Advancing Scientific Practice through Agricultural Statistics

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September 26, 2022

Funded, in part, by

- the Iowa State University Presidential Interdisciplinary Research Initiative on C-CHANGE: Science for a Changing Agriculture
- USDA NIFA: Consortium for Cultivating Human And Naturally reGenerative Enterprises (C-CHANGE Grass2Gas)
- Foundation for Food and Agriculture Research: Prairie Strips for Healthy Soils and Thriving Farms

Collaborators

Prairie STRIPS Collaborators: `http://prairiestrips.org/people`

Gaussian Process Emulators:

Agriculture

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.*

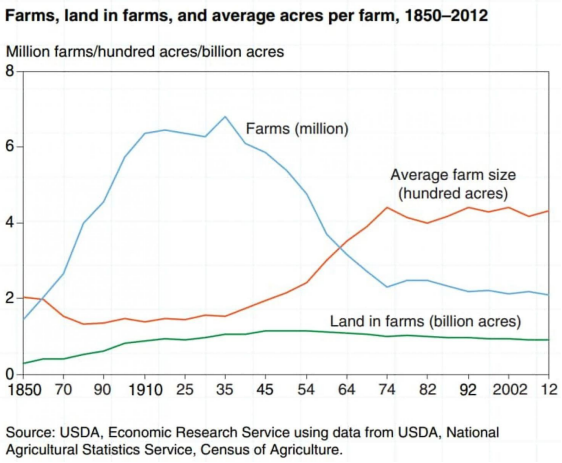


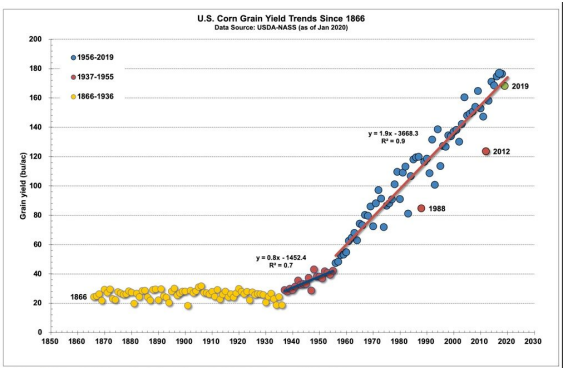


https://www.britannica.com/plant/corn-plant
https://www.nationalhogfarmer.com/marketing/total-pork-production-2014-down-slightly
https://www.medicalnewstoday.com/articles/283659
https://www.midwestfarmreport.com/2019/12/11/state-soybean-yield-contest-entries-announced/

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

Corn production





https://www.iowaagliteracy.org/Article/Family-Farms-Then-and-Now

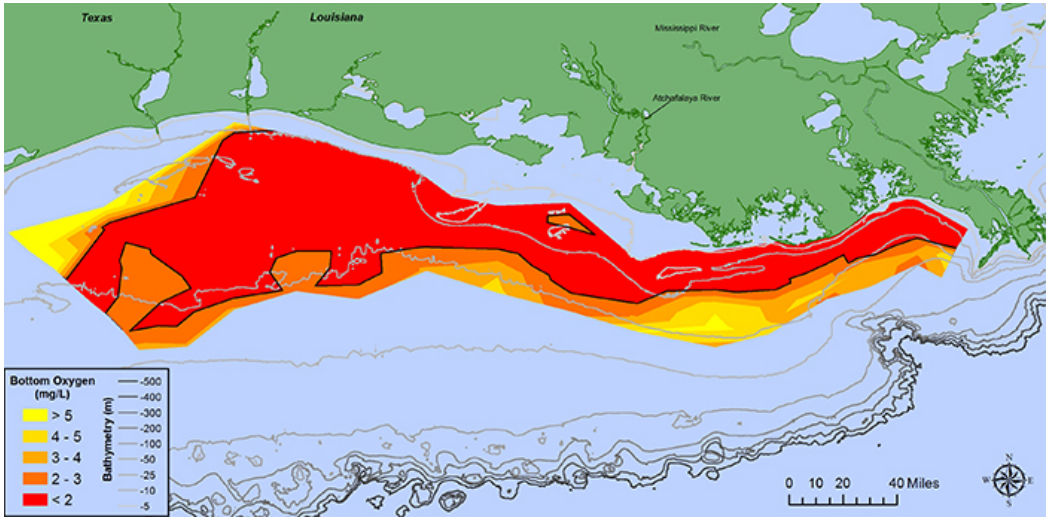
https://extension.entm.purdue.edu/newsletters/pestandcrop/article/historical-corn-grain-yields-in-the-u-s/

