# **To b**[r]**e**[ed] **or not to b**[r]**e**[ed] with [sym][sub-sym] **AI**?

## Towards a framework for AI enabled predictive breeding

Charlie Messina
Professor Horticultural Sciences
Director UF/IFAS Crop Transformation Center
University of Florida

Mark Cooper
Professor Predictive Breeding
ARC Plant Success
University of Queensland

# University of Florida … turn of the century

**Jim Specht**

*Professor Emeritus (formerly the Francis & Dorothy Haskins and Charles E. Bessey Professor of Agronomy and Horticulture)*

*Agronomy and Horticulture*

## A Gene-Based Model to Simulate Soybean Development and Yield Responses to Environment

C. D. Messina,* J. W. Jones, K. J. Boote, and C. E. Vallejos **+ Jim Specht**

**Table 1. List of soybean near-isogenic lines used for model development and for molecular marker evaluation.**

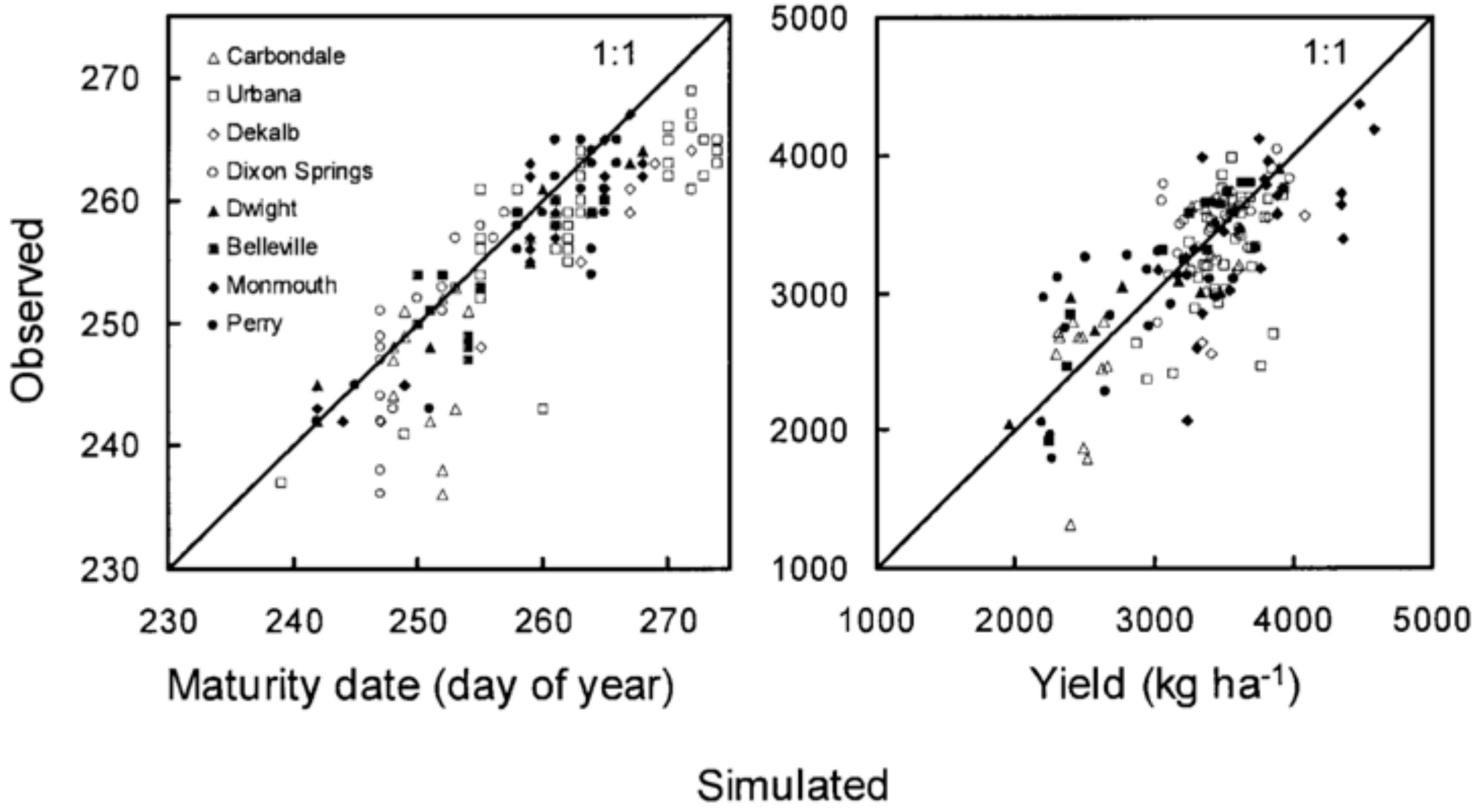
| Near-isogenic line genotype† | Name‡ | Molecular marker evaluation |
|---|---|---|
| *e1 e2 e3 E4 e5 E7* | L71–920 | yes |
| *e1 e2 e3 E4 E5 E7* | L97–2076 | |
| *e1 e2 E3 e4 e5 E7* | L92–21 | yes |
| *e1 e2 E3 E4 e5 E7* | L63–3117 | yes |
| *e1 e2 E3 E4 E5 E7* | L94–1110 | |
| *e1 E2 e3 E4 e5 E7* | L63–2404 | |
| *e1 E2 E3 E4 e5 E7* | Clark | yes |
| *e1 E2 E3 E4 E5 E7* | L92–1195 | |
| *E1 e2 e3 E4 e5 E7* | L80–5914 | |
| *E1 e2 E3 E4 e5 E7* | L66–432 | |
| *E1 e2 E3 E4 E5 E7* | L97–4081 | yes |
| *E1 E2 e3 E4 e5 E7* | L74–441 | yes |
| *E1 E2 E3 E4 e5 E7* | L65–3366 | yes |
| *E1 E2 E3 E4 E5 E7* | L98–2064 | yes |

† Refer to Bernard (1971), Buzzel (1971), Buzzel and Voldeng (1980), Saindon et al. (1989), McBlain and Bernard (1987), and Cober and Voldeng (2001) for genetic analysis of the *E* loci.
‡ Near isogenic lines were provided by Dr. Bernard, University of Illinois.

**Table 5. Associations between *E* loci and genetic coefficients in CROPGRO-Soybean. Dominant and recessive alleles take values of 1 and 0, respectively. NLOCI denotes the sum of dominant alleles.**

| Genetic coefficient† | Linear model | $R^2$ |
|---|---|---|
| CSDL | CSDL = 14.33 – 0.44 NLOCI + 0.27 *E3* – 0.48 *E5* + 0.18 NLOCI *E5* | 0.88 |
| PPSEN | PPSEN = 0.11 + 0.063 NLOCI + 0.58 *E1* – 0.13 *E1* NLOCI | 0.70 |
| EM-FL | EM-FL = 20.77 + 2.1 *E1* + 1.8 *E3* | 0.78 |
| FL-SD | FL-SD = 0.56 FL-VS | – |
| FL-VS | FL-VS = 20.9 + 0.67 NLOCI | 0.47 |
| SD-PM | SD-PM = 35.2 – 1.0 NLOCI – 9.2 *E1* + 2.0 NLOCI *E1* | 0.57 |
| V1-JU | V1-JU = *4.16 E1* | 0.71 |
| R1PRO | R1PRO = 0.1 + 0.066 NLOCI | 0.32 |

CROP SCIENCE, VOL. 46, JANUARY–FEBRUARY 2006




G→P Models

QTLs, RILs, … , ***E* loci**

UF ~ 2000

# Butterfly effect… all started with Jim inspiring a grad student

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Available online at www.sciencedirect.com
SCIENCE DIRECT
Field Crops Research 90 (2004) 145–163
Field Crops Research
www.elsevier.com/locate/fcr

## From genome to crop: integration through simulation modeling

Gerrit Hoogenboom[a,*], Jeffrey W. White[b], Carlos D. Messina[c]
[a]Department of Biological and Agricultural Engineering, University of Georgia, Griffin, Georgia 30223-1797, USA
[b]U.S. Water Conservation Laboratory, USDA-ARS, 4331 E. Broadway Rd., Phoenix AZ 85040, USA
[c]Department of Agricultural and Biological Engineering, University of Florida, Gainesville, Florida 32611, USA

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Journal of Experimental Botany
www.jxb.oxfordjournals.org

REVIEW PAPER

## Yield–trait performance landscapes: from theory to application in breeding maize for drought tolerance

**Carlos D. Messina*, Dean Podlich, Zhanshan Dong, Mitch Samples and Mark Cooper**
Pioneer Hi-Bred, A DuPont Business, 7250 NW 62nd Avenue, Johnston, IA 50131, USA
* To whom correspondence should be addressed. E-mail: charlie.messina@pioneer.com

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Contents lists available at ScienceDirect
European Journal of Agronomy
journal homepage: www.elsevier.com/locate/eja

## Leveraging biological insight and environmental variation to improve phenotypic prediction: Integrating crop growth models (CGM) with whole genome prediction (WGP)

C.D. Messina[a,*], F. Technow[b], T. Tang[a], R. Totir[a], C. Gho[c], M. Cooper[a]
[a] DuPont Pioneer, 8503 NW 62nd Avenue, Johnston, IA, 50131, USA
[b] DuPont Pioneer, 596779 County Road 59N, Woodstock, Ontario, N4S 7W1, Canada
[c] DuPont Pioneer, Semillas Pioneer Chile Ltda., Santa Filomena 1609, Buin, PO Box 267, Chile

Plant Physiology®

## Can we harness digital technologies and physiology to hasten genetic gain in US maize breeding?

Christine H. Diepenbrock[1], Tom Tang,[2] Michael Jines,[3] Frank Technow[4], Sara Lira,[2] Dean Podlich,[2] Mark Cooper[5] and Carlos Messina[2,*,†]

https://doi.org/10.1093/plcell/koac321
THE PLANT CELL 2022: 00: 1–25
THE PLANT CELL

## Breeding crops for drought-affected environments and improved climate resilience

Mark Cooper[1,2,*] and Carlos D. Messina[3]

Theoretical and Applied Genetics (2025) 138:151
https://doi.org/10.1007/s00122-025-04928-6

ORIGINAL ARTICLE

## Toward a general framework for AI-enabled prediction in crop improvement

Carlos Messina[1,2] · Julian Garcia-Abadillo[1] · Owen Powell[2,3] · Shunichiro Tomura[2,3] · Alina Zare[4] · Baskar Ganapathysubramanian[5] · Mark Cooper[2,3]

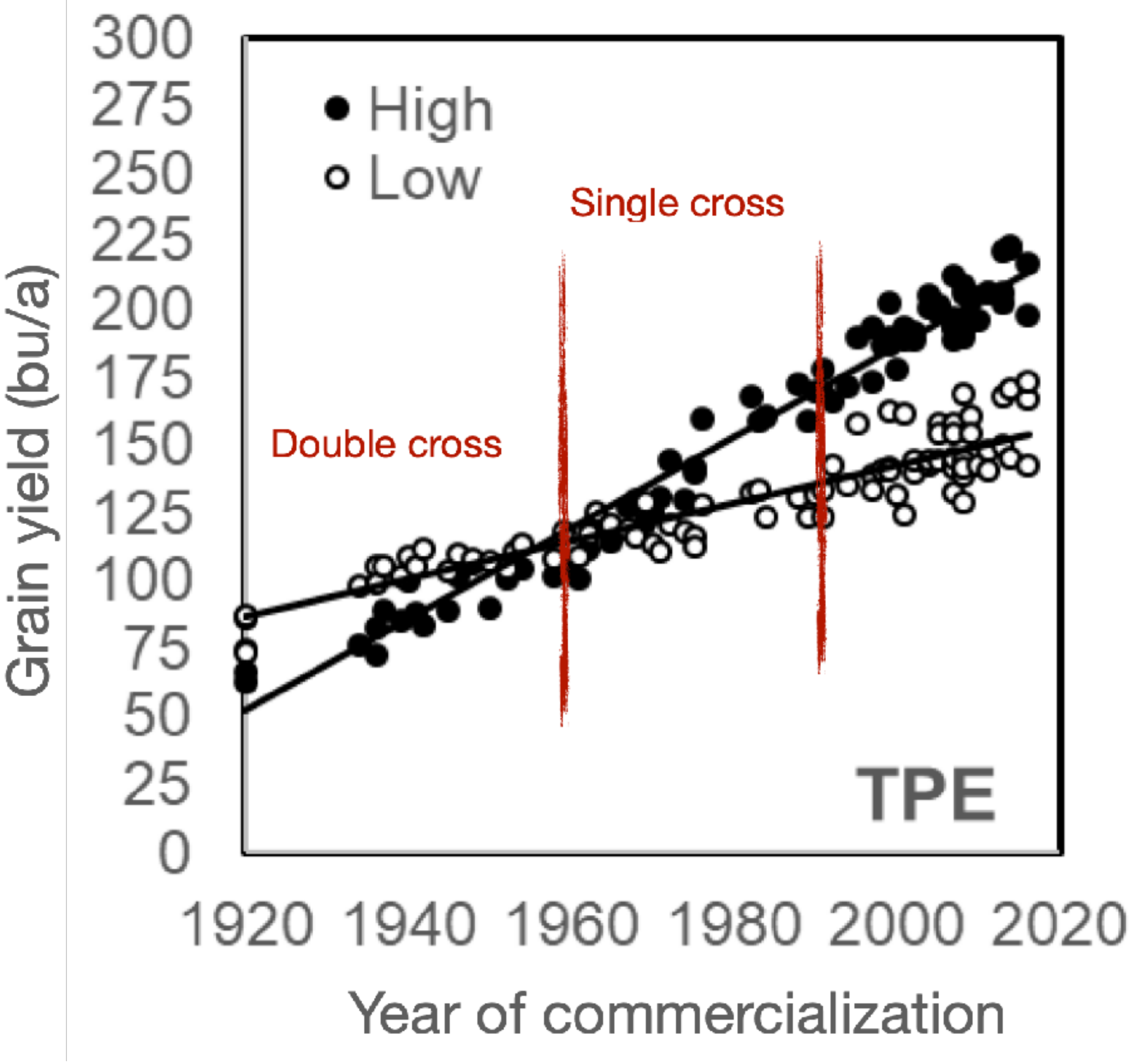
Is there a need for an AI enabled breeding?

