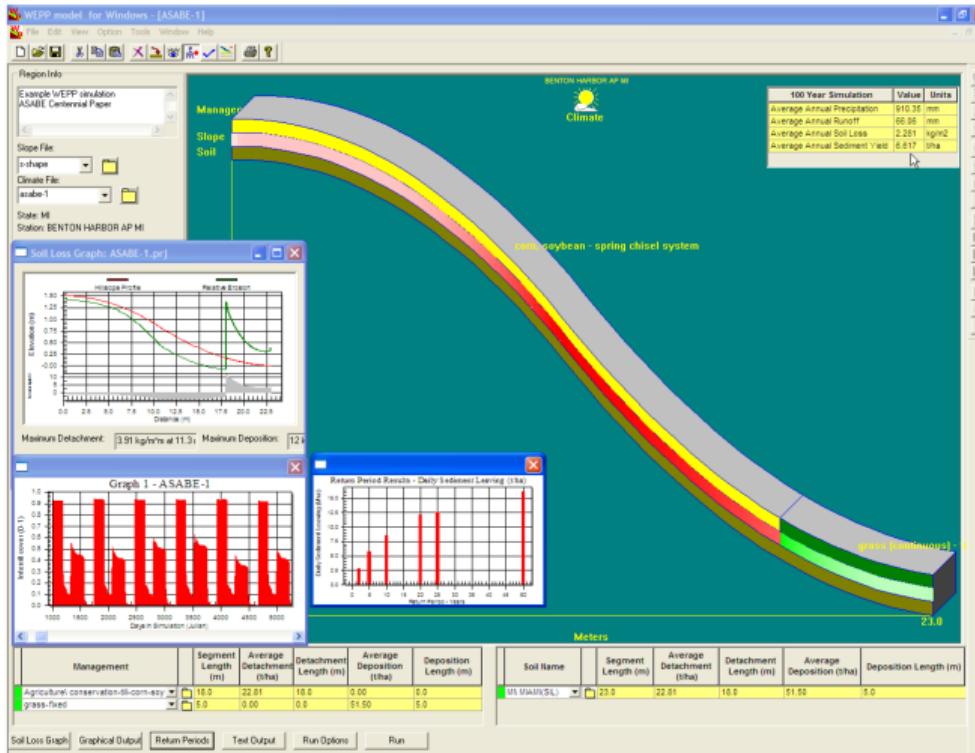


Fig. 1. The agricultural value chain developed through C-CHANGE.

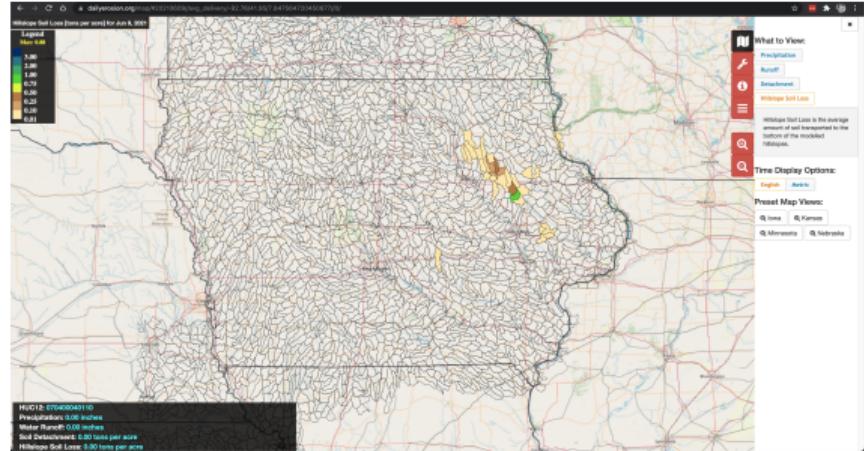
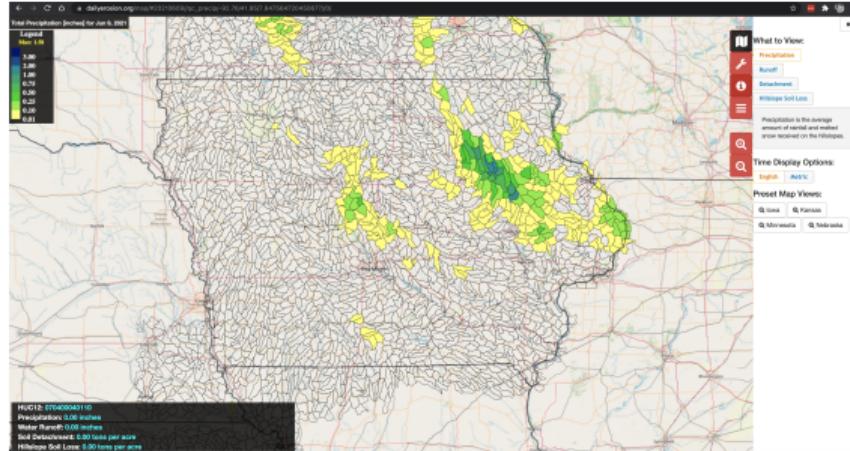
# Computer models

