Research at the interface of environmental protection and mathematics

Presented to the University of Minnesota – Duluth
Department of Mathematics and Statistics

April 29th, 2022

By Nate Pollesch, PhD

United States Environmental Protection Agency
Office of Research and Development, Duluth, MN USA

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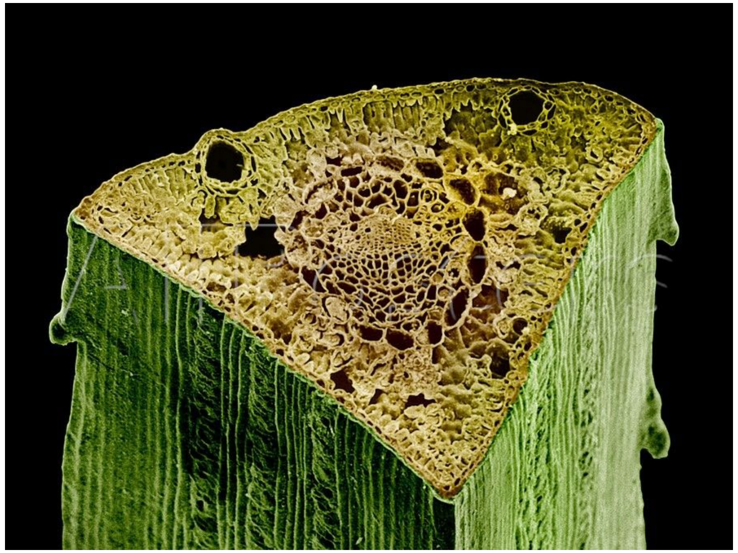
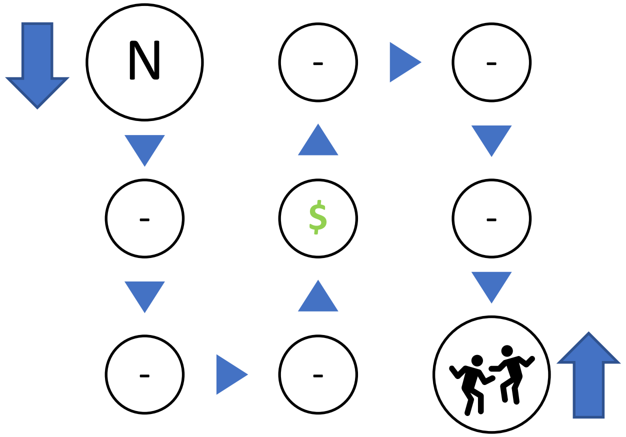


A little personal background:

Motivation:



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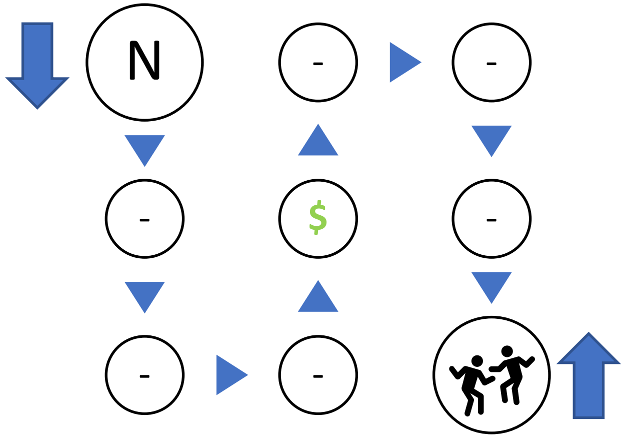
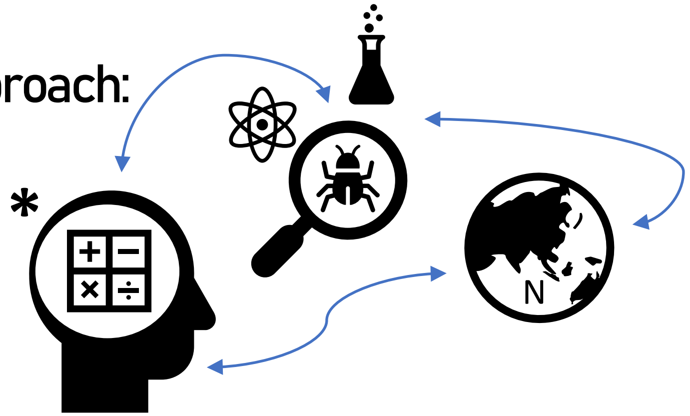


My Approach:



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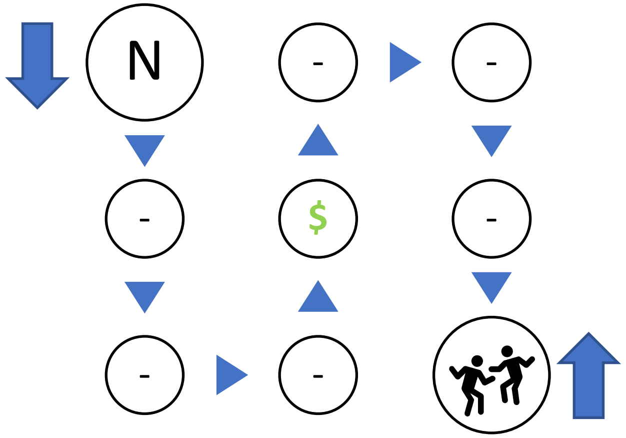

