Emulation of Agricultural Production Systems sIMulator (APSIM)

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

C-CHANGE: Science for a changing agriculture

http://agchange.org

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/

Loss of prairie

85% of Iowa was covered with prairie; today less than 0.1% remains

https://www.facebook.com/NealSmithNWR/photos/a.363116150433606/3093501587395035

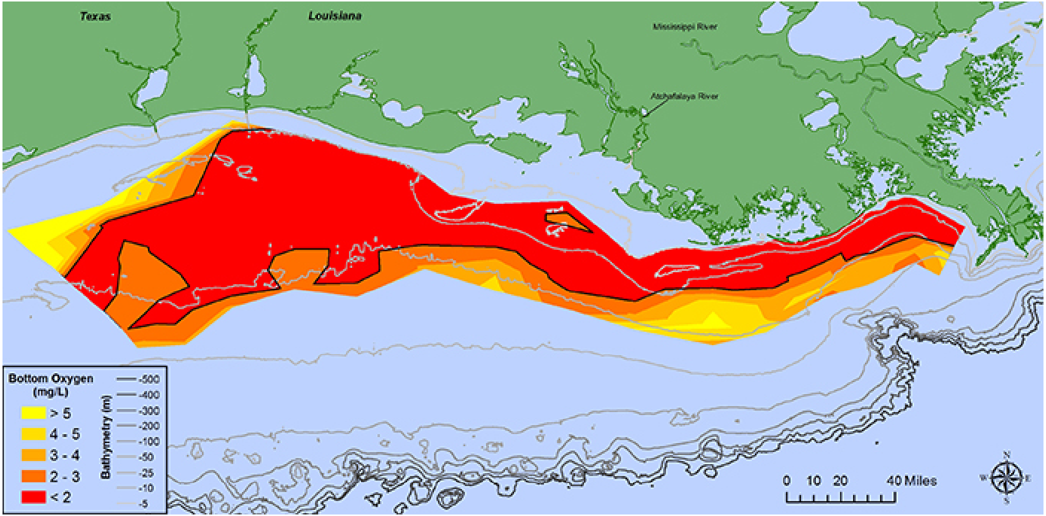
https://dissolve.com/stock-photo/field-young-soybean-plants-showing-corn-stalks-residue-royalty-free-image/101-D869-14-341

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

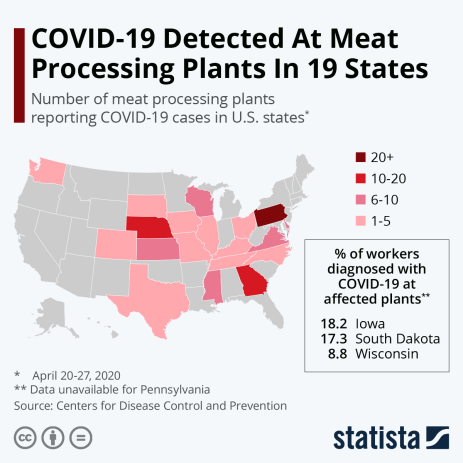
Tedesco Environmental Learning Corridor

https://www.storycountyiowa.gov/1369/Tedesco-Environmental-Learning-Corridor

Manure lagoons

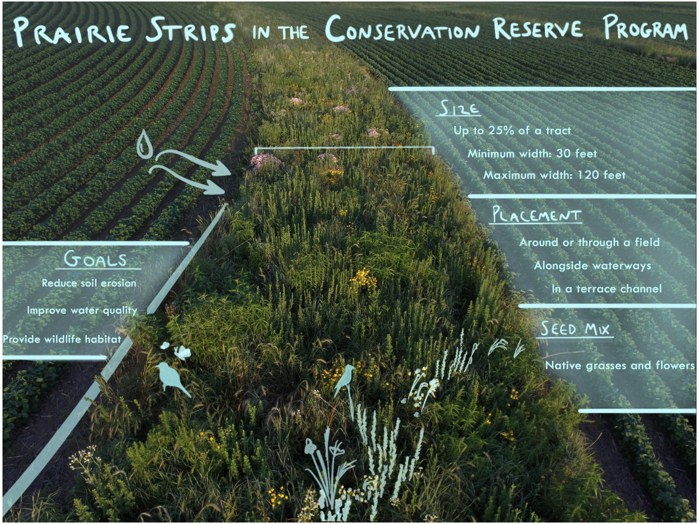
https://www.npr.org/2018/09/22/650698240/hurricane-s-aftermath-floods-hog-lagoons-in-north-carolina