...beyond operational effectiveness initiatives


# Long-term selection in maize

Plant Breeding is a very successful enterprise
Preliminary answer
…may be NO

But maize breeding is expensive



# AI enabled Breeding

## 1 Predictive models

- $ Global data hungry
  ↓
- $ Local knowledge rich

## 2 Experimentation

- $ Sampling
  ↓
- $ Design

Local training
↓
Global testing

## 3 Phenomics

- $ Labor intensive data collection
- $ Robotics and platforms

## 4 Use AI to enable AI

- $ Tech support to breeders
- $ Use of LLM to enable breeders with AI tools

# Prediction Problem

## Dimensionality

$$m \gg p$$

## Information content

$$H = -\sum P(x) \times \log_2 P(x)$$

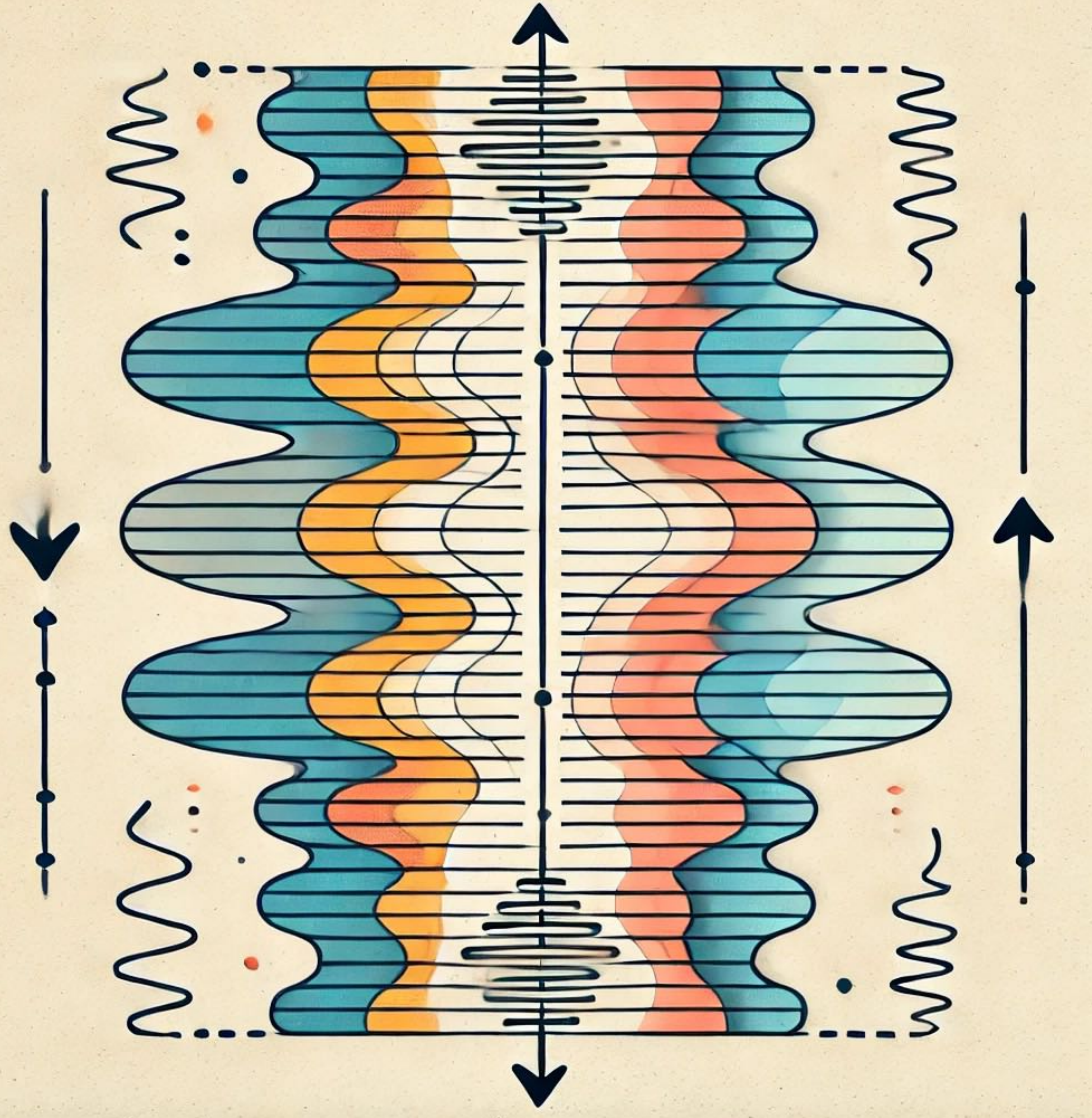
## Emergence Complexity

Properties of the system that the parts don't have and result from their interaction

$$\frac{dp}{dt} = f(p, m)$$

## Upward and Downward causality

*Troublesome to assign causality that increase prediction uncertainty ( $r_a^M$ )*