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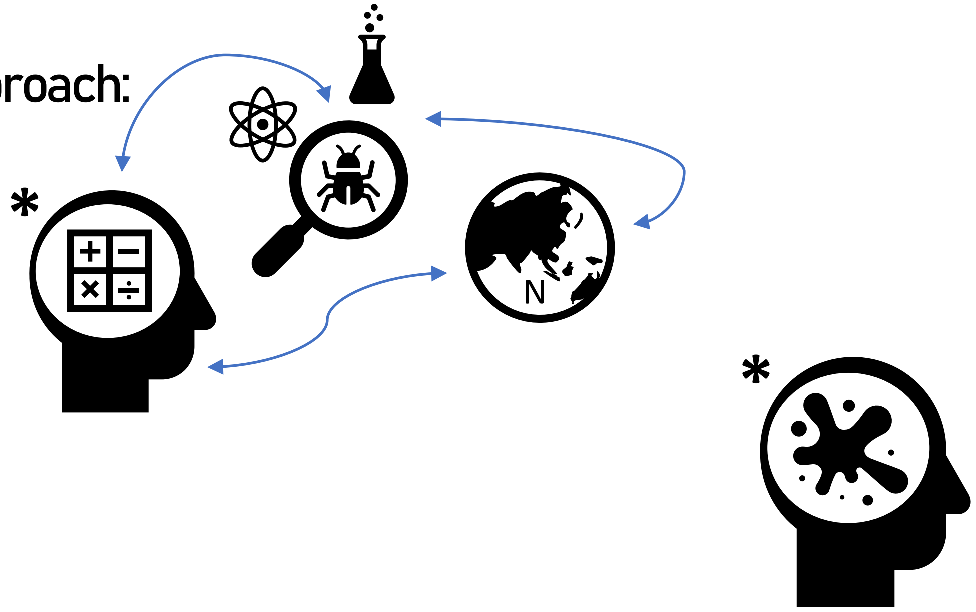
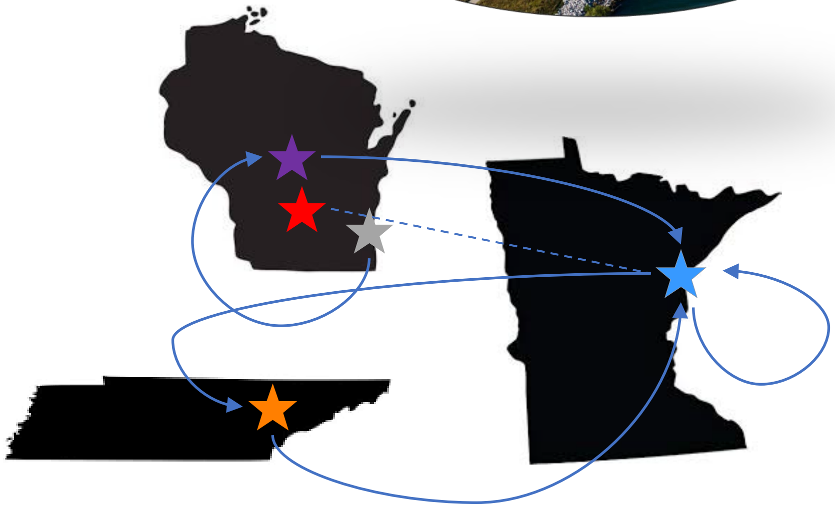


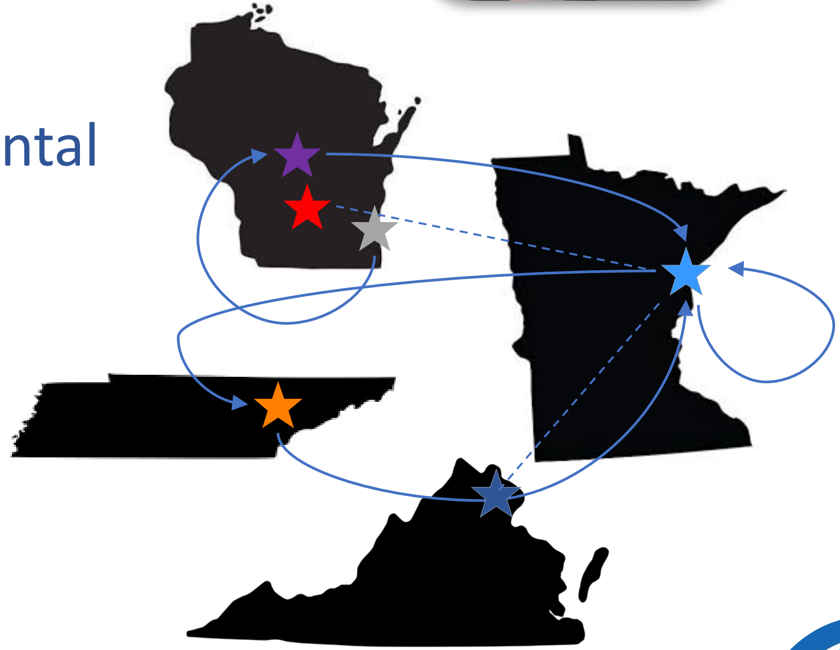
Academic Background

- Milwaukee, WI
- BS Mathematics (Stevens Point, WI)
  - Minor in Chemistry
- MS Applied and Comp. Math (Duluth, MN)
  - Mathematical Ecology
  - Stoichiometric Modeling
- PHD Mathematics (Knoxville, TN)
  - Concurrent MS in Statistics, Markov chain modeling
  - Mathematical Ecology
  - Aggregation theory



Professional Background

- Postdoctoral Research US EPA (Duluth, MN)
  - Ecotoxicological modeling
  - Effects of pesticides on wildlife populations
- Postdoctoral Research UW-Madison/US EPA Cooperative (Madison, WI + Duluth, MN)
  - Ecological Risk Assessment Tool/GUI development
- Senior Ecological Modeler, Waterborne Environmental
  - Ecological modeling focused on endangered species
  - Indirect effects of pesticides
- Mathematician US EPA (Duluth, MN)
  - Ecological Modeling
  - Adverse outcome pathways
  - *Text mining & Natural Language Processing*



I have been fortunate to be able to work on a wide variety of research projects, with collaborators from around the world