- ▶ Water Erosion Prediction Project (WEPP)
  - ▶ Daily Erosion Project (DEP)
- ▶ Agricultural Production Systems sIMulator (APSIM)
  - ▶ Foresite
- ▶ Cycles
- ▶ Iowa Biogas Assessment Model (IBAM)
- ▶ others...

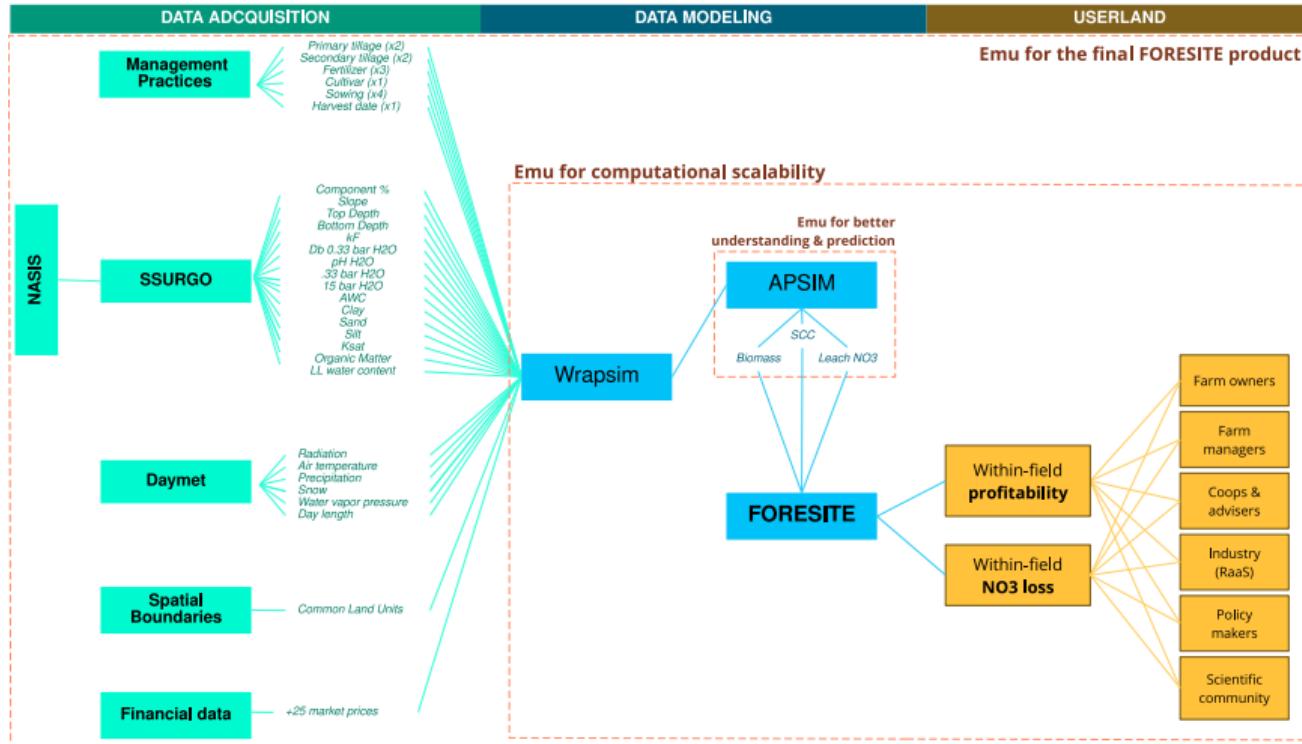
# WEPP



# Daily Erosion Project (DEP) using Water Erosion Prediction Project (WEPP)



# APSIM



# APSIM

## Input space

- ▶ 2,160 run-specific input values
  - ▶ Soil properties 22 functionals  $\times$  16 layers, 2 scalars.
  - ▶ Climate dynamics 4 functionals  $\times$  365 daily values, 2 scalars.
  - ▶ Land management practices, mostly categorical scalars.
- ▶ The input space is...
  - ▶ High dimensional: computational and modeling challenging.
  - ▶ Structured: complex to capture hierarchy.
  - ▶ Vast: large number of runs to explore it.