COVID-19 in Meat Packing Plants



https://www.statista.com/chart/21585/meat-processing-plants-reporting-coronavirus-cases/

Prairie STRIPS



http://prairiestrips.org

Prairie STRIPS

PNAS Proceedings of the National Academy of Sciences of the United States of America

Keyword, Author, or D

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RESEARCH ARTICLE

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

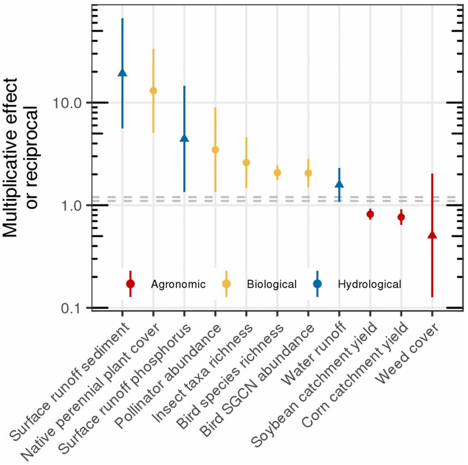
Lisa A. Schulte, Jarad Niemi, Matthew J. Helmers, Matt Liebman, J. Gordon Arbuckle, David E. James, Randall K. Kolka, Matthew E. O'Neal, Mark D. Tomer, John C. Tyndall, Heidi Asbjornsen, Pauline Drobney, Jeri Neal, Gary Van Ryswyk, and Chris Witte

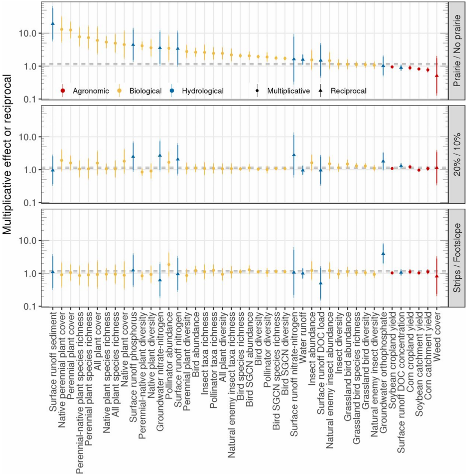
PNAS October 17, 2017 114 (42) 11247-11252; first published October 2, 2017 https://doi.org/10.1073/pnas.1620229114

Edited by David Tilman, University of Minnesota, St. Paul, MN, and approved August 1, 2017 (received for review December 9, 2016)