MATH has been a cool passport for me

UMD

OAK RIDGE National Laboratory

Center for Bioenergy Sustainability

MPE Mathematics of Planet Earth

NIMBioS National Institute for Mathematical and Biological Synthesis

SETAC Society of Environmental Toxicology and Chemistry

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WATERBORNE ENVIRONMENTAL

Aquatic Sciences Center UNIVERSITY OF WISCONSIN–MADISON

CENTER FOR COMPUTATIONAL TOXICOLOGY AND EXPOSURE

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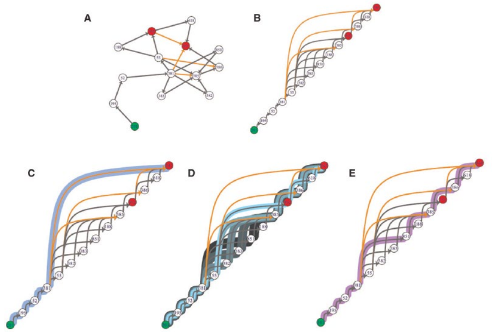
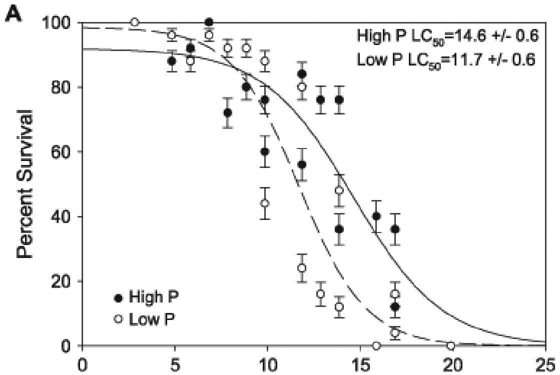
Some research examples



Extracting and benchmarking emerging adverse outcome pathway knowledge
Toxsci Pollesch et al., 2019



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Applications of aggregation theory to sustainability assessment
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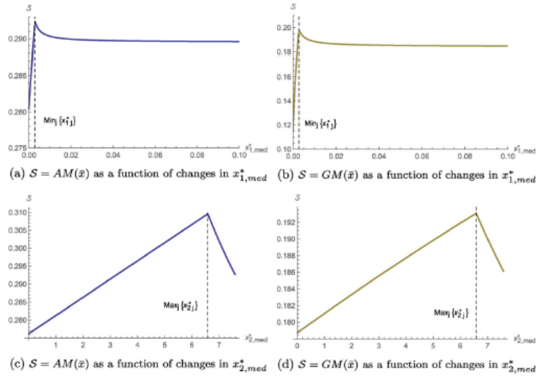

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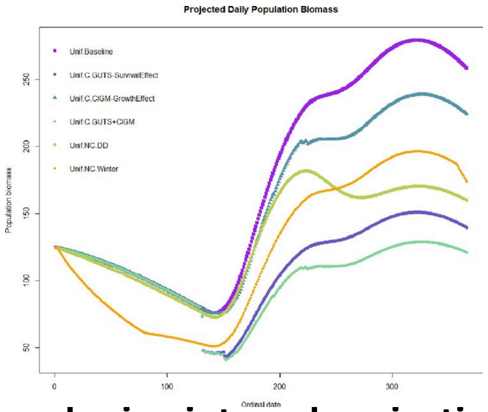
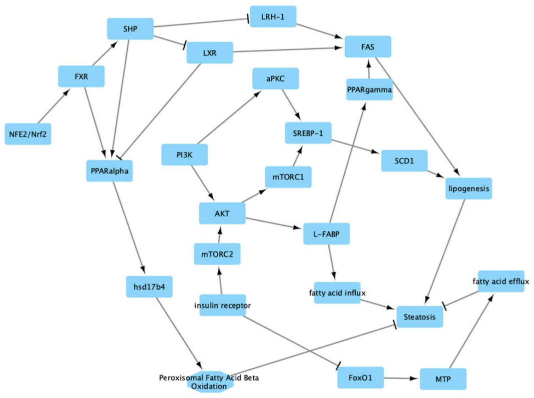


Developing integral projection models for ecotoxicology
Eco Mod Pollesch et al., 2022



Predicting the Probability that a Chemical Causes Steatosis using adverse outcome pathway Bayesian Networks
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$$IS_i = (1-\lambda)\left[\min_j\left(W_j\overline{R}_{ij}\right)\right] + \lambda\sum_{j=1}^{m} W_j\overline{R}_{ij}$$

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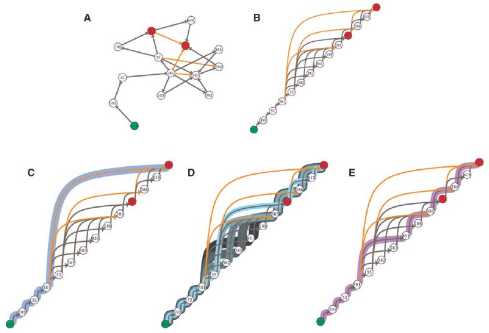

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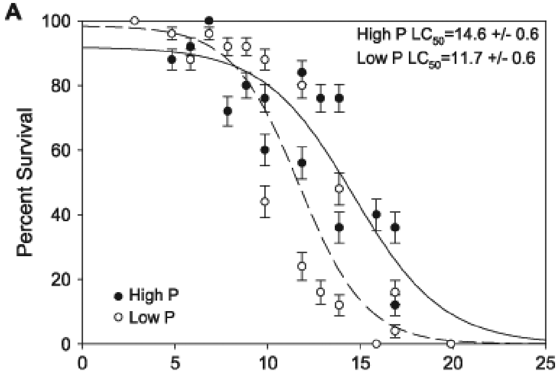

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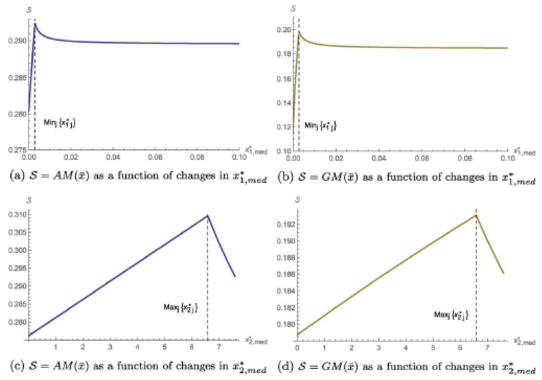

