Emulation of Agricultural Production Systems sIMulator (APSIM)

Jarad Niemi and Luis Damiano

Iowa State University

September 23, 2020

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Funded, in part, by

- 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.*





Loss of prairie

85% of Iowa was covered with prairie;

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

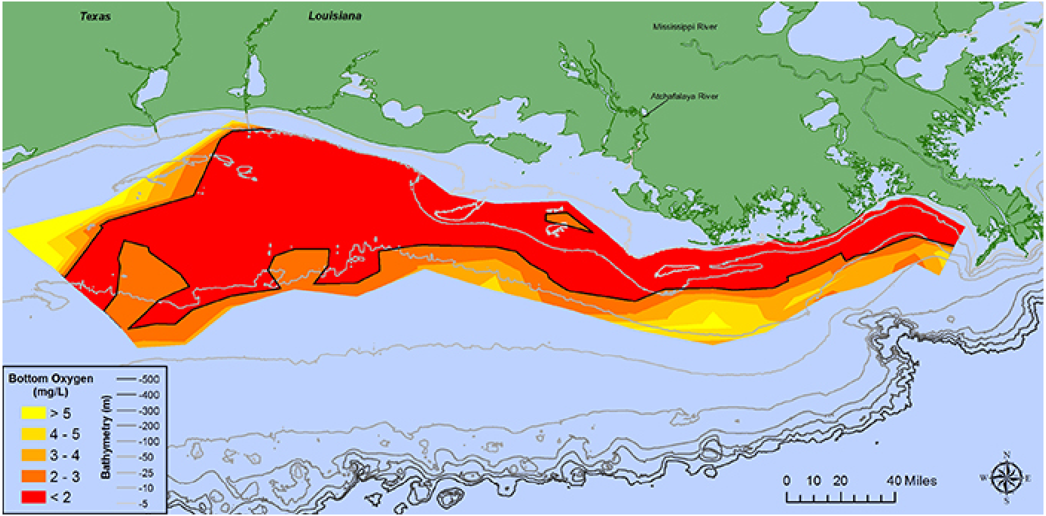
https://dissolve.com/stock-photo/field-young-soybean-plants-showing-corn-stalks-residue-royalty-free-image/101-D869-14-341

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

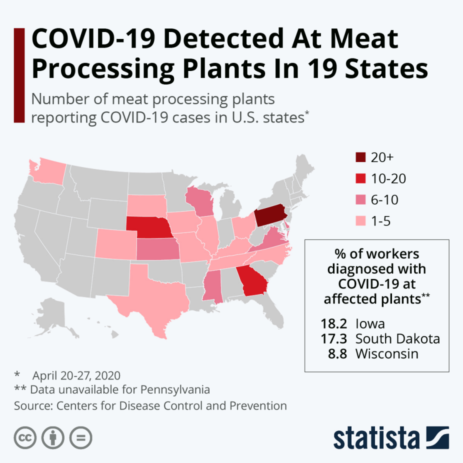
https://www.lwvumrr.org/blog/des-moines-water-works-lawsuit-update

Tedesco Environmental Learning Corridor

Manure lagoons

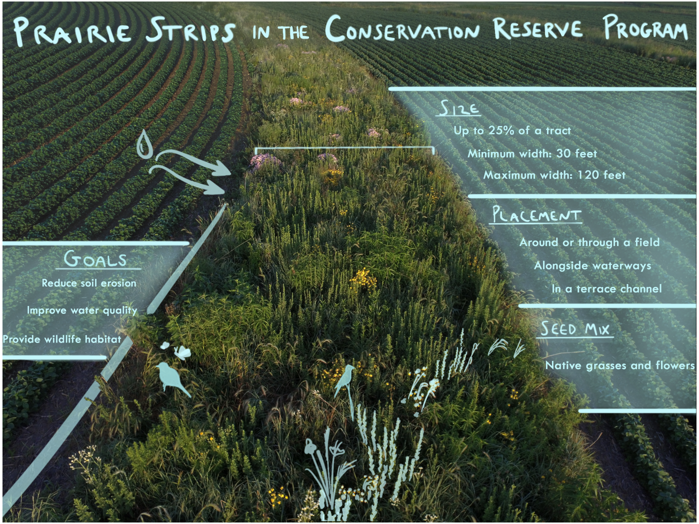
https://www.npr.org/2018/09/22/650698240/hurricane-s-aftermath-floods-hog-lagoons-in-north-carolina