https://www.pnas.org/content/114/42/11247.short

Prairie STRIPS results





https://www.pnas.org/content/114/42/11247/tab-figures-data

USDA NIFA - Biogas production from manure and herbaceous biomass

NIFA PRESS RELEASE

USDA

NATIONAL INSTITUTE OF FOOD AND AGRICULTURE

USDA Scientific Research Program Funds Sustainable Agricultural Systems Projects

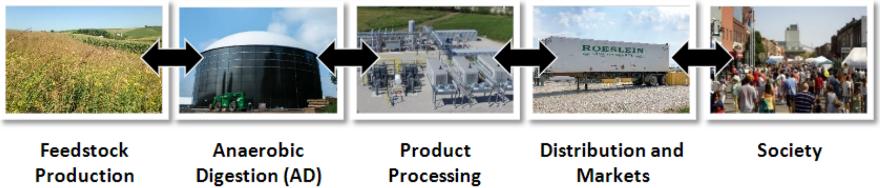


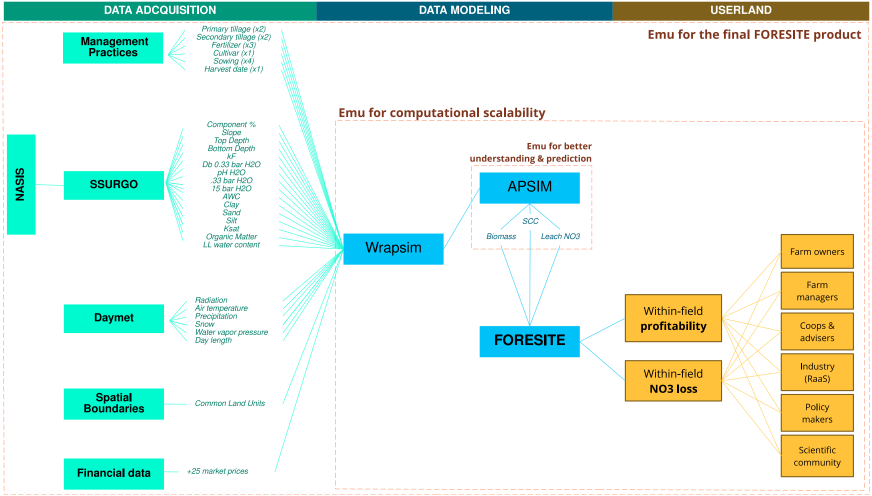
Fig. 1. The agricultural value chain developed through C-CHANGE.

Computer models

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

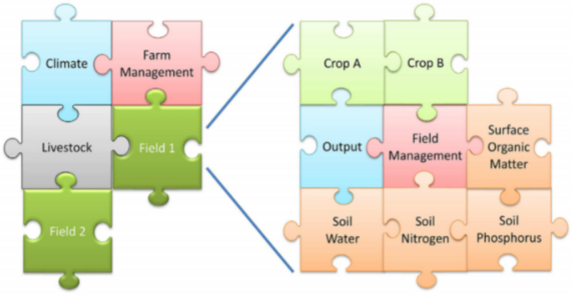
APSIM

Role in the Foresite project



APSIM

Overview



- Physical process based
- Peer-reviewed
- Flexible
- Calibrated for many different climates and countries
- Dedicated, funded team of software engineers working to improve it

APSIM

Emulation goals

- Variable selection: to guide data collection by field scientists.
- Model calibration: APSIM assumes a flat, uniform soil. TWI.
- Identify deficiencies: does APSIM emphasize on soil too much?
- Uncertainty quantification: APSIM is deterministic, real life is not.
- Inform the development & calibration of new crop modules (e.g. cover crops).
- Portability: web interface back end for on-line prediction.
- Assist scientists in studying agronomic hypothesis.

APSIM

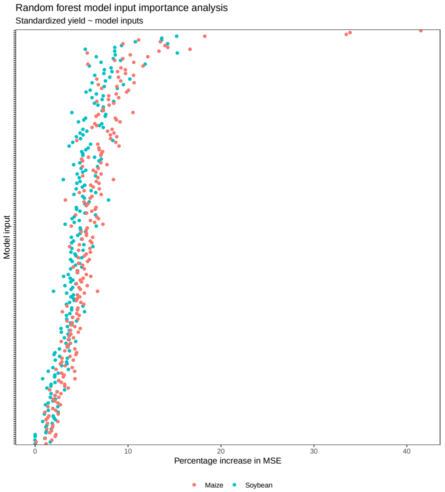
Input space

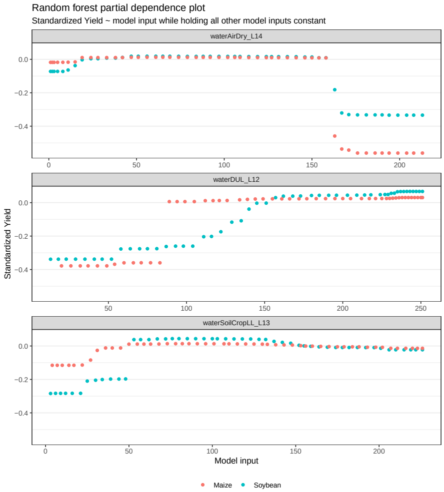
- 2,160 run-specific input values
  - Soil properties 2 functionals x 16 layers, 2 scalars.
  - Climate dynamics 4 functionals x 365 daily values, 2 scalars.
  - Land management practices, but mostly categorical scalars.