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

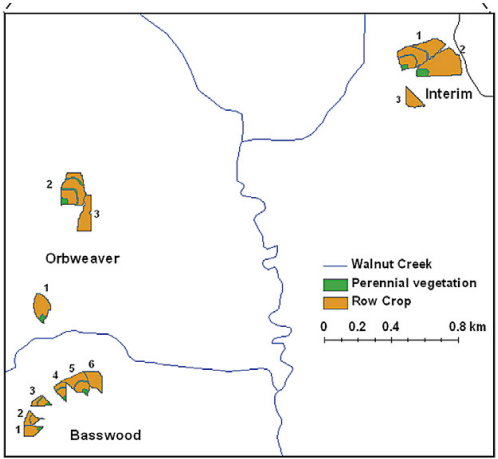
C-CHANGE: Science for a changing agriculture

http://agchange.org

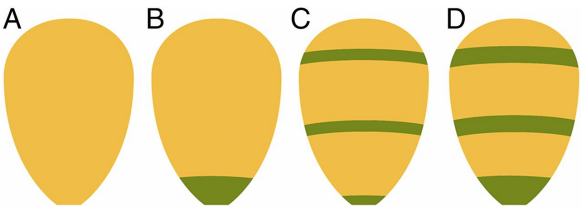
Prairie STRIPS
C-CHANGE PIRIR
C-CHANGE Grass2Gas
Climate Smart Ag