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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NEW RESEARCH IN Physical Sciences Social Sciences

RESEARCH ARTICLE

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

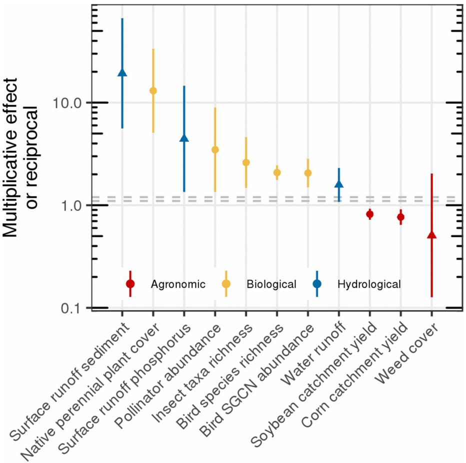
Lisa A. Schulte, Jarad Niemi, Matthew J. Helmers, Matt Liebman, J. Gordon Arbuckle, David E. James, Randall K. Kolka, Matthew E. O'Neal, Mark D. Tomer, John C. Tyndall, Heidi Asbjornsen, Pauline Drobney, Jeri Neal, Gary Van Ryswyk, and Chris Witte

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



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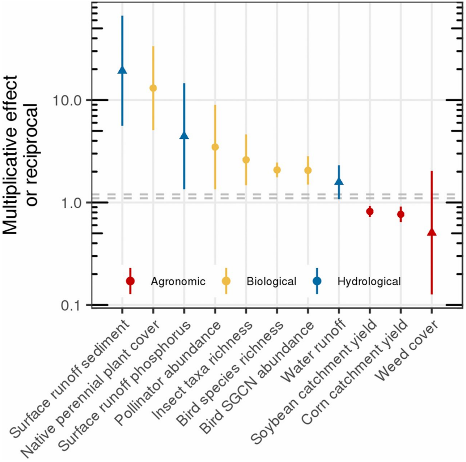

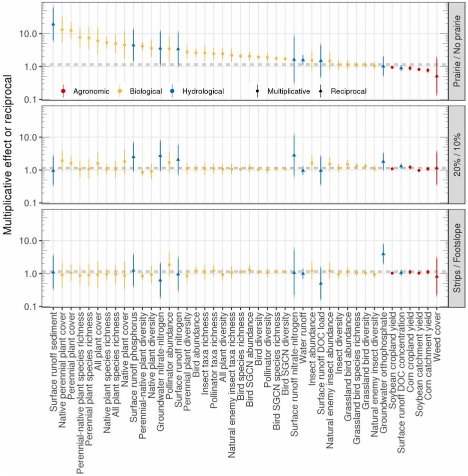

https://www.pnas.org/content/114/42/11247/tab-figures-data

USDA NIFA - Biogas production from manure and herbaceous biomass

NIFA PRESS RELEASE

NATIONAL INSTITUTE OF FOOD AND AGRICULTURE

USDA Scientific Research Program Funds Sustainable Agricultural Systems Projects

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USDA

NATIONAL INSTITUTE OF FOOD AND AGRICULTURE

USDA Scientific Research Program Funds Sustainable Agricultural Systems Projects

Feedstock Production | Anaerobic Digestion (AD) | Product Processing | Distribution and Markets | Society

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

Computer models

- Water Erosion Prediction Project (WEPP)

Computer models

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  - Daily Erosion Project (DEP)

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Computer models

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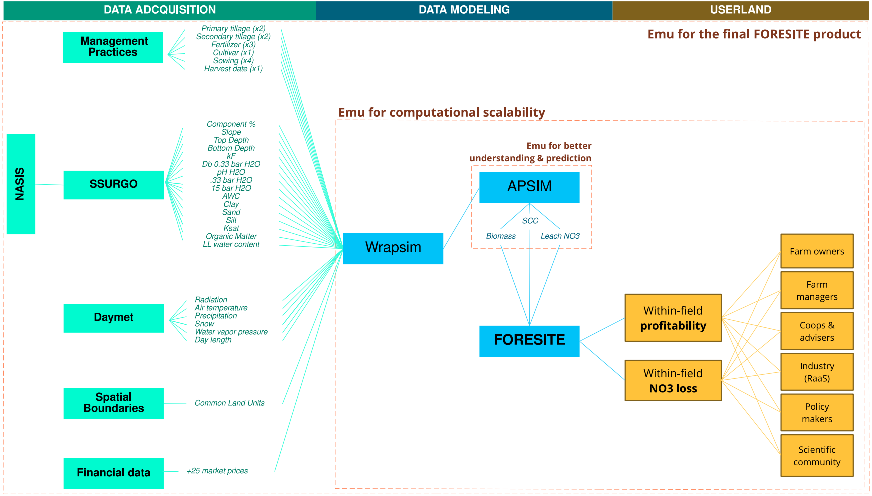
  - Foresite
- Cycles
- Iowa Biogas Assessment Model (IBAM)
- others...