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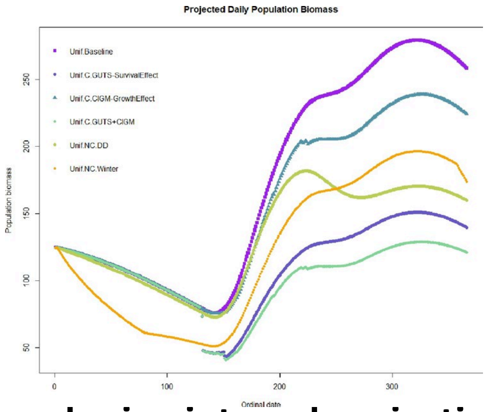

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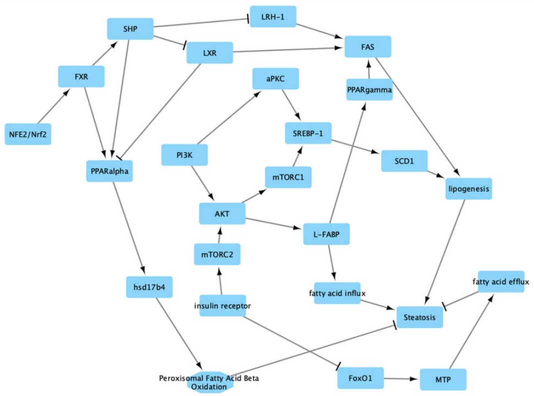

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Oak Ridge National Laboratory

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Applications of aggregation theory to sustainability assessment
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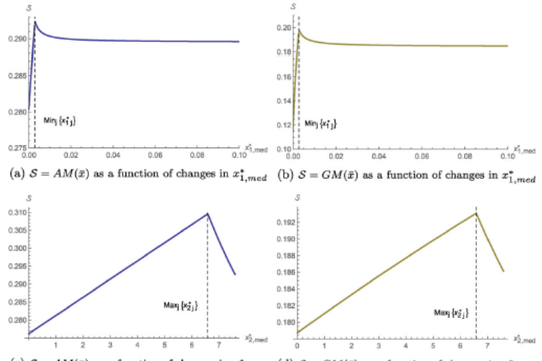
(a) $S = AM(\bar{x})$ as a function of changes in $x^*_{1,med}$ (b) $S = GM(\bar{x})$ as a function of changes in $x^*_{1,med}$
(c) $S = AM(\bar{x})$ as a function of changes in $x^*_{2,med}$ (d) $S = GM(\bar{x})$ as a function of changes in $x^*_{2,med}$

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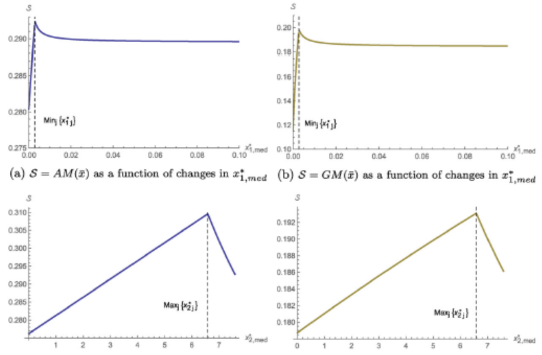

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https://bioenergykdf.net/indicator-checklist

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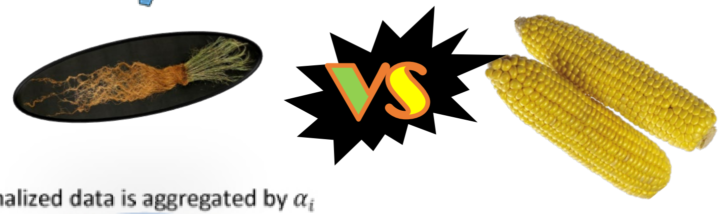

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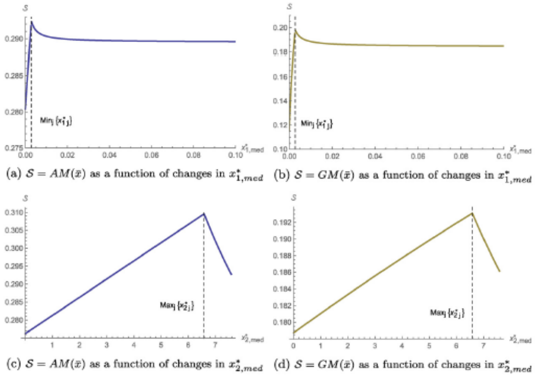

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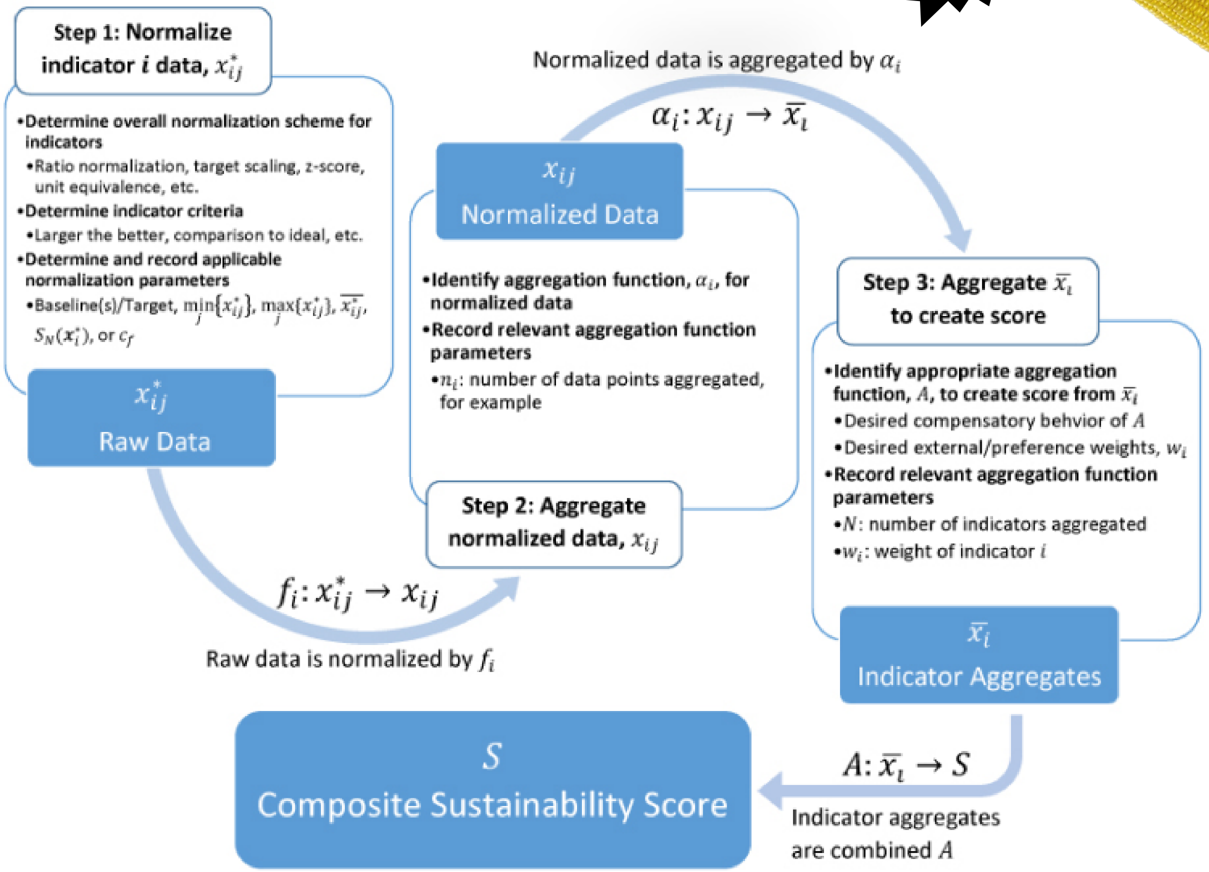