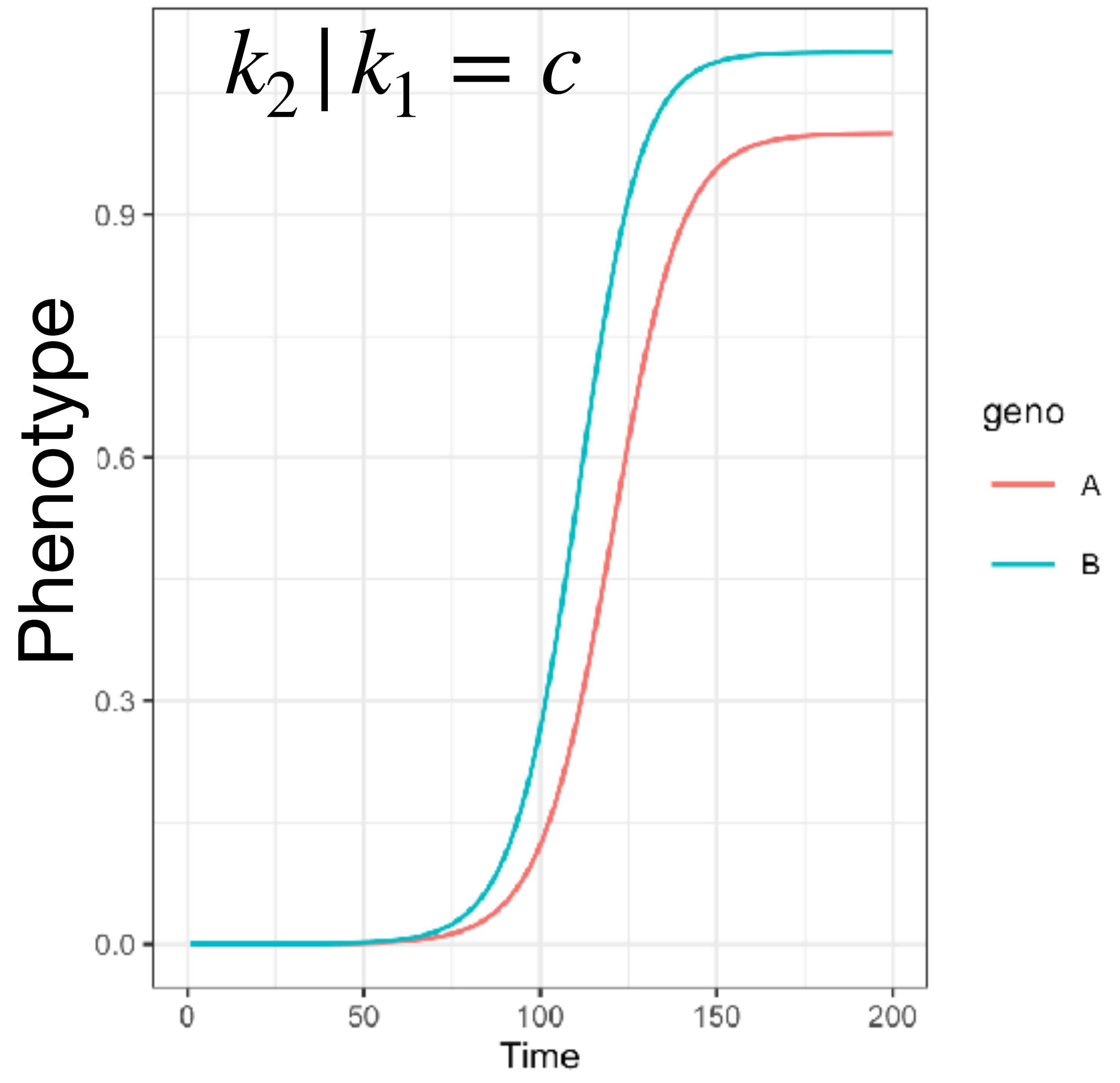


# Transdisciplinary science problem: Semantics to enable convergence s

**Molecular biology**

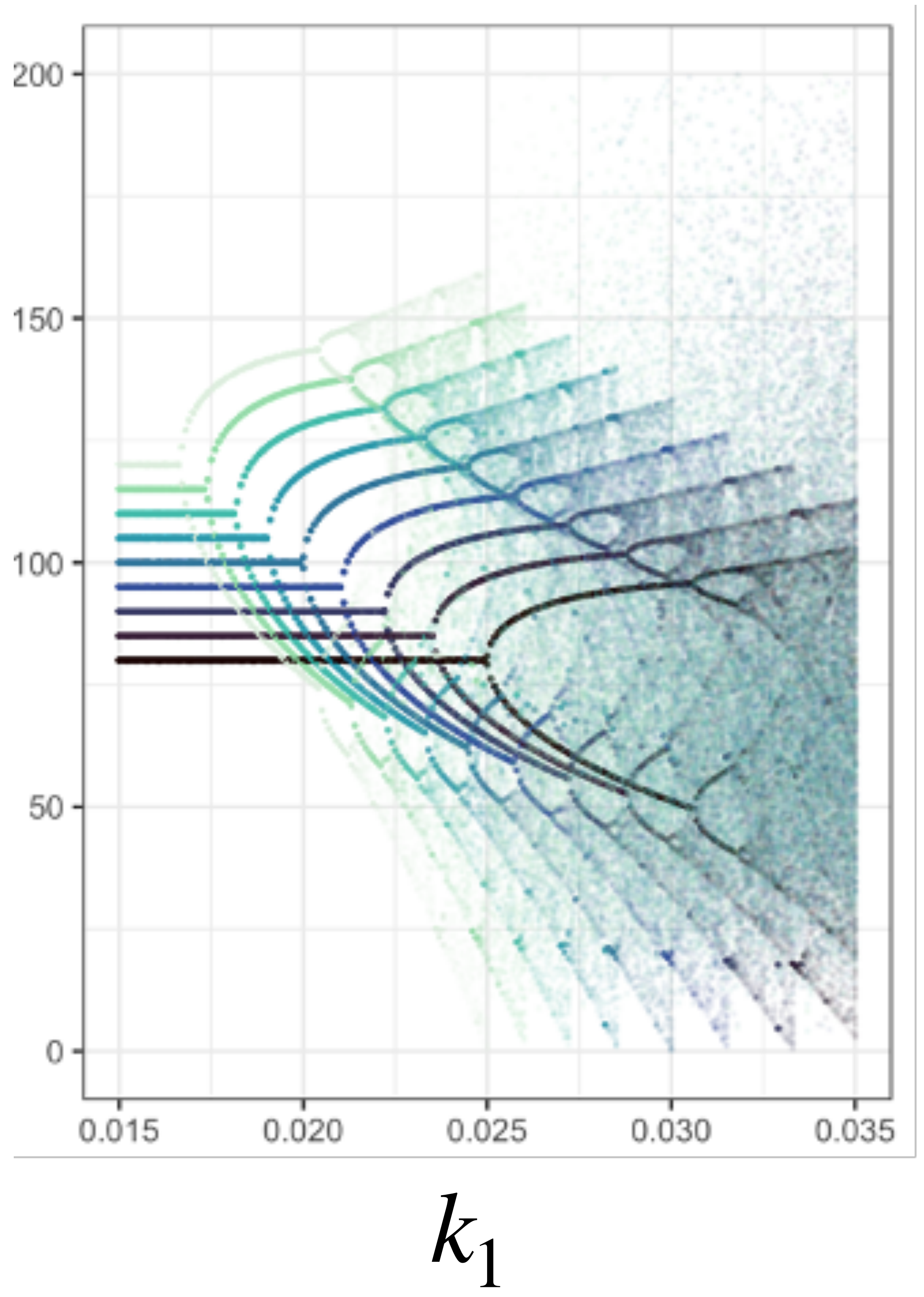
Science of the Plant

$$x_{t+1} = k_1 x_t (k_2 - x_t)$$



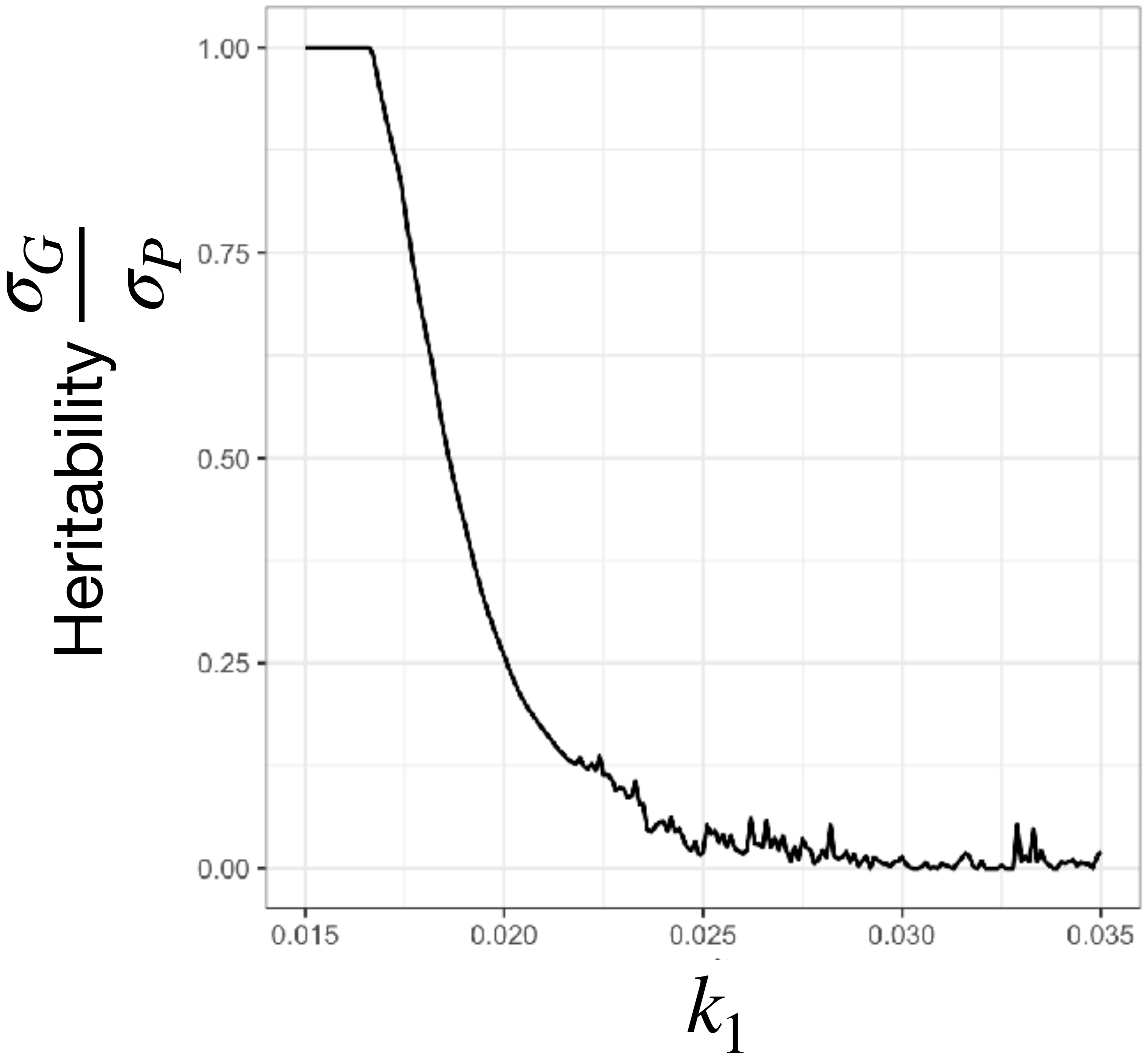

**Organismal Science**

Science of the Crop




**Breeding**

Science of the population and systems



# Why it matters?

## (Rate and Uncertainty)

$$\Delta G_{M,T} = i^{M} \times r_{a}^{M} \times r_{g}^{M,T} \times \sigma_{a}^{T}$$

$\Delta G$ Average predicted response to selection over ALL environments (one cycle of selection)

$i^{M}$ Standardized selection differential (1%, 5%,…)

$r_{a}^{M}$ Prediction accuracy of the model trained with phenotypes determined by the mixture of environmental conditions sampled in multi-environment trials (M)

$r_{M,T}$ Genetic correlation between the multi-environment trials (M) and the target population of environments (T)

$\sigma_{a}^{T}$ Square root of the additive genetic variance in the target population of environments T

# Why it matters?

## (Rate and Uncertainty)

$$\underbrace{\underbrace{\Delta G_{M,T}}} = i^M \times \underbrace{r_a^M} \times r_g^{M,T} \times \sigma_a^T$$

$\Delta G$ Average predicted response to

$i^M$ Standardized selection differen

$r_a^M$ Prediction accuracy of the mod
of environmental conditions sa

$r_{M,T}$ Genetic correlation between th
of environments (T)

$\sigma_a^T$ Square root of the additive genetic variance in the target population of environments T

For the current reality, linear models work for linearized systems ( $r_a^M$ is large)

Expect a change for cropping systems that support a Circular Bioeconomy

Why it matters?

(Rate and Uncertainty)

$$\Delta G_{M,T} = i^{M} \times r_a^{M} \times r_g^{M,T} \times \sigma_a^{T}$$

$\Delta G$ Average predicted re

$i^M$ Standardized select

$r_a^M$ Prediction accuracy
of environmental co

$r_{M,T}$ Genetic correlation
of environments (T)

$\sigma_a^T$ Square root of the a

For the linearized systems of today, the correlation between training and testing environments $r_g^{M,T}$ is high

Change in climate extremes and cropping systems, may lead to much lower $r_g^{M,T}$

# CGM-GS Framework for abductive reasoning

Would be World

Real system is not bijective

Inductive reasoning (sub symbolic AI) has limitations due to feedback and feedforward mechanisms that can lead to ***emergence***

Harness prior scientific knowledge

Crop growth model-genomic selection

$$\frac{dW}{dt} = P_m(1 - e^{-Q \cdot PAR \cdot (1 - e^{-k_1 \cdot W \cdot \kappa})}) \cdot f(\theta) - k_2 \cdot W$$

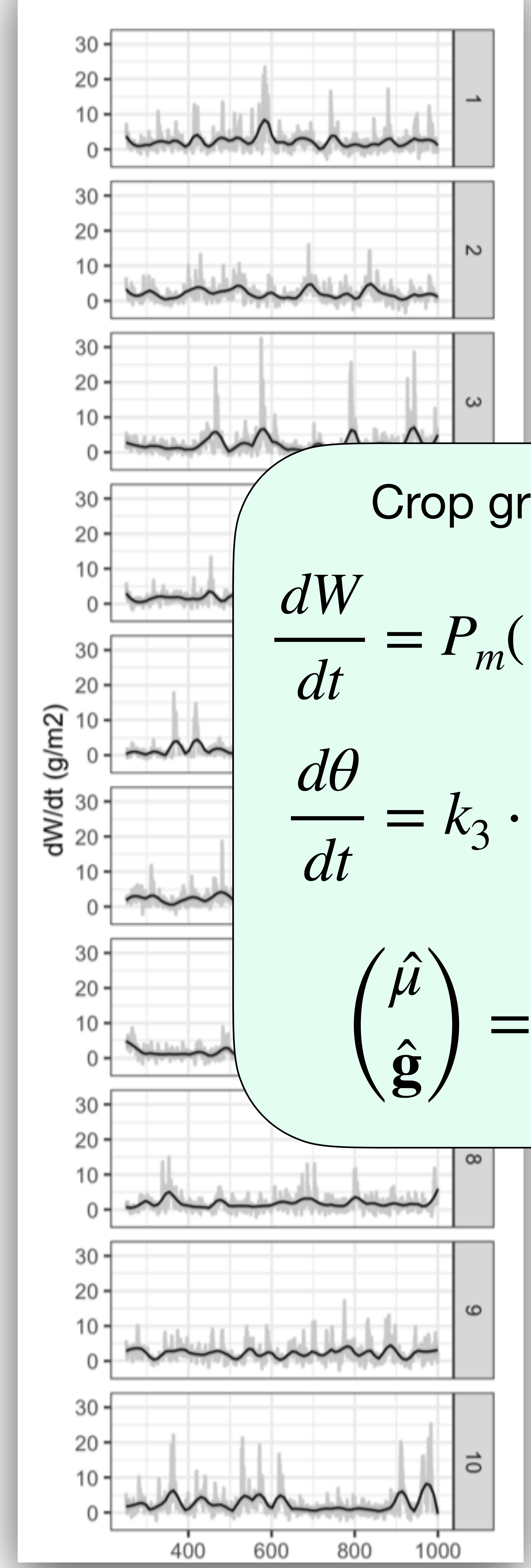
$$\frac{d\theta}{dt} = k_3 \cdot R + kl \cdot (\theta - \theta_0) - \frac{f(W) \cdot (e_s - e)}{\Omega}$$

$$\begin{pmatrix} \hat{\mu} \\ \hat{\mathbf{g}} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n'\mathbf{1}_n & \mathbf{1}_n\mathbf{X} \\ \mathbf{X}'\mathbf{1}_n & \mathbf{X}'\mathbf{X} + \mathbf{I}\lambda \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{1}_n'\hat{\boldsymbol{\Omega}} \\ \mathbf{X}'\hat{\boldsymbol{\Omega}} \end{pmatrix}$$

***Emergence:*** collective properties of a system that parts don't have and arise upon their interaction

# CGM-GS Framework for abductive reasoning

System of equations can generate disorder in the form of recurrent but not periodic pattern and order in form of linear associations with dispersion




Crop growth model-genomic selection

$$\frac{dW}{dt} = P_m(1 - e^{-Q \cdot PAR \cdot (1 - e^{-k_1 \cdot W \cdot \kappa})}) \cdot f(\theta) - k_2 \cdot W$$