# Gaussian Process Emulators

Consider a computer model  $f(\cdot)$  with

$$Y_i = f(X_i, \psi) = f(X_i), \quad i = 1, \dots, N$$

where

- ▶  $\psi$  are model parameters,
- ▶  $X_i$  are inputs, and
- ▶  $Y_i$  are outputs.

We assume a Gaussian Process prior

$$f \sim \mathcal{GP}(m, k) \implies y \sim N(m_x, \Sigma_{x,x})$$

where  $\Sigma_{x,x}(x, x') = k(x, x')$ .

Two research directions:

- ▶ Computational tractability for large  $N$
- ▶ Dealing with functional  $X_i$

# Training a GP

Find the maximum likelihood estimator (MLE) for  $\theta = (\tau^2, \sigma^2, \phi)$ ,

$$\hat{\theta} = \operatorname{argmax}_{\theta} p(y|\theta) = \operatorname{argmax}_{\theta} N(y; m_x, \tau^2 I + \Sigma(\theta))$$

where  $y = (y_1, \dots, y_N)$ . The log-likelihood is

$$\begin{aligned} \log \mathcal{N}(y; m_x, \tau^2 I + \Sigma_{\theta}) = & C \\ & -\frac{1}{2} \log |\tau^2 I + \Sigma(\theta)| \\ & -\frac{1}{2} y^\top [\tau^2 I + \Sigma(\theta)]^{-1} y \end{aligned}$$

If there are  $N$  observations,  $\Sigma(\theta)$  is an  $N \times N$  covariance matrix and thus the computational time scales as  $\mathcal{O}(N^3)$ .

This is doable if  $N \approx 1,000$  but not when you start getting larger and larger data sets.

# Fully Independent Conditional (FIC) Approximation

Introduce a set of knots  $x^\dagger = \{x_1^\dagger, \dots, x_K^\dagger\}$  with  $K \ll N$ , such that

$$p(f_x, f_{x^\dagger} | \theta) = p(f_x | f_{x^\dagger}, \theta)p(f_{x^\dagger} | \theta).$$

where

$$\begin{aligned} f_x | f_{x^\dagger}, \theta &\sim \mathcal{N}(m_x + \Sigma_{xx^\dagger} \Sigma_{x^\dagger x^\dagger}^{-1} (f_{x^\dagger} - m_{x^\dagger}), \Lambda) \\ f_{x^\dagger} | \theta &\sim \mathcal{N}(m_{x^\dagger}, \Sigma_{x^\dagger x^\dagger}) \end{aligned}$$

with  $\Lambda = \text{diag}(\Sigma_{xx} - \Sigma_{xx^\dagger} \Sigma_{x^\dagger x^\dagger}^{-1} \Sigma_{x^\dagger x})$ .

This joint implies the following marginal distribution for  $f_x$ :

$$f_x | \theta \sim \mathcal{N}(m_x, \Lambda + \Sigma_{xx^\dagger} \Sigma_{x^\dagger x^\dagger}^{-1} \Sigma_{x^\dagger x})$$

which has the correct marginal means and variances, but the covariances are controlled by the knots.

# Train FIC Model

Let  $\Psi_{xx} \equiv \Lambda(\theta) + \Sigma_{xx^\dagger}(\theta)\Sigma_{x^\dagger x^\dagger}(\theta)^{-1}\Sigma_{x^\dagger x}(\theta)$ , then

$$Y|x^\dagger, \theta \sim \mathcal{N}(m_x, \tau^2 I + \Psi_{xx}).$$

Train the model by finding

$$\hat{x}^\dagger, \hat{\theta} = \operatorname{argmax}_{x^\dagger, \theta} \mathcal{N}(y; m_x, \tau^2 I + \Psi_{xx}).$$

which has computational complexity of  $\mathcal{O}(NK^2)$ .

Appealing due to similarity with Full GP MLE approach and massively reduced computational complexity, but there are a number of questions:

- ▶ how many knots are needed?
- ▶ where should the knots be?