Prairie STRIPS

STRIPS1 - Neal Smith National Wildlife Refuge

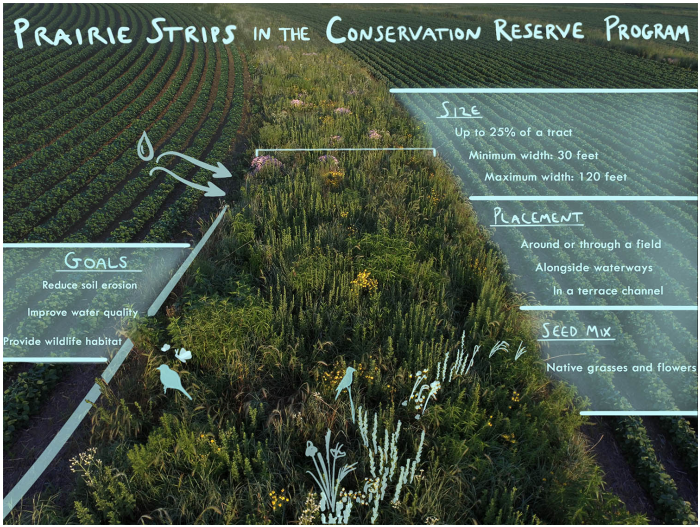


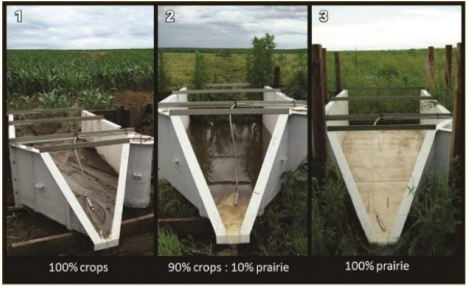
Find on Google Maps



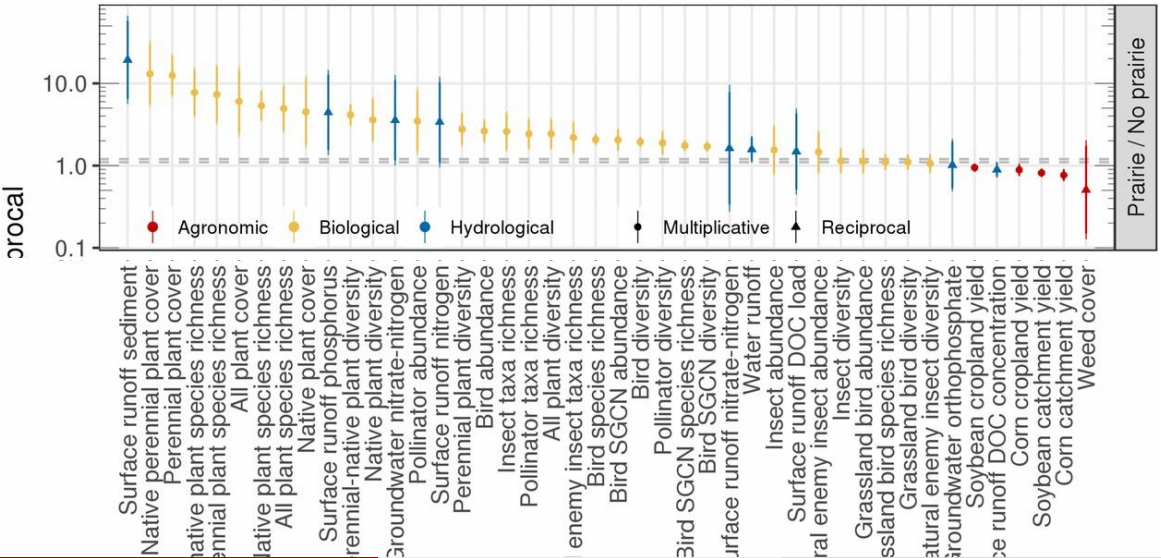
	Treatment			
Block	Control	10% B	10% S	20%
Interim	X	X	X	
Orbweaver	X	X		X
Basswood-South		X	X	X
Basswood-North	X		X	X

STRIPS1 - Science





STRIPS1 - PNAS



USDA CRP: CP-43

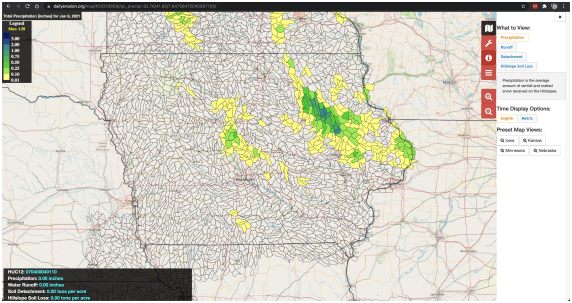
Prairie strips improve biodiversity and the delivery of multiple ecosystem services from corn–soybean croplands

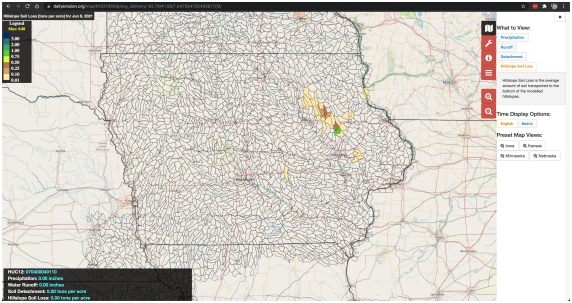
Lisa A. Schulte, Jarad Niemi, Matthew J. Helmers, +11, and Chris Witte Authors Info & Affiliations