Notation: x^*_{ij} non-normalized measurement j of indicator i, f_i normalization function for indicator i, x_{ij} normalized measurement j for indicator i, α_i aggregation function for normalized measures of i, $\bar{x}_i$ aggregate of normalized measures of indicator i, and A is the aggregation function for indicator aggregates $\bar{x}_1, \bar{x}_2, \ldots$

$$IS_i = (1-\lambda)\left[\min_j\left(W_j\overline{R}_{ij}\right)\right] + \lambda\sum_{j=1}^{m} W_j\overline{R}_{ij}$$

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Table 1
Example aggregation functions.

Function name	Formula	Assumptions/notes
Arithmetic mean	$A(x) := \frac{1}{n}\sum_{i=1}^{n} x_i$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$
Weighted arithmetic mean	$A(x) := \sum_{i=1}^{n} w_i x_i$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I} (w_1, \ldots, w_n) \in [0,1]^n \sum_{i=1}^{n} w_i = 1$
Ordered weighted average	[a]$A(x) := \sum_{i=1}^{n} w_i x_{(i)}$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$ $(w_1, \ldots, w_n) \in [0,1]^n \sum_{i=1}^{n} w_i = 1$
Geometric mean	$A(x) := (\prod_{i=1}^{n} x_i)^{1/n}$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$ [b]If $n > 1$ then $\mathbb{I} \subseteq (0, \infty)$
Weighted geometric mean	$A(x) := \prod_{i=1}^{n} x_i^{w_i}$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$ $(w_1, \ldots, w_n) \in [0,1]^n \sum_{i=1}^{n} w_i = 1$ If $n > 1$ then $\mathbb{I} \subseteq (0, \infty)$
Minimum	$A(x) := min\{x_1, \ldots, x_n\}$ (or $OS_1(x) := x_{(1)}$)	Also written $\min(x) = \bigwedge_{i=1}^{n} x_i$ and OS_1 is the 1st order statistic
Maximum	$A(x) := max\{x_1, \ldots, x_n\}$ (or $OS_n(x) := x_{(n)}$)	Also written $\max(x) = \bigvee_{i=1}^{n} x_i$ and OS_n is the nth order statistic

[a] $x_{(i)}$ represents the *i*th lowest coordinate of *x*, s.t. $x_{(1)} \le \cdots \le x_{(k)} \le \cdots \le x_{(n)}$.
[b] The geometric means are not aggregation functions on every domain, specifically, for $n > 1$ then $\mathbb{I}$ must satisfy $\mathbb{I} \subseteq (0, \infty)$.

Table 3
Internality, conjunctivity, and disjunctivity properties.

Property	Definition	Interpretation/notes
Conjunctive	[a]$F : \mathbb{I}^n \to \overline{\mathbb{R}}, x \in \mathbb{I}^n$ F is *conjunctive* if $\inf \mathbb{I} \le F(x) \le \mathrm{Min}(x)$	The output of the function F must be bounded (above) by the min(x) function. This condition means that, in a conjunctive function, no low input component can be compensated for by a high input component.
Disjunctive	$F : \mathbb{I}^n \to \overline{\mathbb{R}}, x \in \mathbb{I}^n$ F is *disjunctive* if $\max(x) \le F(x) \le \sup \mathbb{I}$	Similar to conjunctivity, but the output of the function F must be bounded (below) by the max(x) function. Meaning that no low input component values may compensate for a high input component value.
Internal	$F : \mathbb{I}^n \to \overline{\mathbb{R}}, x \in \mathbb{I}^n$ F is *internal* if $\min(x) \le F(x) \le \max(x)$	Internal aggregation functions allow for *compensatory effects* between input component values. Here compensatory effects are taken to mean those that allow, for example, high input components to offset low input components in the aggregate output. Averages or mean aggregation functions are internal functions.