- The input space is...
  - High dimensional: computational and modeling challenging.
  - Structured: complex to capture hierarchy.
  - Vast: large number of runs to explore.

APSIM

Exploratory Analyses





One-at-a-time knot selection

Training a GP

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

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

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

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

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.

One-at-a-time knot selection

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

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

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:

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

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

[Seeger et al., 2003, Quiñonero-Candela and Rasmussen, 2005, Snelson and Ghahramani, 2006, Banerjee et al., 2008, Finley et al., 2009, Titsias, 2009, Cao et al., 2013]

One-at-a-time knot selection

Knot selection algorithm

Algorithm 1. OAT knot selection algorithm.

Initialize: $x^\dagger = \{x_i^\dagger\}_{i=1}^{K_I}$;
$\hat{\theta} = \text{argmax}_\theta p(y|x, x^\dagger, \theta)$;
repeat
  propose new knot $x^{\dagger^*} \leftarrow J(y, x, x^\dagger, \hat{\theta})$;
  $(\hat{x}^{\dagger^*}, \hat{\theta}) = \text{argmax}_{(x^{\dagger^*}, \theta)} p(y|x, \{x^\dagger, x^{\dagger^*}\}, \theta)$;
  $x^\dagger = \{x^\dagger, \hat{x}^{\dagger^*}\}$;
until $|x^\dagger| = K_{max}$ *or convergence*;

[Garton et al., Garton]

One-at-a-time knot selection

Knot proposal algorithm

Algorithm 2. Knot proposal algorithm. Set the minimum (T_{min}) and maximum (T_{max}) number of marginal likelihood evaluations.

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set the mean of the meta GP equal to $\log p\left(y \middle| x, \left\{x^\dagger, \cdot\right\}, \hat{\theta}\right)$;

sample $x_1^\dagger, ..., x_{T_{min}}^\dagger$ without replacement from x ;

augment known marginal likelihood values $w_j = \log p\left(y \middle| x, \left\{x^\dagger, x_j^\dagger\right\}, \hat{\theta}\right)$ for $j = 1, \ldots, k$ with evaluations of the marginal likelihood at the new knots, that is $w_{k+j} = \log p\left(y \middle| x, \left\{x^\dagger, x_j^\dagger\right\}, \hat{\theta}\right)$ for $j = 1, ..., T_{min}$;

for $t = T_{min} + 1, ..., T_{max}$ **do**

  update covariance parameters in meta GP ;

  $x_t^* = \text{argmax}_{z \in x \setminus \{x_l^\dagger\}_{l=1}^{t-1}} \alpha\left(z; w, \left\{x_1^\dagger, \ldots, x_{t-1}^\dagger\right\}\right)$;

  $w_t = \log p\left(y \middle| x, \left\{x^\dagger, x_t^*\right\}, \hat{\theta}\right)$;

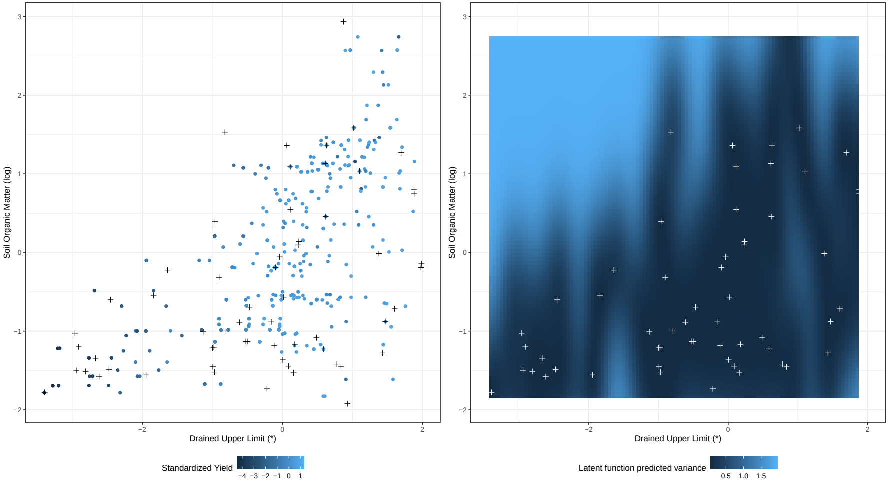
end

return x_j^* such that $j = \text{argmax}_t\, w_t$

[Garton et al., Garton]

OAT Knot selection

Visualization



(*) Content of water retained after gravitational flow.