# One-at-a-time (OAT) selection

We developed a **one-at-a-time (OAT) knot selection** that

- ▶ Begins with a small number of knots
- ▶ Optimizes the knot locations according to the marginal likelihood or variational objective function
- ▶ Iteratively adds knots until no improvement is seen in the objective function

Manuscripts:

- ▶ Nate Garton, Jarad Niemi, and Alicia Carriquiry. (2020) "Knot Selection in Sparse Gaussian Processes with a Variational Objective." *Statistical Analysis and Data Mining.* 13(4): 324-336.
- ▶ Nate Garton, Jarad Niemi, and Alicia Carriquiry. "Knot Selection in Sparse Gaussian processes." arXiv:2002.09538

# Vector-input Gaussian Process (viGP)

For observation  $i$ , we have response  $Y_i \in \mathbb{R}$  and input  $X_i = (X_{i,1}, \dots, X_{i,D})$ . Our computer model is  $f()$  with  $Y_i = f(X_i)$ .

Assume  $f$  is a zero-mean Gaussian process with

$$\text{Cov}(Y_i, Y_j) = \sigma^2 e^{-\frac{1}{2}D(X_i, X_j, \omega)}$$

and

$$D(X_i, X_j, \omega) = \sum_{d=1}^D \omega_d (x_{i,d} - x_{j,d})^2.$$

# Functional-input Gaussian Process

For observation  $i$ , we have  $Y_i \in \mathbb{R}$  and  $X_i(t)$  for  $t \in [0, T]$ . Our computer model is  $f()$  with  $Y_i = f(X_i(t))$ .

The functional-input Gaussian Process has

$$\text{Cov}(Y_i, Y_j) = \sigma^2 e^{-\frac{1}{2}D(X_i(t), X_j(t), \omega)}$$

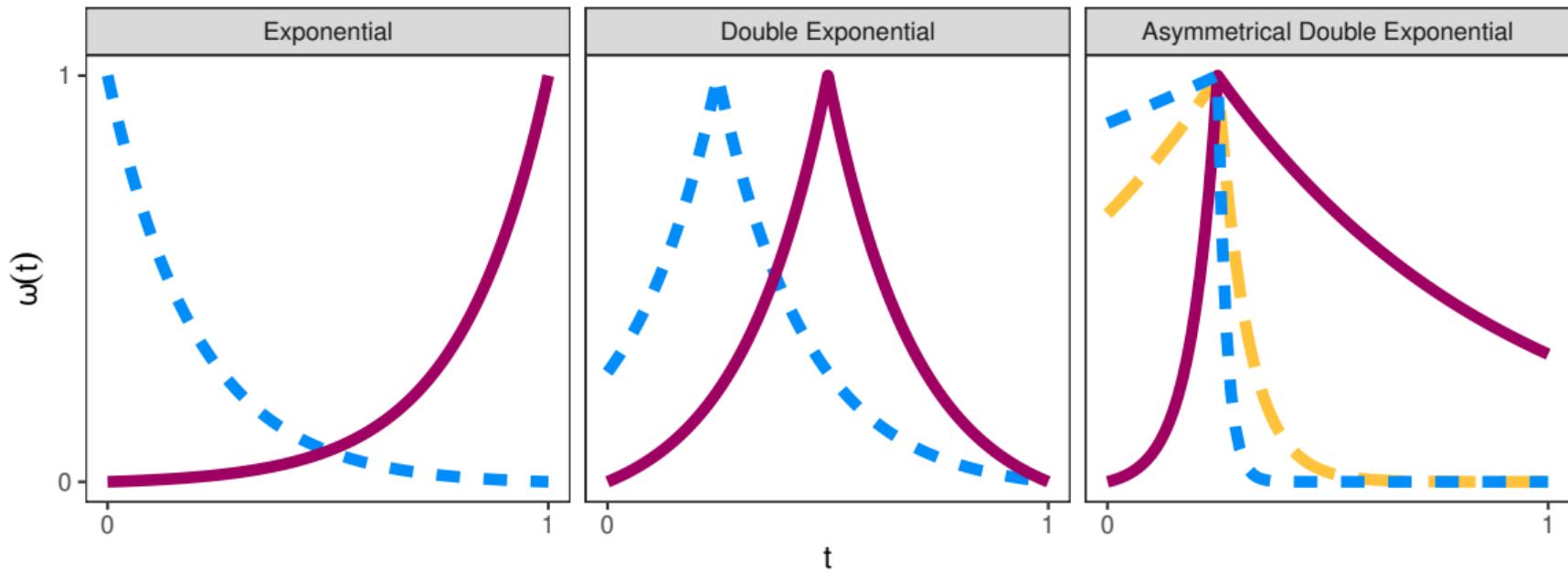
$$D(X_i, X_j, \omega) = \int_0^T \omega(t)(X_i(t) - X_j(t))^2 dt \approx \sum_{d=1}^D \omega(t_d)(X_i(t_d) - X_j(t_d))^2.$$