[a] $\overline{\mathbb{R}} = [-\infty, \infty]$ represents the *extended real line* and $\mathbb{I} \subseteq \overline{\mathbb{R}}$.

$$IS_i = (1-\lambda)\left[\min_j\left(W_j\bar{R}_{ij}\right)\right] + \lambda\sum_{j=1}^{m} W_j\bar{R}_{ij}$$

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Weighted arithmetic mean	$A(x) := \sum_{i=1}^{n} w_i x_i$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I} (w_1, ,.., .,w_n) \in [0,1]^n \sum_{i=1}^{n} w_i = 1$
Ordered weighted average	[a] $A(x) := \sum_{i=1}^{n} w_i x_{(i)}$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$ $(w_1,..., w_n) \in [0,1]^n \sum_{i=1}^{n} w_i = 1$
Geometric mean	$A(x) := (\prod_{i=1}^{n} x_i)^{1/n}$	$A : \mathbb{I}^n \to \mathbb{I}, x : \in \mathbb{I}$ [b] If $n > 1$ then $\mathbb{I} \subseteq (0, \infty)$
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Minimum	$A(x) := min\{x_1,..., x_n\}$ (or $OS_1(x) := x_{(1)}$)	Also written $\min(x) = \bigwedge_{i=1}^{n} x_i$ and OS_1 is the 1st order statistic
Maximum	$A(x) := max\{x_1,..., x_n\}$ (or $OS_n(x) := x_{(n)}$)	Also written $\max(x) = \bigvee_{i=1}^{n} x_i$ and OS_n is the nth order statistic

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Internality, conjunctivity, and disjunctivity properties.

Property	Definition	Interpretation/notes
Conjunctive	[a] $F : \mathbb{I}^n \to \bar{\mathbb{R}}, x \in \mathbb{I}^n$ F is *conjunctive* if $inf\ \mathbb{I} \le F(x) \le \mathrm{Min}(x)$	The output of the function F must be bounded (above) by the min(x) function. This condition means that, in a conjunctive function, no low input component can be compensated for by a high input component.
Disjunctive	$F : \mathbb{I}^n \to \bar{\mathbb{R}}, x \in \mathbb{I}^n$ F is *disjunctive* if $\max(x) \le F(x) \le sup\ \mathbb{I}$	Similar to conjunctivity, but the output of the function F must be bounded (below) by the max(x) function. Meaning that no low input component values may compensate for a high input component value.
Internal	$F : \mathbb{I}^n \to \bar{\mathbb{R}}, x \in \mathbb{I}^n$ F is *internal* if $\min(x) \le F(x) \le \max(x)$	Internal aggregation functions allow for *compensatory effects* between input component values. Here compensatory effects are taken to mean those that allow, for example, high input components to offset low input components in the aggregate output. Averages or mean aggregation functions are internal functions.

[a] $\bar{\mathbb{R}} = [-\infty, \infty]$ represents the *extended real line* and $\mathbb{I} \subseteq \bar{\mathbb{R}}$.

"Weak vs Strong" Sustainability Assessment

Category	Indicator	Units	Measurability Scale
Soil quality	1. Total organic carbon (TOC)	Mg/ha	Ratio scale
	2. Total nitrogen (N)	Mg/ha	Ratio scale
	3. Extractable phosphorus (P)	Mg/ha	Ratio scale
	4. Bulk Density	g/cm^3	Ratio scale
Water quality and quantity	5. Nitrate concentration in streams (and export)	Concentration: mg/L; export: kg/ha/year	Ratio scale; ratio scale
	6. Total phosphorus (P) concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	7. Suspended sediment concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	8. Herbicide concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	9. Peak storm flow	L/s	Ratio scale
	10. Minimum base flow	L/s	Ratio scale
	11. Consumptive water use (incorporates base flow)	Feedstock production: m^3/ha/day; biorenery: m^3/day	Ratio scale; ratio scale
Greenhouse gases	12. CO_2 equivalent emissions (CO_2 and N_2O)	kg C_{eq}/GJ	Ratio scale
Biodiversity	12. Presence of taxa of special concern	Presence	**
	14. Habitat area of taxa of special concern	ha	Ratio scale
Air Quality	15. Tropospheric ozone	ppb	Ratio scale
	16. Carbon monoxide	ppm	Ratio scale
	17. Total particulate matter less than 2.5μm diameter ($PM_{2.5}$)	$\mu g/m^3$	Ratio scale
	18. Total particulate matter less than 10μm diameter (PM_{10})	$\mu g/m^3$	Ratio scale
Productivity	19. Aboveground net primary productivity (ANPP)/yield	g C/m^2/year	Ratio scale

Table 7
Meaningfulness of common aggregation functions *adapted from* Grabisch et al. (2009).

Aggregation function	R.S.I.	S.R.S.	I.R.S.	I.S.I.	S.I.S.	I.I.S.
Arithmetic mean	✓	✓		✓	✓	
Geometric mean	✓	✓	✓			
[a]$P_k(x) := x_k$	✓	✓	✓	✓	✓	✓
[b]$OS_k(x) := x_{(k)}$	✓	✓		✓	✓	
Weighted arithmetic mean	✓	✓		✓	✓	
Weighted geometric mean	✓	✓	✓			
Ordered weighted average	✓	✓		✓	✓	
$\sum_{i=1}^{n} x_i$	✓	✓			✓	
$\prod_{i=1}^{n} x_i$	✓	✓				

Ratio scale invariant (R.S.I.), meaningful on a single ratio scale (S.R.S.) meaningful on independent ratio scales (I.R.S.), interval scale invariant (I.S.I), meaningful on a single interval scale (S.I.S.), and meaningful on an independent interval scales (I.I.S).
[a] $P_k(x)$ is the projection onto the *kth* element, x_k of the input vector x.
[b] $OS_k(x)$ is the projection on the *kth* ordered element, $x_{(k)}$ of the input vector x (All other function definitions may be found in Table 1).