APSIM

Role in the Foresite project



APSIM

Overview

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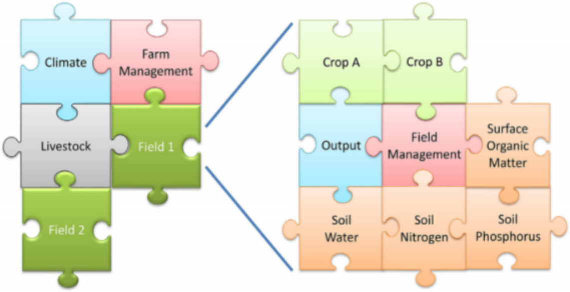

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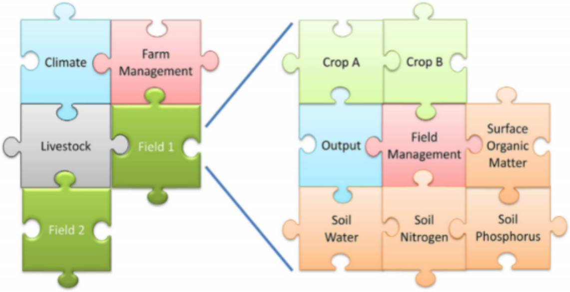

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APSIM

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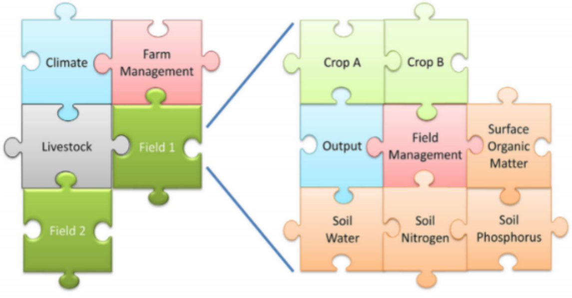

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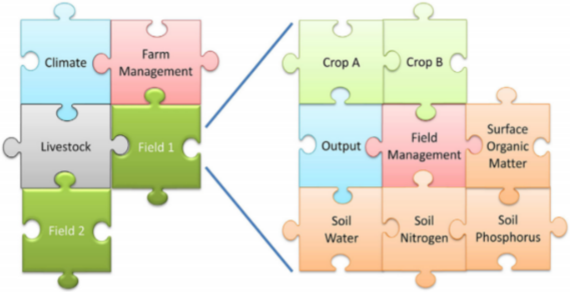

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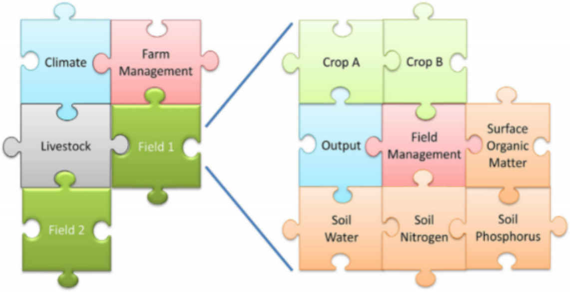

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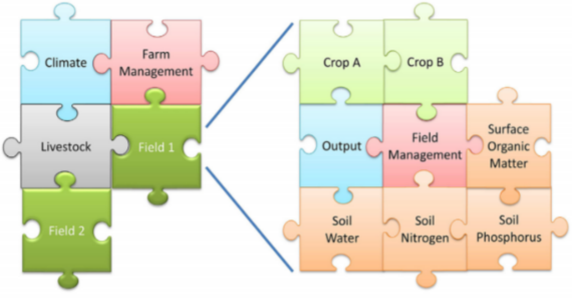

- Physical process based
- Peer-reviewed
- Flexible
- Calibrated for many different climates and countries
- Dedicated, funded team of software engineers working to improve it

APSIM

Emulation goals

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- Assist scientists in studying agronomical hypothesis.