Gaussian Process Emulators

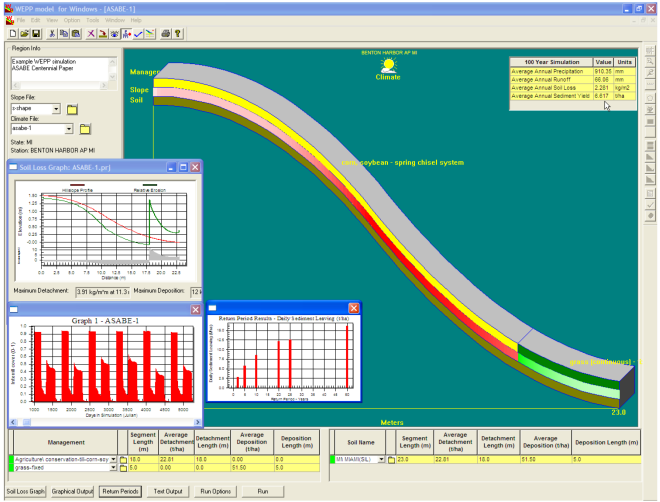
Daily Erosion Project (DEP)

using Water Erosion Prediction Project (WEPP)





Water Erosion Prediction Project (WEPP)



Gaussian Process Emulators

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

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

where

- X_i are inputs and
- Y_i are outputs.

We assume a Gaussian Process prior

$$f \sim \mathcal{GP}(m, k) \implies Y \sim N(m_x, \Sigma)$$

where (often) $m_x = 0$ and, for scalar inputs, $\Sigma_{ij} = k(x_i, x_j) = \sigma^2 e^{-(x_i - x_j)^2/\phi}$.

Two research directions:

- Computational tractability for large N
- Dealing with functional inputs

Training a GP

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

$$\hat{\theta} = \text{argmax}_\theta \, p(y|\theta) = \text{argmax}_\theta \, N\left(y; 0, \Sigma(\theta)\right)$$

where $y = (y_1, \ldots, y_N)$.

The log-likelihood is

$$\log \mathcal{N}(y; 0, \Sigma(\theta) \propto C - \log|\Sigma(\theta)| - y^\top \Sigma(\theta)^{-1} y$$

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.

OAT Algorithm

Fully Independent Conditional (FIC) Approximation

Introduce a set of knots $x^\dagger = \left\{x_1^\dagger, \ldots, x_K^\dagger\right\}$ with $K << N$, such that

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

where

$$\begin{aligned} f_{x^\dagger}|\theta &\sim \mathcal{N}(0, \Sigma_{x^\dagger x^\dagger}) \\ f_x|f_{x^\dagger}, \theta &\sim \mathcal{N}\left(\Sigma_{xx^\dagger}\Sigma_{x^\dagger x^\dagger}^{-1}(f_{x^\dagger}), \Lambda\right) \end{aligned}$$

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

This joint implies the following marginal distribution for f_x:

$$f_x|\theta \sim \mathcal{N}(0, \Lambda + \Sigma_{xx^\dagger}\Sigma_{x^\dagger x^\dagger}^{-1}\Sigma_{x^\dagger x})$$

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

Train FIC Model

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

$$Y|x^\dagger, \theta \sim \mathcal{N}(0, \Psi(x^\dagger, \theta)).$$

Train the model by finding

$$\hat{x}^\dagger, \hat{\theta} = \text{argmax}_{x^\dagger, \theta}\mathcal{N}(y; 0, \Psi(x^\dagger, \theta)).$$

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

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

Summary of results:

- Prediction is equivalent to Full GP and simultaneous knot optimization
- Formally, OAT has computational complexity of $\mathcal{O}(NK^2)$
- Practically, OAT is much faster than Full GP and simultaneous knot optimization

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

Functional inputs

Vector-input Gaussian Process (viGP)

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

Assume f is a zero-mean Gaussian process with

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

and

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

Some call this automatic relevance determination.