Category	Indicator	Units	Measurability Scale
Soil quality	1. Total organic carbon (TOC)	Mg/ha	Ratio scale
	2. Total nitrogen (N)	Mg/ha	Ratio scale
	3. Extractable phosphorus (P)	Mg/ha	Ratio scale
	4. Bulk Density	g/cm^3	Ratio scale
Water quality and quantity	5. Nitrate concentration in streams (and export)	Concentration: mg/L; export: kg/ha/year	Ratio scale; ratio scale
	6. Total phosphorus (P) concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	7. Suspended sediment concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	8. Herbicide concentration in streams (and export)	Concentration: mg/L; export kg/ha/year	Ratio scale; ratio scale
	9. Peak storm flow	L/s	Ratio scale
	10. Minimum base flow	L/s	Ratio scale
	11. Consumptive water use (incorporates base flow)	Feedstock production: m^3/ha/day; biorenery: m^3/day	Ratio scale; ratio scale
Greenhouse gases	12. CO_2 equivalent emissions (CO_2 and N_2O)	kg C_{eq}/GJ	Ratio scale
Biodiversity	12. Presence of taxa of special concern	Presence	**
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Air Quality	15. Tropospheric ozone	ppb	Ratio scale
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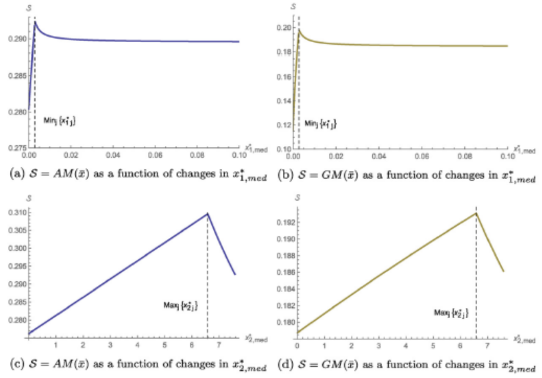
Table 7
Meaningfulness of common aggregation functions *adapted from* Grabisch et al. (2009).

Aggregation function	R.S.I.	S.R.S.	I.R.S.	I.S.I.	S.I.S.	I.I.S.
Arithmetic mean	✓	✓		✓	✓	
Geometric mean	✓	✓	✓			
[a] $P_k(x) := x_k$	✓	✓	✓	✓	✓	✓
[b] $OS_k(x) := x_{(k)}$	✓	✓		✓	✓	
Weighted arithmetic mean	✓	✓		✓	✓	
Weighted geometric mean	✓	✓	✓			
Ordered weighted average	✓	✓		✓	✓	
$\sum_{i=1}^{n} x_i$	✓	✓			✓	
$\prod_{i=1}^{n} x_i$	✓	✓				

Ratio scale invariant (R.S.I.), meaningful on a single ratio scale (S.R.S.) meaningful on independent ratio scales (I.R.S.), interval scale invariant (I.S.I), meaningful on a single interval scale (S.I.S.), and meaningful on an independent interval scales (I.I.S).

[a] $P_k(x)$ is the projection onto the *kth* element, x_k of the input vector x.

[b] $OS_k(x)$ is the projection on the *kth* ordered element, $x_{(k)}$ of the input vector x (All other function definitions may be found in Table 1).



(a) $S = AM(\bar{x})$ as a function of changes in $x^*_{1,med}$ (b) $S = GM(\bar{x})$ as a function of changes in $x^*_{1,med}$

(c) $S = AM(\bar{x})$ as a function of changes in $x^*_{2,med}$ (d) $S = GM(\bar{x})$ as a function of changes in $x^*_{2,med}$

Normalization in sustainability assessment: Methods and implications
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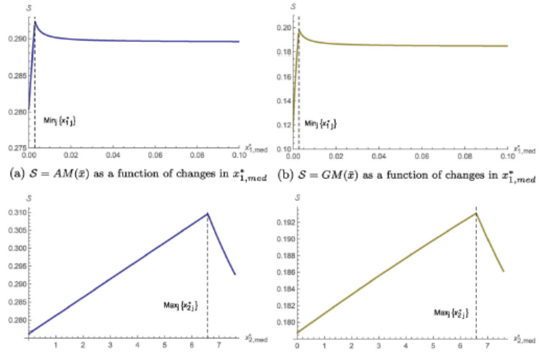
Table 2.1: Common normalization function definitions and notations: Internal normalization functions, those for which the normalized value of x_j depends on the entire data set $\boldsymbol{x}^*$, and the normalization functions that create dimensionless quantities are identified

Scheme, notation, and definition	Indicator Bearing	Internal	Dimensionless
Ratio Normalization			
$R_{L,j}(\boldsymbol{x}^*) = \frac{x_j^*}{\max\{\boldsymbol{x}^*\}}$	LTB	✓	✓
$R_{S,j}(\boldsymbol{x}^*) = \frac{\min\{\boldsymbol{x}^*\}}{x_j^*}$	STB	✓	✓
$R_{D,j}(x_j^*, T) = \frac{\min\{x_j^*, T\}}{\max\{x_j^*, T\}}$	DTI		✓
Z-Score Normalization			
$Z_j(\boldsymbol{x}^*) = \frac{x_j^* - \bar{x}^*}{S_N(\boldsymbol{x}^*)}$	n/a	✓	✓
where $\bar{x}^* = \frac{1}{n}\sum_{j=1}^n x_j^*$, $S_N = \left(\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2\right)^{1/2}$			
Unit Equivalence			
$C_j(x_j^*, c_f) = x_j^* c_f$	n/a		
where c_f is a *conversion factor* from x_j^*'s to desired units			
Target Normalization to Interval [0, 1]			
$T_{L,j}(x_j^*, T, B) = \begin{cases} 0, & x_j^* \le B \\ 1 - \frac{T - x_j^*}{T - B}, & B < x_j^* < T \\ 1, & x_j^* \ge T \end{cases}$	LTB		✓
$T_{S,j}(x_j^*, T, B) = \begin{cases} 1, & x_j^* \le T \\ 1 - \frac{x_j^* - T}{B - T}, & T < x_j^* < B \\ 0, & x_j^* \ge B \end{cases}$	STB		✓
$T_{D,j}(x_j^*, T, B_l, B_u) = \begin{cases} 1 - \frac{T - x_j^*}{T - B_l}, & B_l < x_j^* < T \\ 1, & x_j^* = T \\ 1 - \frac{x_j^* - T}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$	DTI		✓

Note: LTB: Larger-the-better, STB: Smaller-the-better, DTI: Distance-to-ideal, $\boldsymbol{x}^* = \{x_1^*, x_2^*, ..., x_n^*\}$, T is a target or ideal value for a given indicator, B is a baseline or non-ideal value for a given indicator (B_l and B_u used when an upper and lower baseline are required), $\bar{x}^*$ is the sample mean, S_N is the sample standard deviation, and c_f is a conversion factor to change units of $\boldsymbol{x}^*$ to alternate units (ex. dollars or greenhouse gas equivalents).