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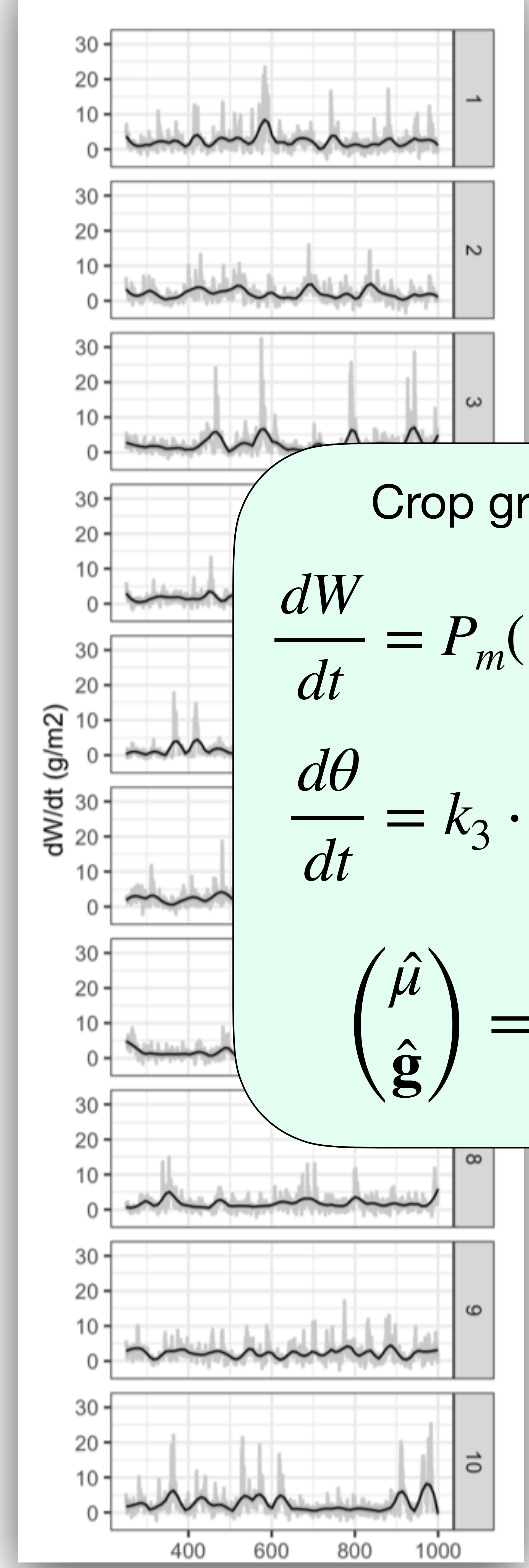
# CGM-GS Framework for abductive reasoning

System of equations can generate disorder in the form of recurrent but not periodic pattern and order in form of linear associations with dispersion

Yet, it can generate order and stable realistic patterns, such as water use efficiency

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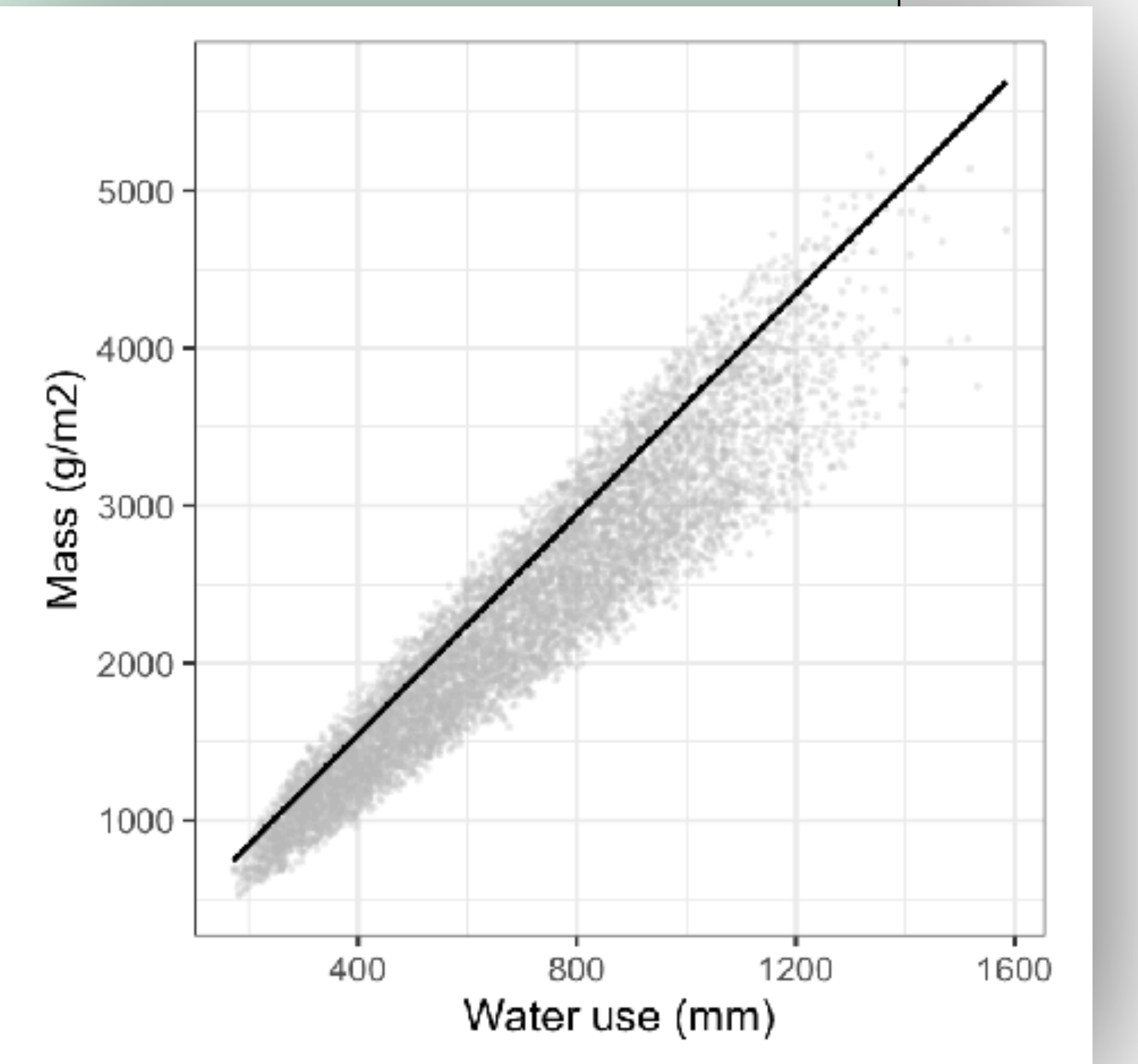
$$\frac{d\theta}{dt} = k_3 \cdot R + kl \cdot (\theta - \theta_0) - \frac{f(W) \cdot (e_s - e)}{\Omega}$$

$$\begin{pmatrix} \hat{\mu} \\ \hat{\mathbf{g}} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_n'\mathbf{1}_n & \\ \mathbf{X}'\mathbf{1}_n & \mathbf{X}' \end{pmatrix}$$



# CGM-GS Framework for abductive reasoning

Definitions

Symbolic AI: Crop growth model

subSymbolic AI: Statistical learning

Bayesian methodology to estimate parameters given a set of data and a likelihood function (here CGM)

## Artificial Intelligence

Deductive, Inductive and Abductive reasoning to solve the system of equations Messina et al. 2018

$$P(\Theta/D) \propto P(D/\Theta)$$

## Crop growth model-genomic selection

$$\frac{dW}{dt} = P_m(1 - e^{-Q \cdot PAR \cdot (1 - e^{-k_1 \cdot W \cdot \kappa})}) \cdot f(\theta) - k_2 \cdot W$$

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# CGM-GS Framework for abductive reasoning

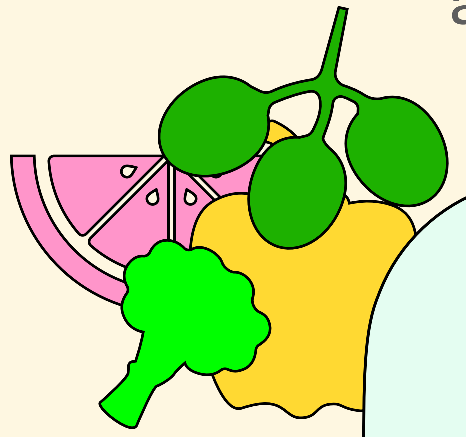
Phenomics informed by CGM is crucial to create **INFORMATIVE** data sets

Limit issues with equifinality and estimability

$$H = -\sum P(x) \times \log_2 P(x)$$

## Phenomics (IoT)

Measure the state of the system at relevant points in time to allow estimation of parameters (physiological and genetic)



## Artificial Intelligence

Deductive, Inductive and Abductive reasoning to solve the system of equations
Messina et al. 2018

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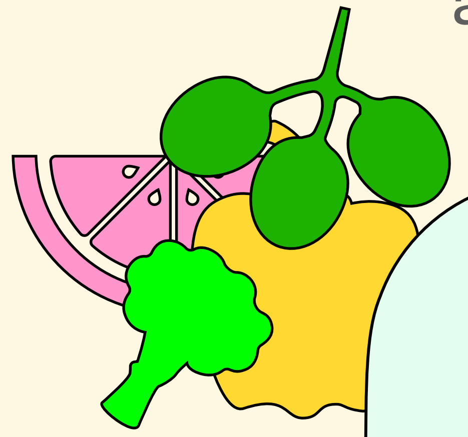
# CGM-GS Framework for abductive reasoning

Enviromics: soil, weather, management and other measurements of inputs to the model

## Phenomics (IoT)

Measure the state of the system at relevant points in time to allow estimation of parameters (physiological and genetic)



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Deductive, Inductive and Abductive reasoning to solve the system of equations Messina et al. 2018

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## Crop growth model-genomic selection

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Monitor the environment to quantify the realized value of the random variables that are inputs to the system of equations (e.g. R)

## Environmics (IoT)

# CGM-GS Framework for abductive reasoning

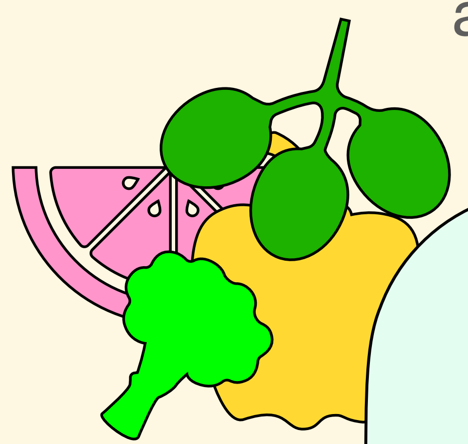
Genomics informed by genetics, and germplasm is crucial to create **INFORMATIVE** data sets

Constrain solution space

$$H = -\sum P(x) \times \log_2 P(x)$$

## Phenomics (IoT)

Measure the state of the system at relevant points in time to allow estimation of parameters (physiological and genetic)



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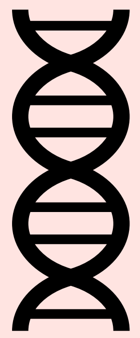


Methods to characterize the genotype of each individual in the training and prediction sets to allow estimation and prediction of performance $\int f(x)dx$

## Genomics

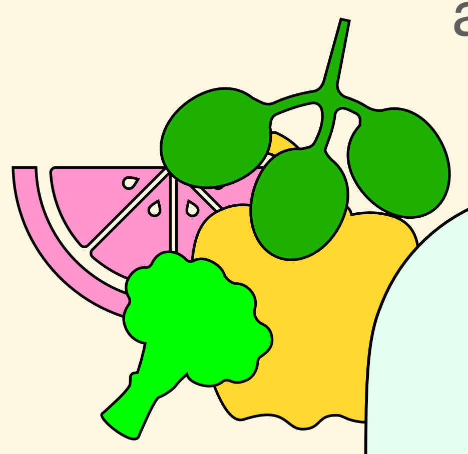
# CGM-GS Framework for abductive reasoning

Integrating symbolic (CGM) and sub symbolic (GS) provides the framework to inform Phenomics, Enviromics and Genomics.