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

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

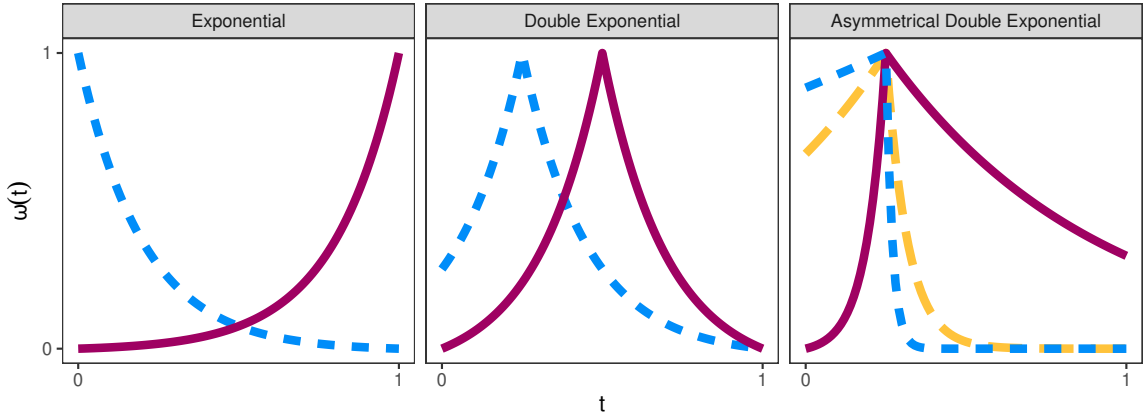
$$D(X_i, X_j, \omega) = \int_0^T \omega(t)(X_i(t) - X_j(t))^2 dt \approx \sum_{d=1}^{D} \omega(t_d)(X_i(t_d) - X_j(t_d))^2.$$

For the functional length-scale, we assume

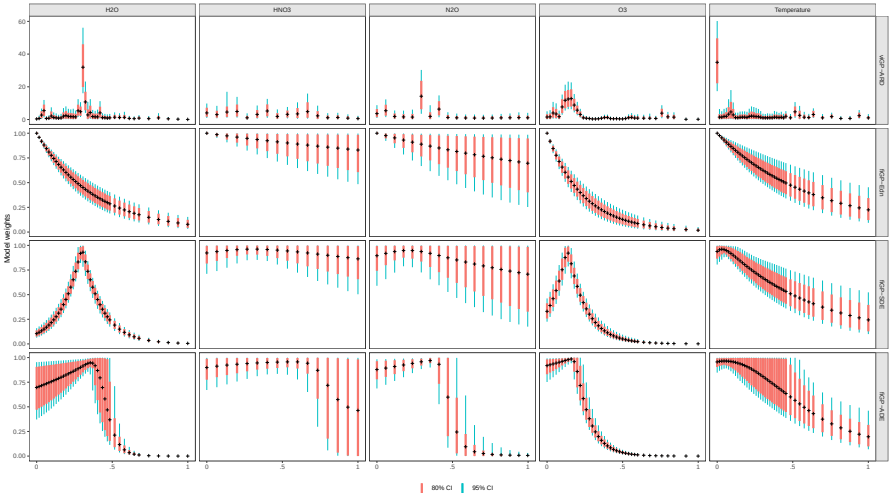
$$\omega(t) = \exp\left(2\sigma_\ell^2 t^\eta\right).$$

We'll refer to this as fiGP and dynamic automatic relevance determination.

Theoretical fiGP functional length-scale



Estimated fiGP functional length-scale



Summary

Research/policy advances

- Prairie strips impact on agroecosystem services and inclusion in CRP as CP-43
- OAT algorithm for knot selection to deal with computational intractability due to large n
- fiGP/DARD model for functional inputs

These slides are available at

- `https://github.com/jarad/ISU2022`
- `http://www.jarad.me/research/presentations.html`

Thank you!

Other links:

- `http://www.jarad.me/`
- `http://www.youtube.com/jaradniemi`