APSIM
Input space

- 2,160 run-specific input values

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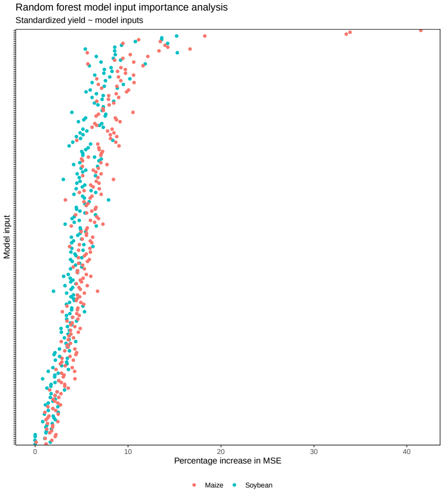
- The input space is...
  - High dimensional: computational and modeling challenging.
  - Structured: complex to capture hierarchy.
  - Vast: large number of runs to explore it.

APSIM

Exploratory Analyses

APSIM

Exploratory Analyses



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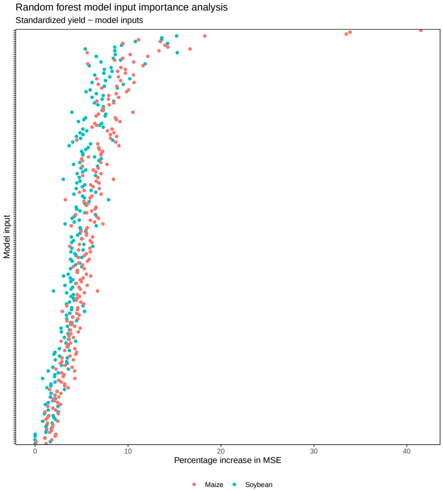

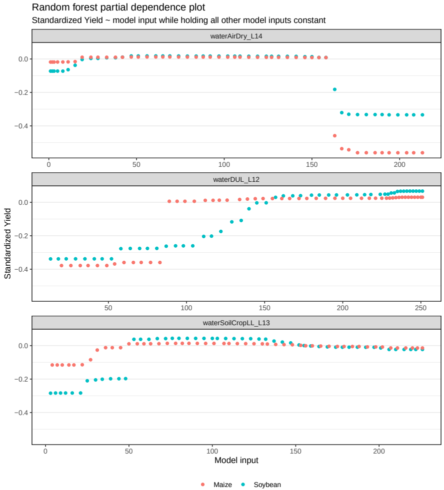

One-at-a-time knot selection

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

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

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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.

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Fully Independent Conditional (FIC) Approximation

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[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]

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Algorithm 1. OAT knot selection algorithm.

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  $x^\dagger = \{x^\dagger, \hat{x}^{\dagger^*}\}$;

until $|x^\dagger| = K_{max}$ *or convergence*;

[Garton et al., Garton]

One-at-a-time knot selection

Knot proposal algorithm

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set the mean of the meta GP equal to log p(y | x, {x†, ·}, θ̂) ;
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    update covariance parameters in meta GP ;
    x*_t = argmax_{z ∈ x \ {x†_l}_{l=1}^{t-1}} α(z; w, {x†_1, ..., x†_{t-1}}) ;
    w_t = log p(y | x, {x†, x*_t}, θ̂)
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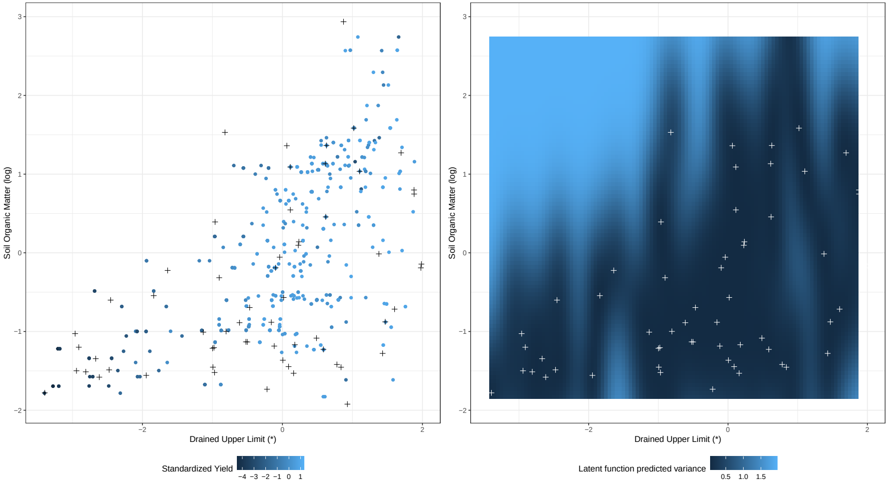
    $w_t = \log p\left(y \middle| x, \left\{x^\dagger, x^*_t\right\}, \hat{\theta}\right)$;
end
return x^*_j such that $j = \text{argmax}_t\, w_t$

[Garton et al., Garton]

OAT Knot selection

Visualization



(*) Content of water retained after gravitational flow.