Goal is to estimate parameter set $[P_m, Q, k_1, k_2, \ldots, k_m, kl, \lambda, \Omega]$

## Phenomics (IoT)

Measure the state of the system at relevant points in time to allow estimation of parameters (physiological and genetic)



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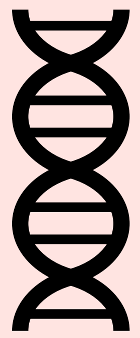
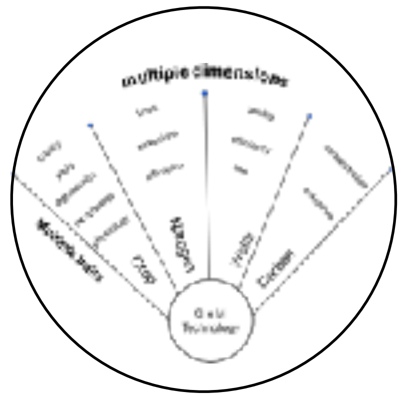
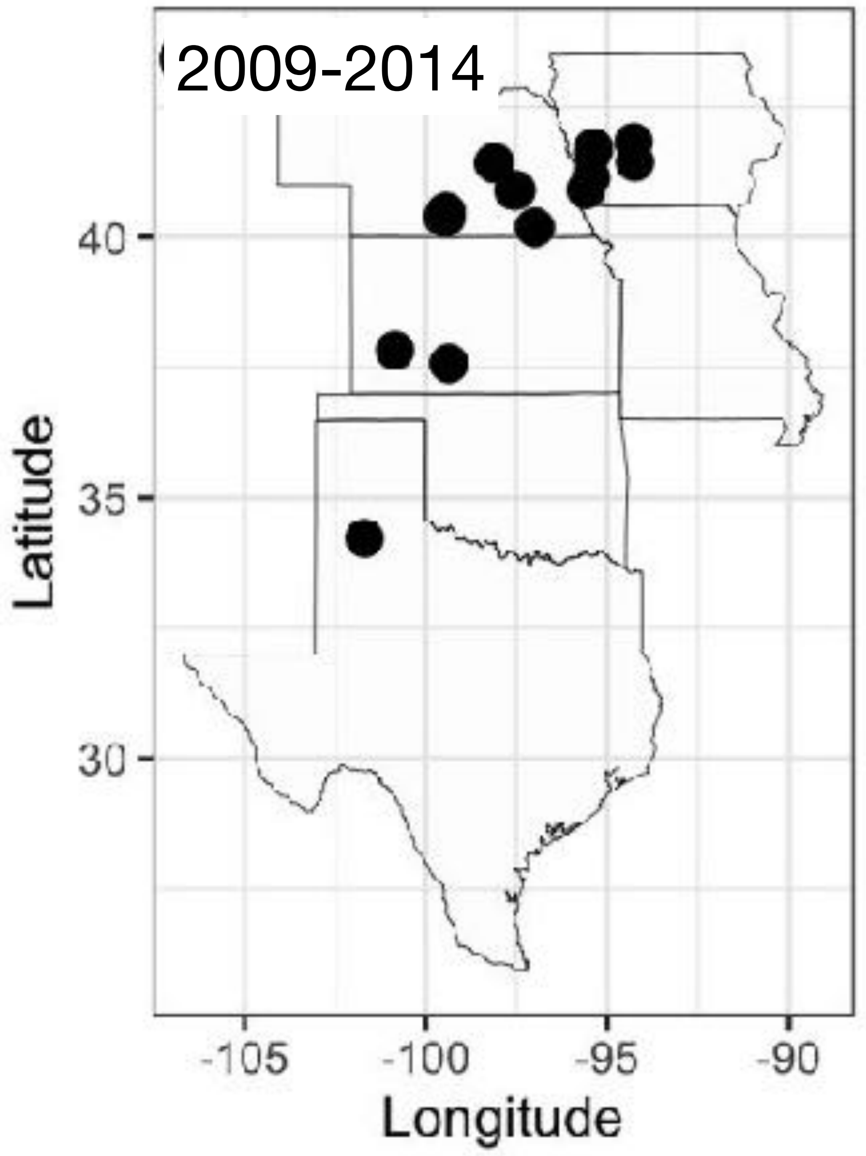


Methods to characterize the genotype of each individual in the training and prediction sets to allow estimation and prediction of performance $\int f(x)dx$

## Genomics

# Predictive accuracy using a Crop Model as the State Space generating function

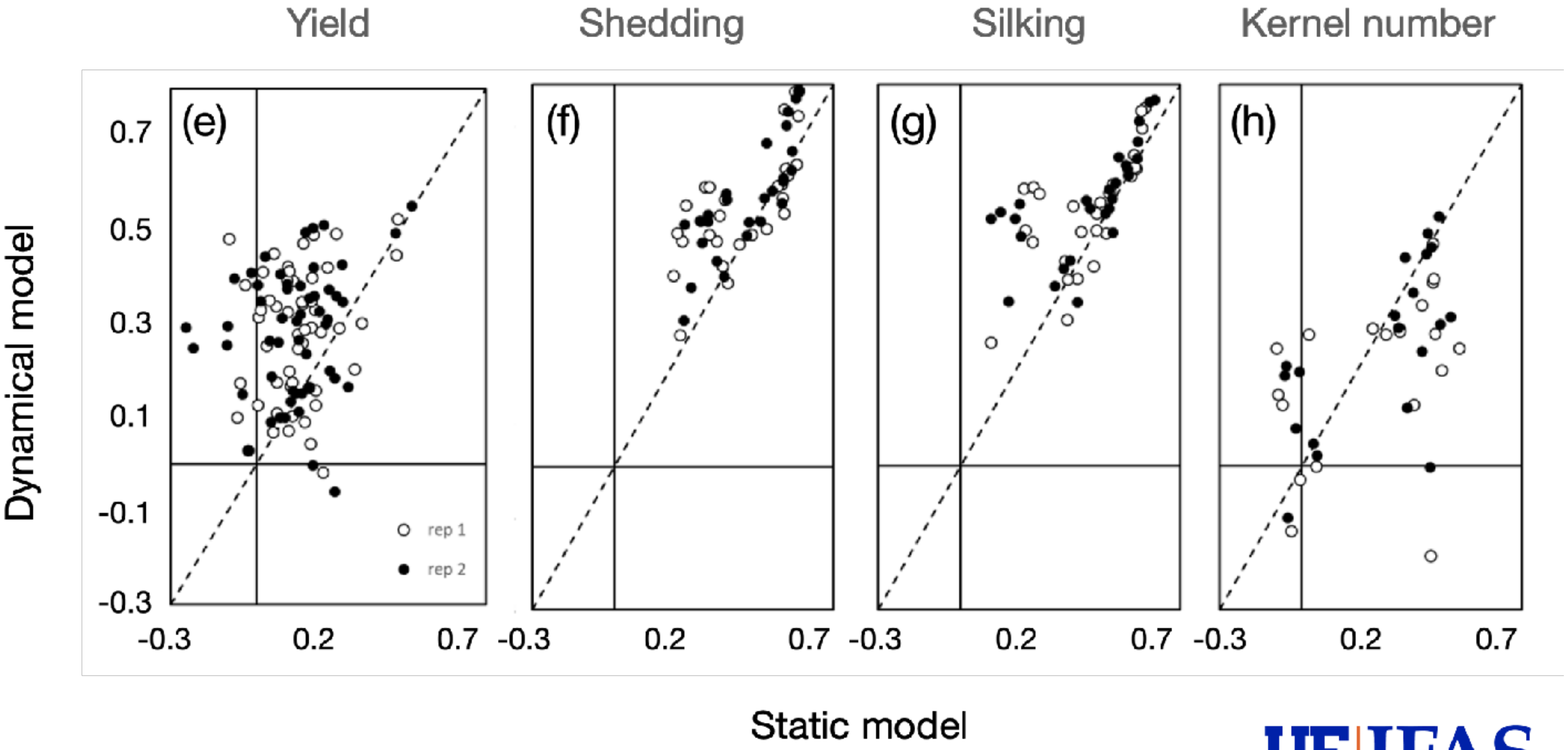





7615
hybrids

Messina et al. (2022) Journal of the ASABE. 65(3): 491-504.

**Prediction skill ($r_a^M$)**

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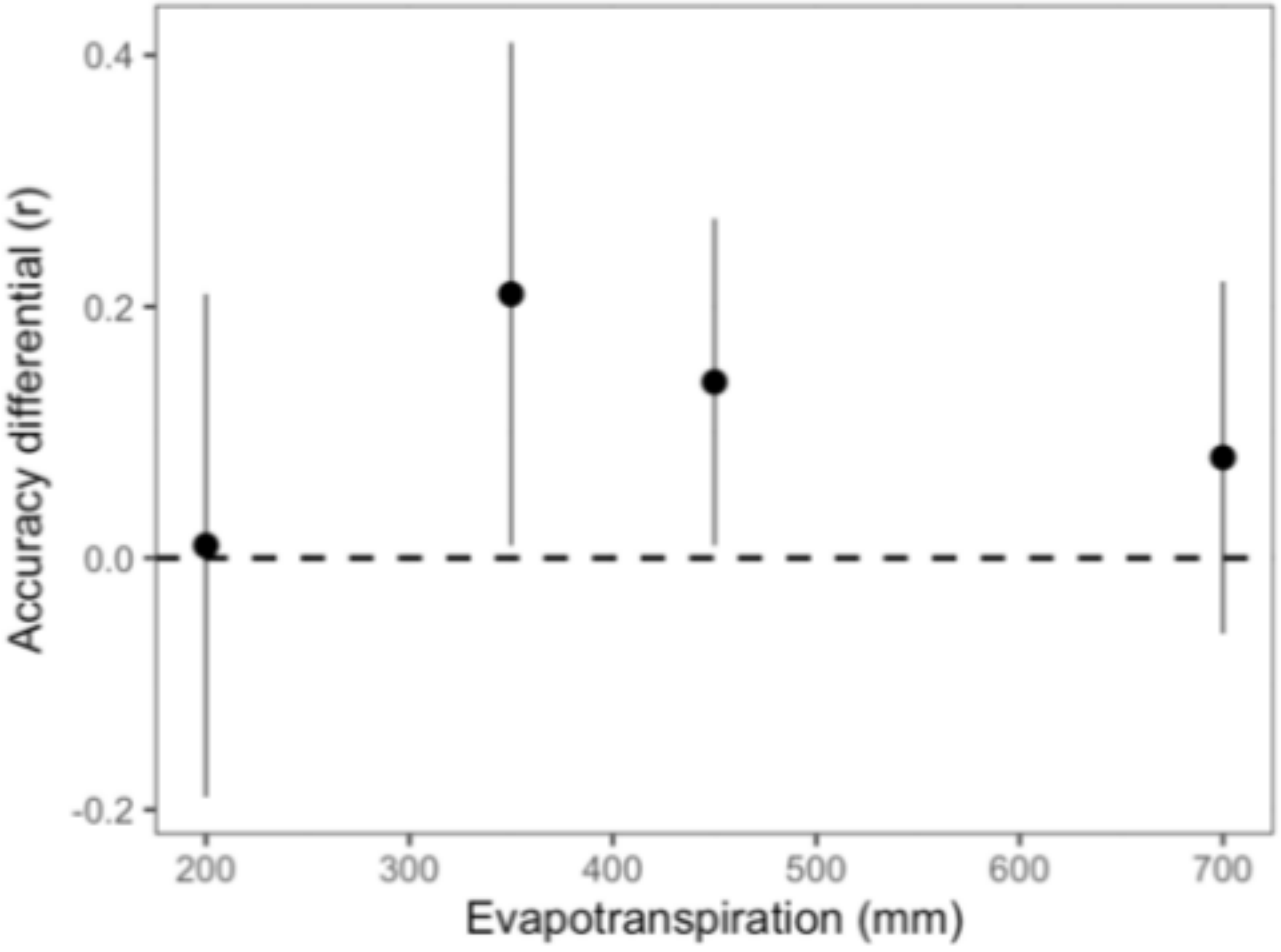
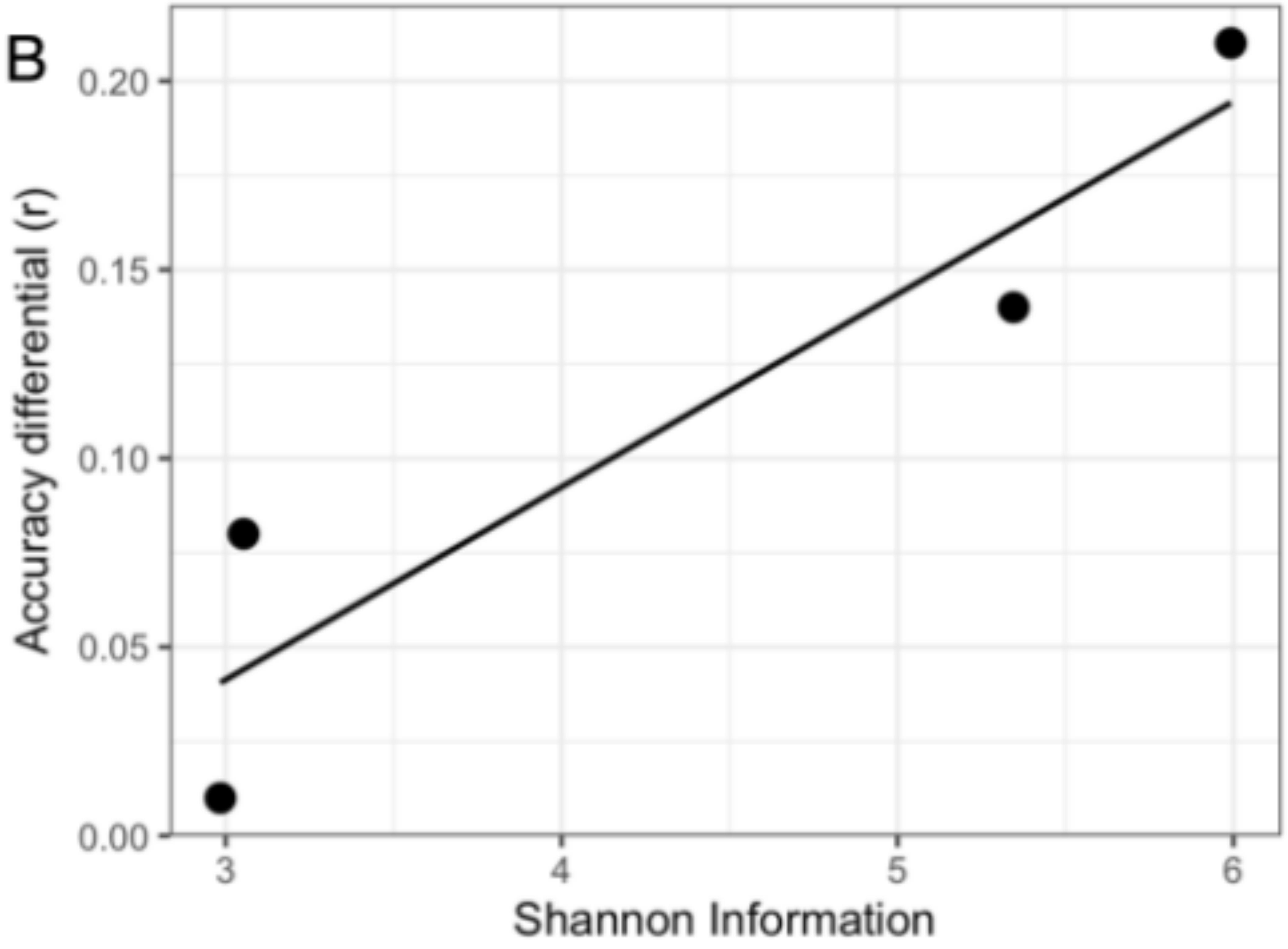
# Prediction accuracy differential ($r^M_{a,+CGM} - r^M_{a,-CGM}$) increase with increasing system complexity