Future Efforts

Extending Morris' correlation distance for unknown weight function

- Let $Y \in \mathbb{R}$ be a scalar-valued output
- Let $\mathbf{X}$ be a D-sized input vector, $D \in \mathbb{N}$
- Assume $Y = f(\mathbf{X})$
- Assume $Y \sim GP(\mu, \sigma^2)$, $\mu \in \mathbb{R}$ and $\sigma^2 > 0$
- Recall the SE Kernel with ARD

$$k(\mathbf{X_i}, \mathbf{X_j}) = \sigma^2_{ard} e^{-\frac{1}{2} D(\mathbf{X_i}, \mathbf{X_j}, \mathbf{w})}$$

$$D(\mathbf{X_i}, \mathbf{X_j}, \mathbf{w}) = \sum_{d=1}^{D} w_d (X_{i,d} - X_{j,d})^2$$

For a continuous index $t \in [0, T], T \in \mathbb{R}^+$

$$D(\cdot) = \int_0^t w(t-s)(X_i(s) - X_j(s))^2 ds$$

$$w : \mathbb{R}^+ \to \mathbb{R}^+$$

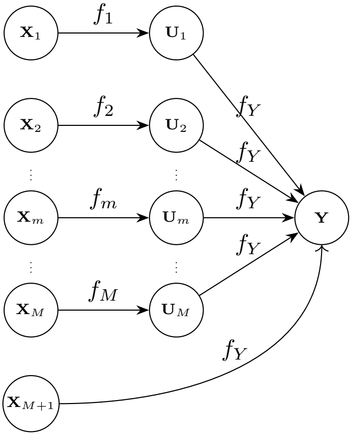
The model now becomes as follows

$$\begin{aligned} \mu_w &\sim \pi(\mu_w) \\ \sigma^2_w &\sim \pi(\sigma_w) \\ \log w(t) &\sim GP(\mu_w, \sigma^2_w) \\ Y &\sim GP(\mu_Y, \sigma^2_Y) \end{aligned}$$

for some priors $\pi(\mu_w)$, $\pi(\sigma_w)$

Future Efforts

Deep Gaussian Process



- High-dimensional input vector $\mathbf{X}$ with $M \in \mathbb{N}$ functional inputs.
- Let $\mathbf{X} \in \mathbb{R}^{D_1} \times \cdots \times \mathbb{R}^{D_M} \times \mathbb{R}^{D_{M+1}}$, where $D_1, \ldots, D_M, D_{M+1} \in \mathbb{N}$, be a $D = \sum_{m=1}^{M} D_m + D_{M+1}$ dimensional vector.
- For each functional $m \in \{1, \ldots, M\}$, let $\mathbf{U_m} = \mathbf{f_m}(\mathbf{X_m}) + \varepsilon_m$ and assume $\mathbf{f_m} \sim GP(\mu_\mathbf{m}, \sigma_\mathbf{m})$ for $\mu_\mathbf{m} \in \mathbb{R}^{D_m}$
- $\tilde{\mathbf{X}} = (\mathbf{U_1}, \ldots, \mathbf{U_M}, \mathbf{X_{M+1}})$
- $Y = f_Y(\tilde{\mathbf{X}}) + \varepsilon_y$ and $f_Y \sim GP(\mu_Y, \sigma_Y)$

Summary

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

- Automatically selects the number of knots
- Similar predictive performance to simultaneous knot selection
- Better represents full GP compared to simultaneous knot selection
- Reduced runtimes compared to simultaneous knot selection

Future work

- Extending the functional input correlation function for unknown weights
- Deep Gaussian Process for the emulation of functional

These slides are available at

- `https://github.com/jarad/LANL2020`
- `http://www.jarad.me/research/presentations.html`

Thank you!

Other links:

- `http://www.jarad.me/`
- `https://luisdamiano.github.io/`

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