For the **functional length-scale**, we assume

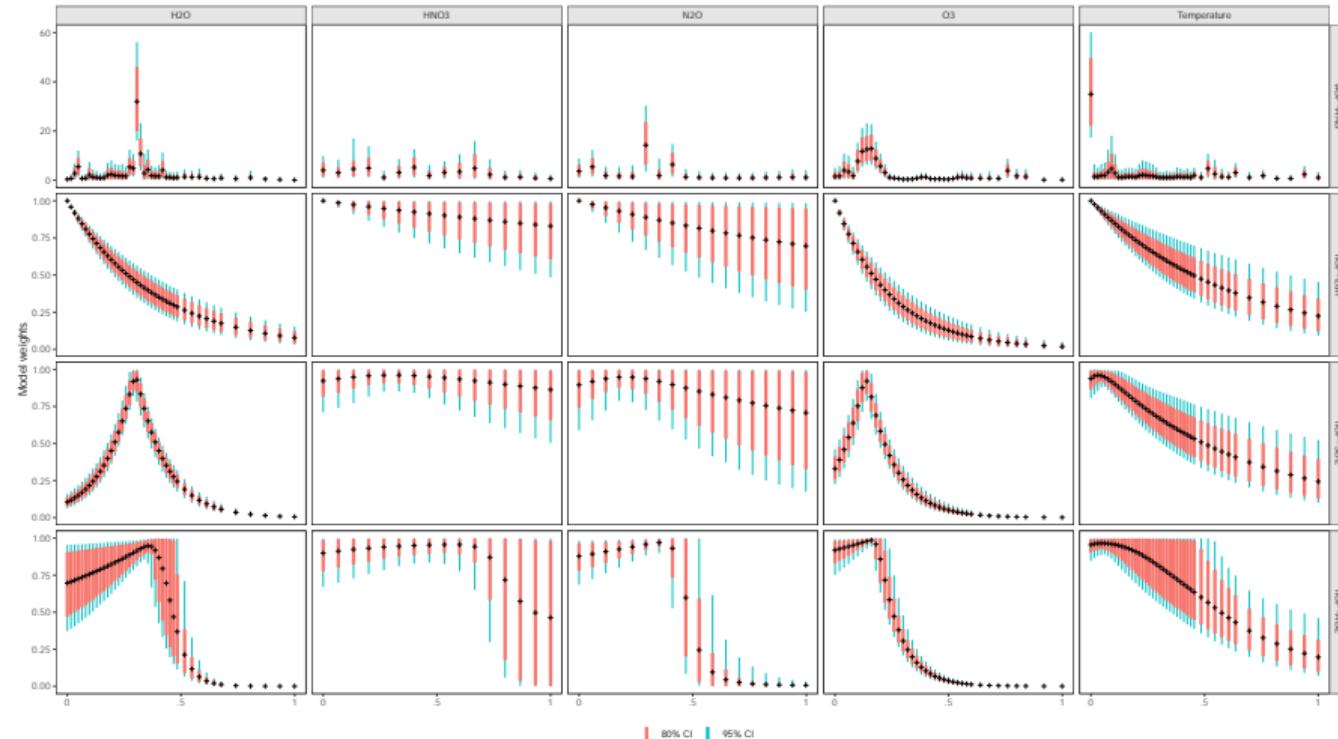
$$\omega(t) = \exp(2\sigma_\ell^2 t^\eta).$$

We'll refer to this as **fiGP**.

# Theoretical fiGP functional length-scale



# Estimated fiGP functional length-scale



# Summary

Research advances

- ▶ OAT algorithm for knot selection to deal with computational intractability due to large  $n$
- ▶ fiGP model for functional inputs

These slides are available at

- ▶ [https://github.com/jarad/NCCC170\\_2022](https://github.com/jarad/NCCC170_2022)
- ▶ <http://www.jarad.me/research/presentations.html>

Thank you!

Other links:

- ▶ <http://www.jarad.me/>
- ▶ <https://www.youtube.com/c/jaradniemi>