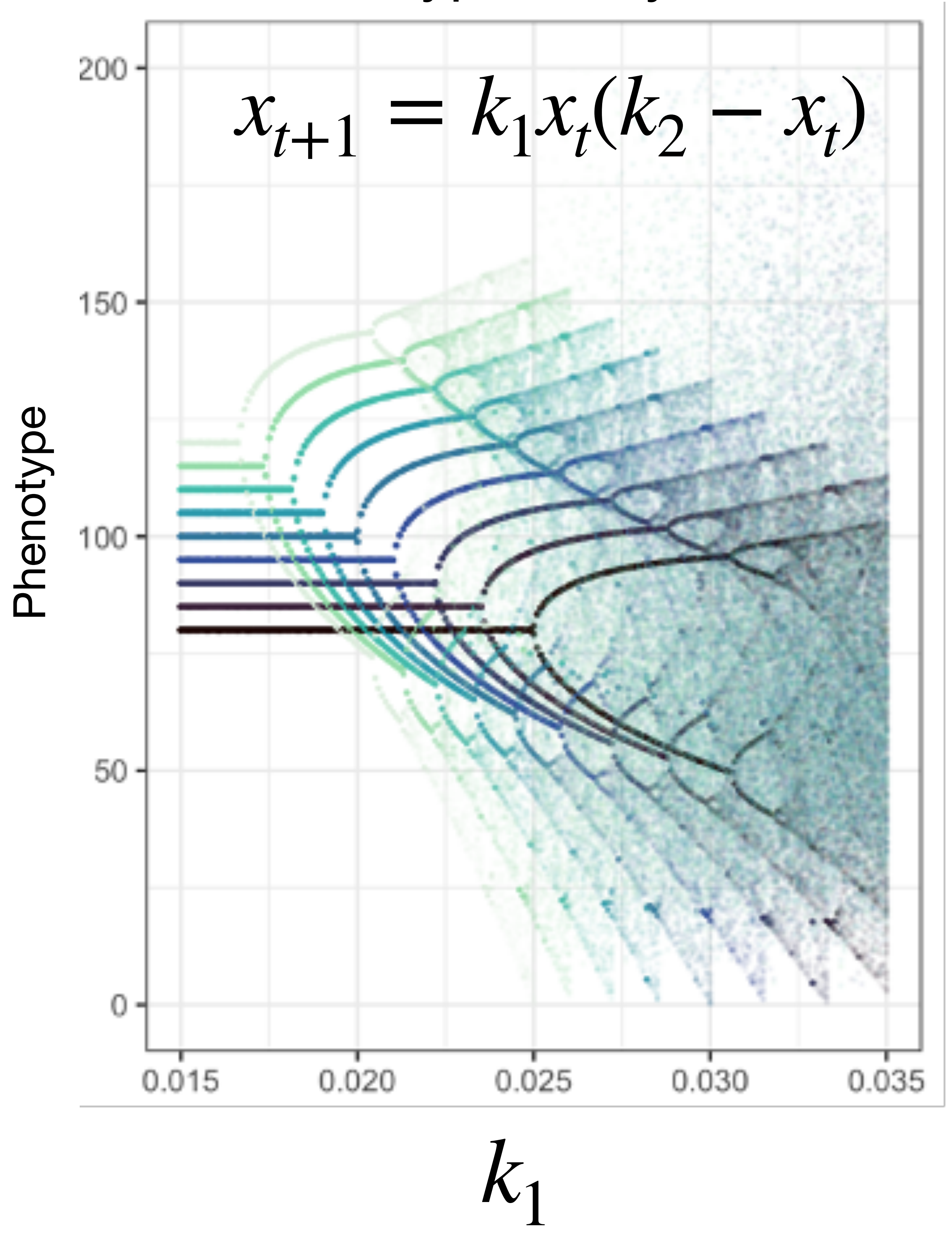


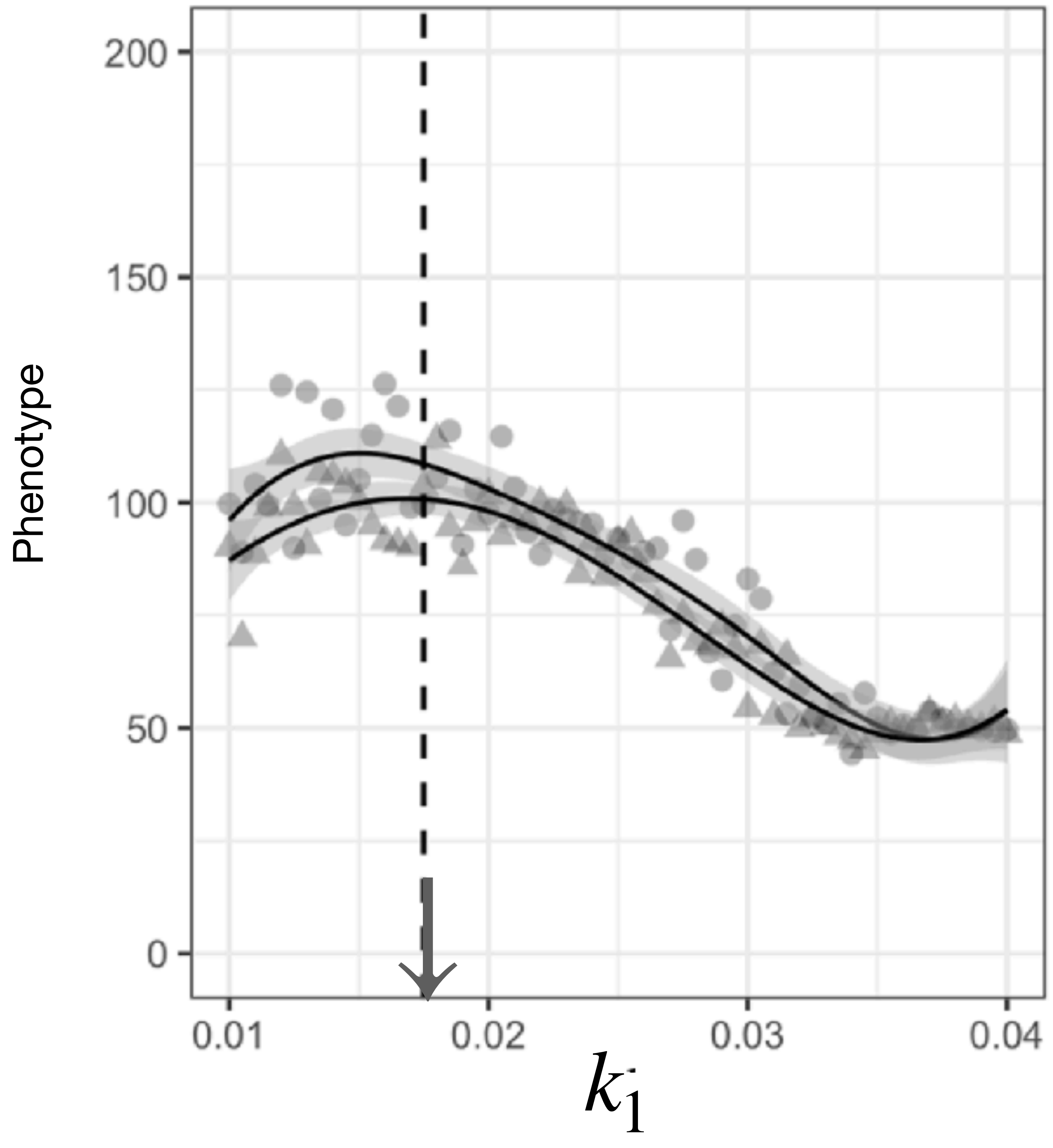
# Simple growth model

## *Estimate $k_2$ for each genotype and predict phenotype*

Phenotypic space
Phenotypes vary with $k_1$




GBLUP by level of $k_1$




Limited predictive skill even when phenomics is perfect

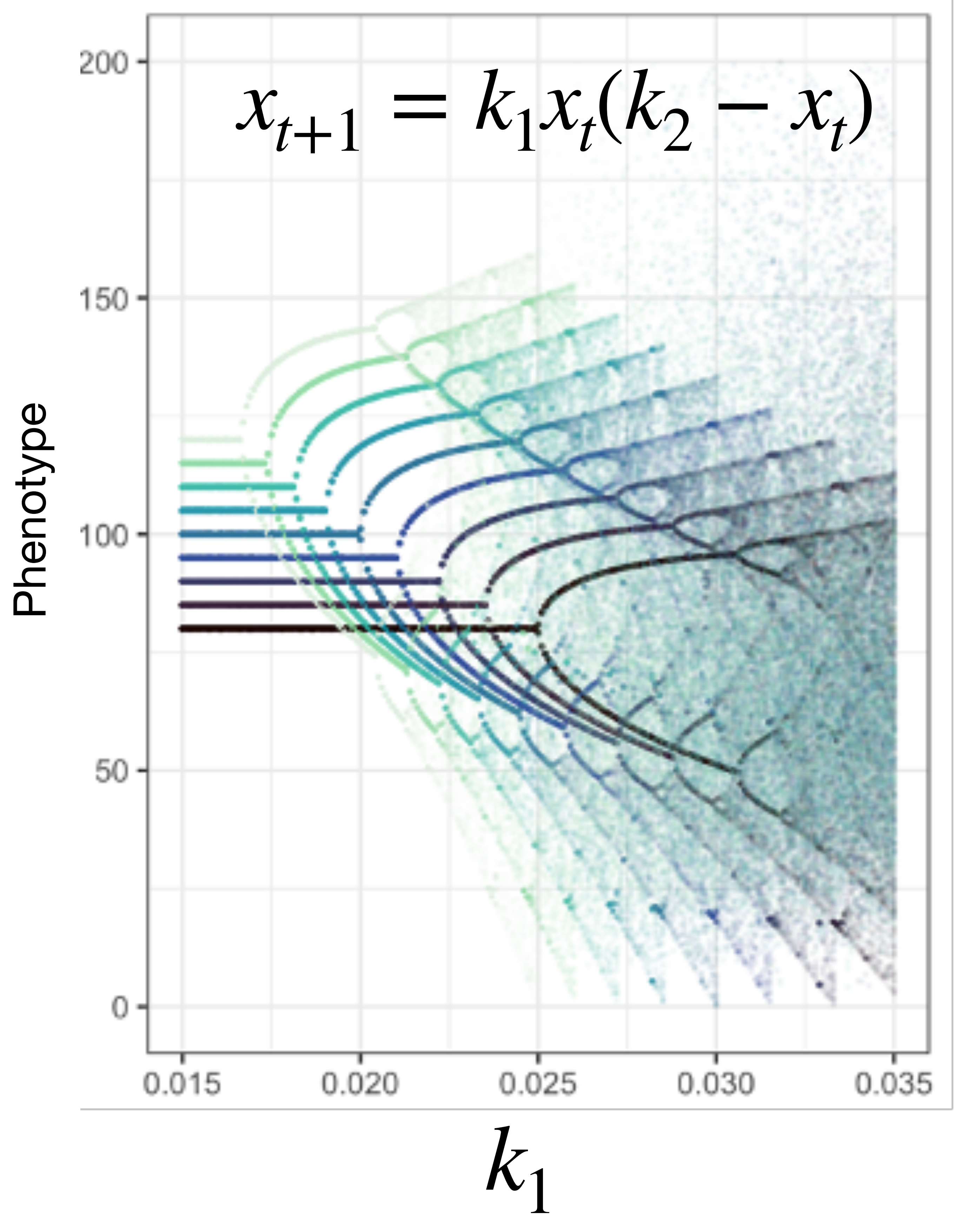
Rankings may be recovered
… but with limited resemblance of reality