Future Efforts

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- Recall the SE Kernel with ARD

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

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

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

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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

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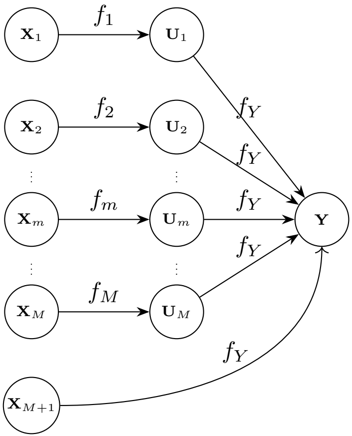

Future Efforts

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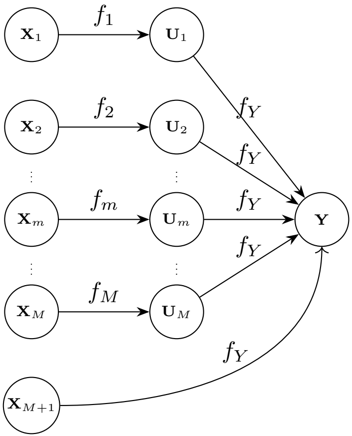

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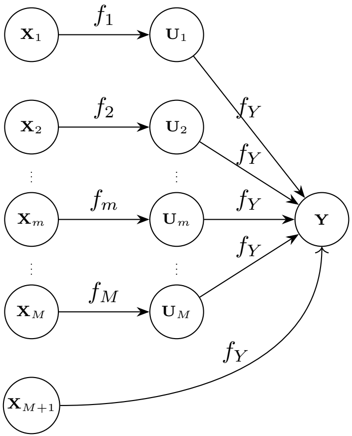

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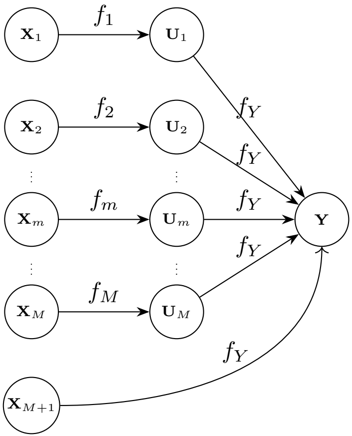

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- For each functional $m \in \{1, \ldots, M\}$, let $\mathbf{U_m} = \mathbf{f_m}(\mathbf{X_m}) + \varepsilon_m$ and assume $\mathbf{f_m} \sim GP(\mu_\mathbf{m}, \sigma_\mathbf{m})$ for $\mu_\mathbf{m} \in \mathbb{R}^{D_m}$

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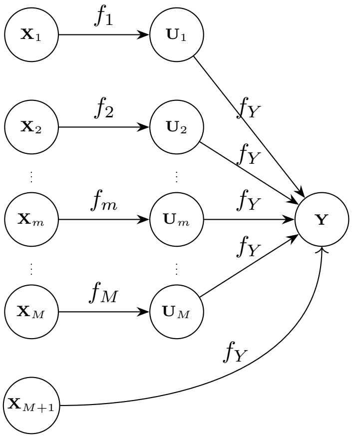

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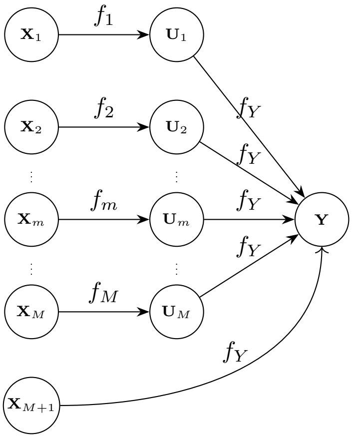

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- $\tilde{\mathbf{X}} = (\mathbf{U_1}, \ldots, \mathbf{U_M}, \mathbf{X_{M+1}})$
- $Y = f_Y(\tilde{\mathbf{X}}) + \varepsilon_y$ and $f_Y \sim GP(\mu_Y, \sigma_Y)$

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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