Difficult to separate
(recall reduction in $h^2$)

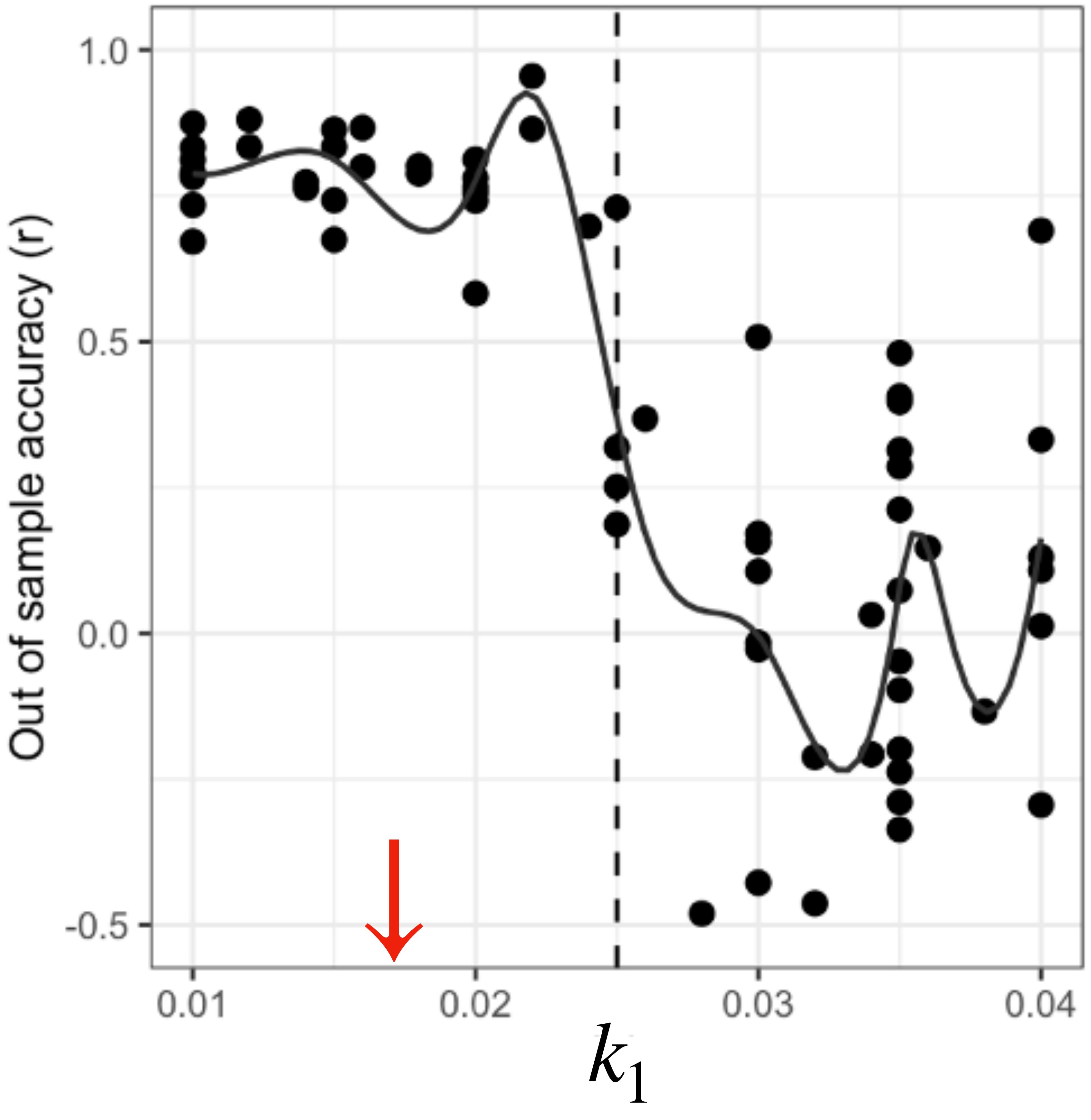
# Simple growth model

## *Estimate $k_2$ for each genotype and predict phenotype*

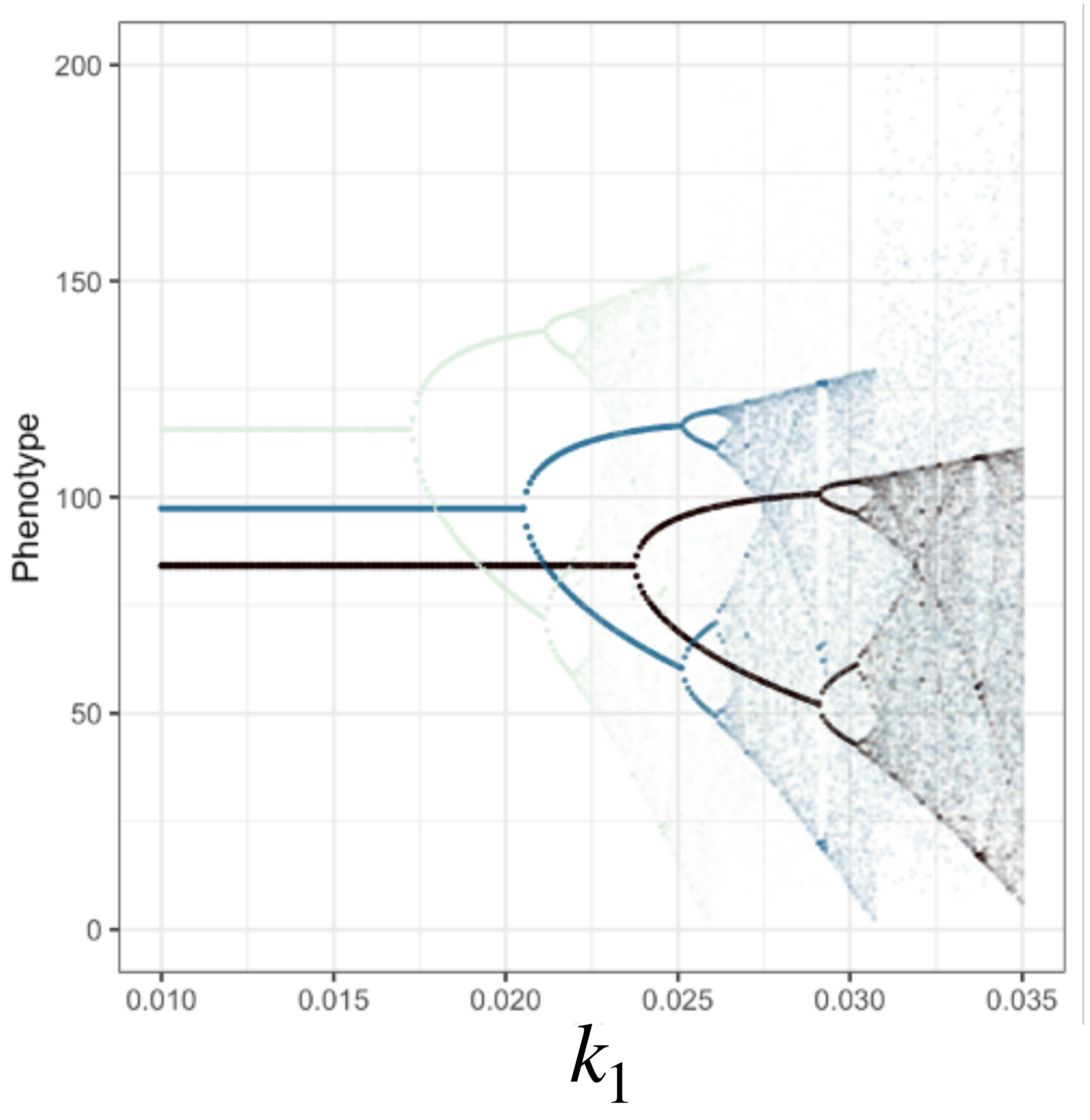
Phenotypic space
Phenotypes vary with $k_1$




Recover parameter $k_2$ for each genotype




Predict Phenotypic space for each genotype $k_2$



# Predictive breeding as model ensembles

$$E(P_{ij}) = \frac{1}{n}\sum_n g(NK)_{in}^{D} + \frac{1}{s}\sum_s \Gamma(\mathrm{o}(E(NK))_p, \mathbf{Q}, \mathbf{I}_t)_{ijs}^{D} + e_{ij}$$

Ensemble mean

Expectation over Genomic Prediction models

Expectation over Dynamical Models

Expectation over a sample of gene networks *NK*

# Diversity prediction theorem

$$(\widehat{x^M} - x^T)^2 = \sum_{i=1}^{N} \frac{(x_i^M - x^T)^2}{N} - \sum_{i=1}^{N} \frac{(x_i^M - \widehat{x^M})^2}{N}$$

Model prediction ensemble

True

Diversity model (M) term

Ensembles of diverse models outperform any single model.

# Perspectives I

**Continue developing a New paradigm in AI enabled prediction**

**Neuroscience**

Science of the brain

Objective and quantitative

System
Parts and Connections

Mark Rothko

Jackson Pollock

**Psychology**

Science of the mind

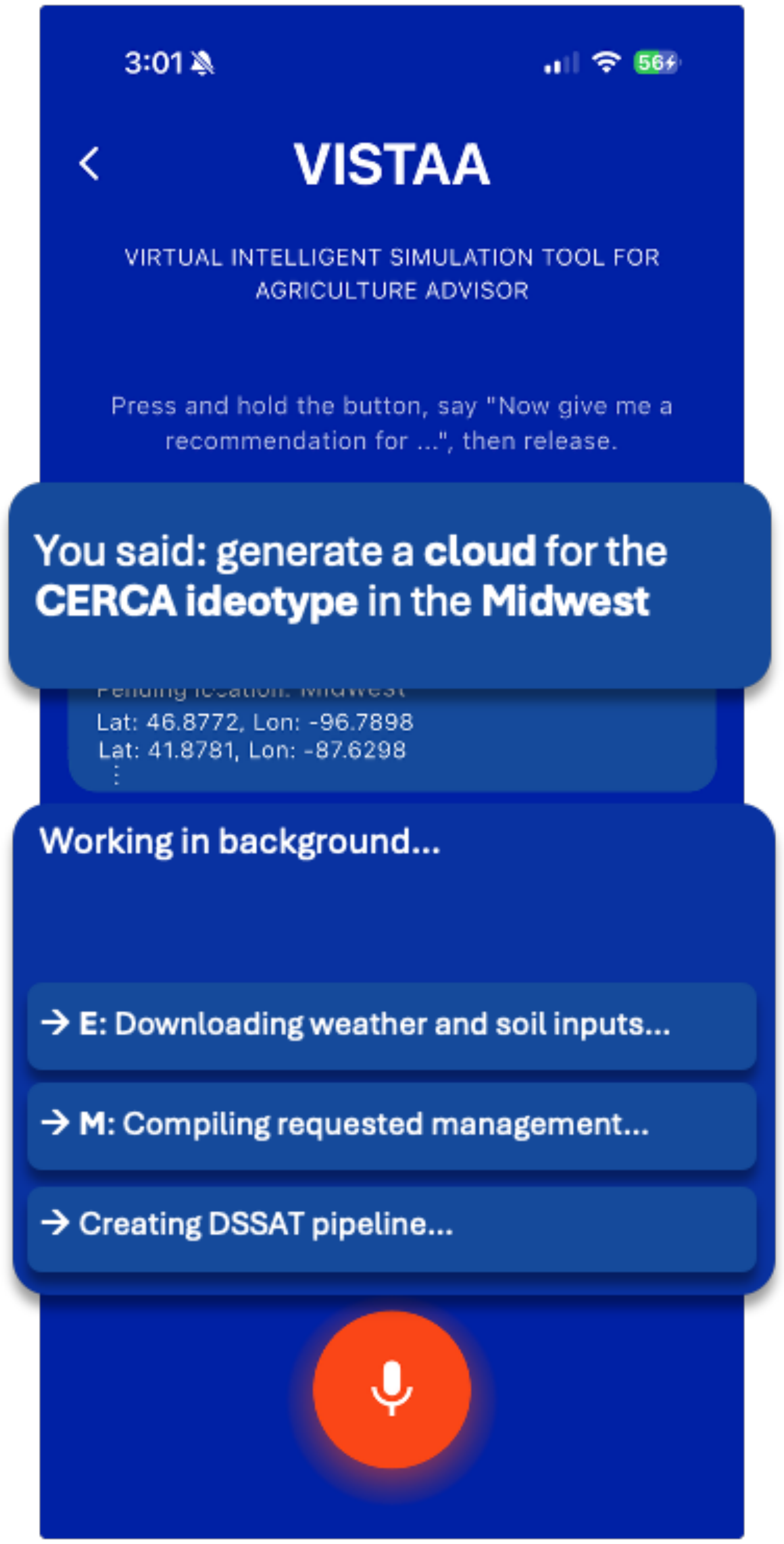
Subjective and holistic

System
Output & Behavior

**Neuropsychology search for a unified theory of the brain and the mind**

## Emergence Crop Modeling reconciles order and chaos

# Perspective II: Use AI to enables AI for breeders

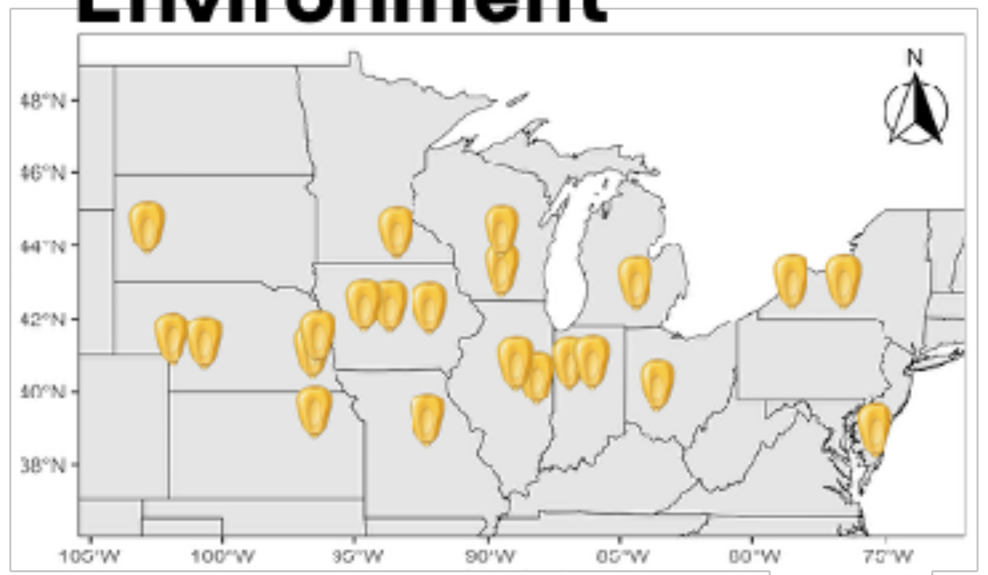



User-LLM interaction

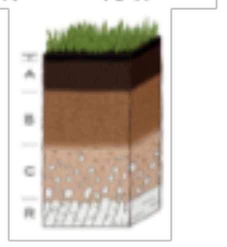
## Genotype

- Growth
- Development
- Environmental sensitivities
- Stress responses
  - **Extended growing season**
  - **Cold tolerance**
  - **Low protein content**

## Environment



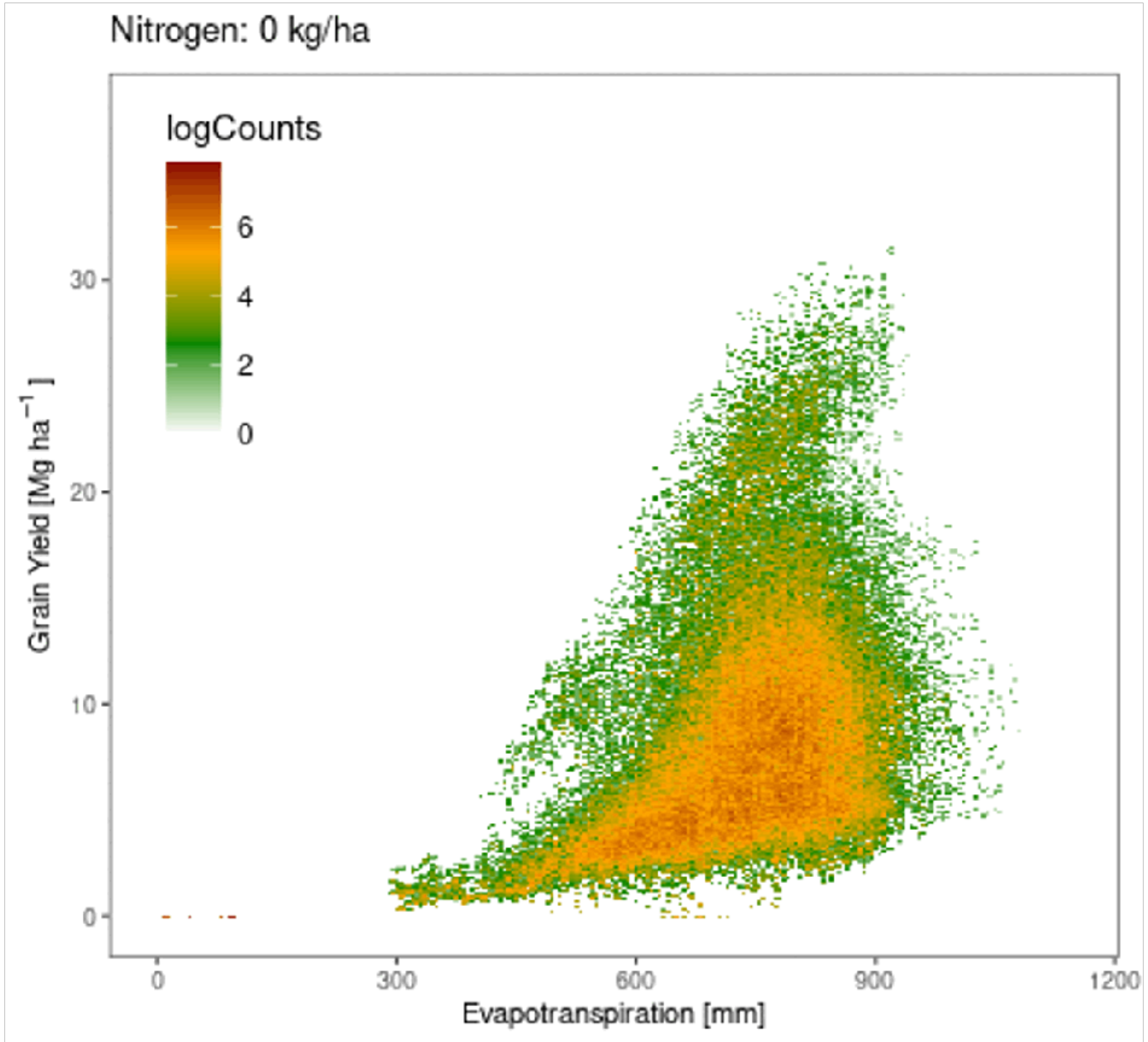
POWER
Prediction Of Worldwide Energy Resources



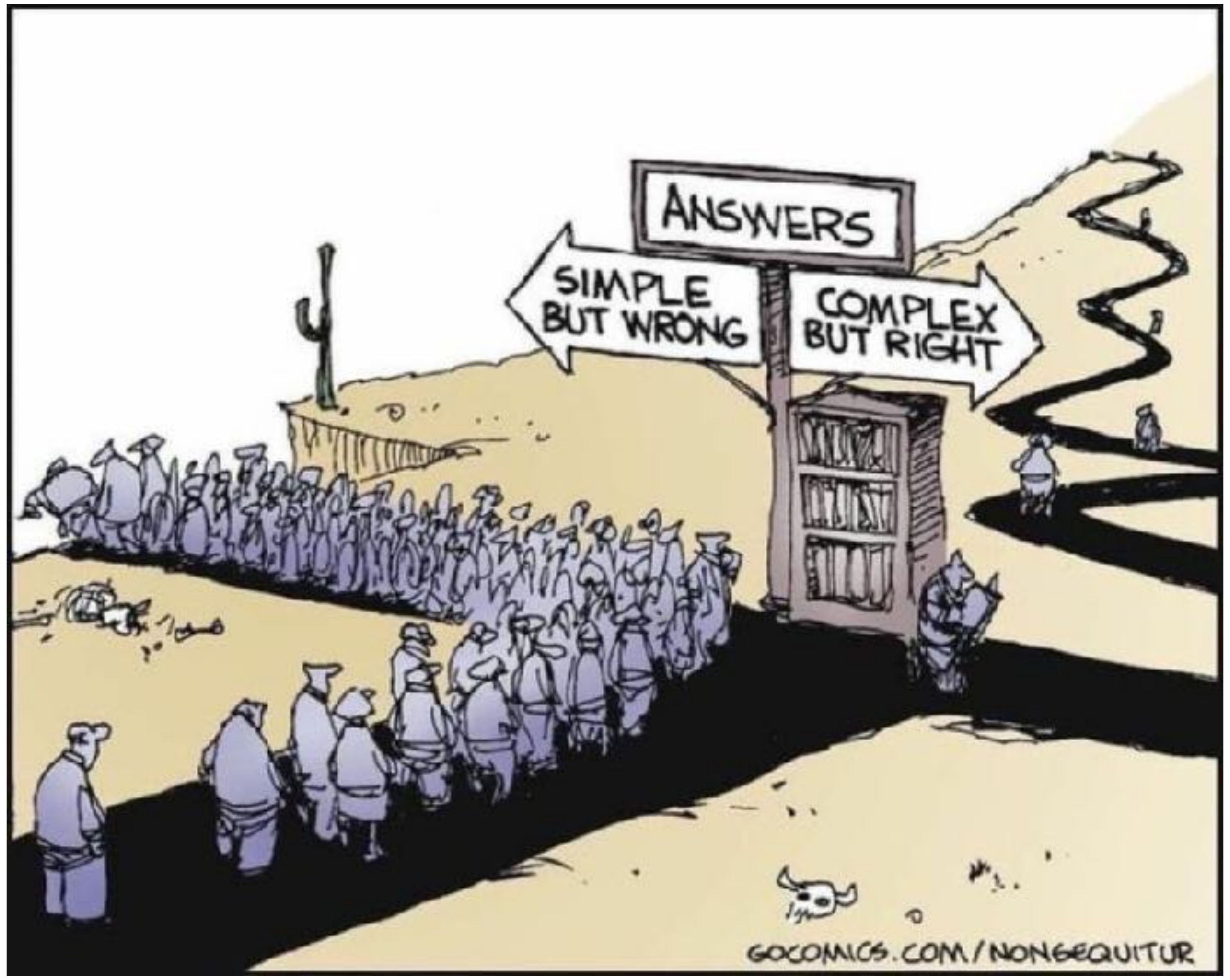
## Management

- Planting date
  - **Early planting**
- Irrigation
- Fertilization rate

CGM: Cloud processing



# Perspective III: AI enabled breeding that harness ensembles will have impact across the complexity continuum




***Dynamical Bayesian framework (Crop Model + Genomic selection — or variations)***

- Manage complexity
- Enable systems level thinking
- Crop design (and breeding for cropping systems)
- Breed crops at the right pace and the right place

# Thank you for having me!

U.S. National Science Foundation

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