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Normalization in sustainability assessment: Methods and implications

Ecol Econ Pollesch and Dale, 2016

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$R_{S,j}(\boldsymbol{x}^*) = \frac{\min\{\boldsymbol{x}^*\}}{x_j^*}$	STB	✓	✓
$R_{D,j}(x_j^*, T) = \frac{\min\{x_j^*, T\}}{\max\{x_j^*, T\}}$	DTI		✓
Z-Score Normalization			
$Z_j(\boldsymbol{x}^*) = \frac{x_j^* - \bar{x}^*}{S_N(\boldsymbol{x}^*)}$	n/a	✓	✓
where $\bar{x}^* = \frac{1}{n}\sum_{j=1}^n x_j^*$, $S_N = \left(\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2\right)^{1/2}$			
Unit Equivalence			
$C_j(x_j^*, c_f) = x_j^* c_f$	n/a		
where c_f is a *conversion factor* from x_j^*'s to desired units			
Target Normalization to Interval $[0,1]$			
$T_{L,j}(x_j^*, T, B) = \begin{cases} 0, & x_j^* \le B \\ 1 - \frac{T - x_j^*}{T - B}, & B < x_j^* < T \\ 1, & x_j^* \ge T \end{cases}$	LTB		✓
$T_{S,j}(x_j^*, T, B) = \begin{cases} 1, & x_j^* \le T \\ 1 - \frac{x_j^* - T}{B - T}, & T < x_j^* < B \\ 0, & x_j^* \ge B \end{cases}$	STB		✓
$T_{D,j}(x_j^*, T, B_l, B_u) = \begin{cases} 1 - \frac{T - x_j^*}{T - B_l}, & B_l < x_j^* < T \\ 1, & x_j^* = T \\ 1 - \frac{x_j^* - T}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$	DTI		✓

Note: LTB: Larger-the-better, STB: Smaller-the-better, DTI: Distance-to-ideal, $\boldsymbol{x}^* = \{x_1^*, x_2^*, ..., x_n^*\}$, T is a target or ideal value for a given indicator, B is a baseline or non-ideal value for a given indicator (B_l and B_u used when an upper and lower baseline are required), $\bar{x}^*$ is the sample mean, S_N is the sample standard deviation, and c_f is a conversion factor to change units of $\boldsymbol{x}^*$ to alternate units (ex. dollars or greenhouse gas equivalents).

Table 2.3: Normalization function derivatives: Using functions defined in Table 2.1, change in normalized value with respect to a change in the data point, x_j^*, is presented

Change in normalized value with respect to change in x_j^*

Ratio Normalization

$$\frac{\partial}{\partial x_j^*}(R_{L,j}(\boldsymbol{x}^*)) = \begin{cases} \frac{1}{\max\{\boldsymbol{x}^*\}}, & x_j^* < x_k^* \forall k \neq j \\ 0, & \text{else} \end{cases}$$

$$\frac{\partial}{\partial x_j^*}(R_{S,j}(\boldsymbol{x}^*)) = \begin{cases} \frac{-\min\{\boldsymbol{x}^*\}}{(x_j^*)^2}, & x_j^* < x_k^* \forall k \neq j \\ 0, & \text{else} \end{cases}$$

$$\frac{\partial}{\partial x_j^*}(R_{D,j}(x_j^*, T)) = \begin{cases} \frac{1}{T}, & x_j^* < T \\ 0, & x_j^* = T \\ \frac{-T}{(x_j^*)^2}, & x_j^* > T \end{cases}$$

Z-Score Normalization

$$\frac{\partial}{\partial x_j^*}(Z_j(\boldsymbol{x}^*)) = \frac{\left(\left(\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2\right)^{\frac{1}{2}}\left(1 - \frac{1}{n}\right)\right) - \left(\frac{n^{-1/2}(x_j^* - \bar{x}^*)^2}{\left(\sum_{j=1}^n (x_j^* - \bar{x}^*)^2\right)^{1/2}}\right)\left(\frac{\sum_{k \neq j}(x_k^* - \bar{x}^*)}{-n(x_j^* - \bar{x}^*)} + \left(1 - \frac{1}{n}\right)\right)}{\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2}$$

Unit Equivalence Normalization

$$\frac{\partial}{\partial x_j^*}(C(x_j^*, c_f)) = c_f$$

Target Normalization to Interval [0,1]

$$\frac{\partial}{\partial x_j^*}(T_{L,j}(x_j^*, T, B)) = \begin{cases} \frac{1}{T - B}, & B < x_j^* < T \\ 0, & \text{else} \end{cases}$$

$$\frac{\partial}{\partial x_j^*}(T_{S,j}(x_j^*, T, B)) = \begin{cases} \frac{-1}{B - T}, & T < x_j^* < B \\ 0, & \text{else} \end{cases}$$

$$\frac{\partial}{\partial x_j^*}(T_{D,j}(x_j^*, T, B_l, B_u)) = \begin{cases} \frac{1}{T - B_l}, & B_l < x_j^* < T \\ \frac{-1}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$$

Note: $\boldsymbol{x}^* = \{x_1^*, x_2^*, ..., x_n^*\}$, T is a target or ideal value for a given indicator, B is a baseline or non-ideal value for a given indicator (B_l and B_u used when an upper and lower baseline are required), $S_N = [\frac{1}{n}\sum_{j=1}^n (x_j - \bar{x})^2]^{1/2}$ is the sample standard deviation, $\bar{x}^* = \frac{1}{n}\sum_{j=1}^n x_j^*$ is the sample mean, and c_f is a conversion factor to change units of $\boldsymbol{x}^*$ to alternate units, such as dollars or greenhouse gas equivalents.

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$R_{L,j}(\boldsymbol{x}^*) = \frac{x_j^*}{\max\{\boldsymbol{x}^*\}}$	LTB	✓	✓
$R_{S,j}(\boldsymbol{x}^*) = \frac{\min\{\boldsymbol{x}^*\}}{x_j^*}$	STB	✓	✓
$R_{D,j}(x_j^*, T) = \frac{\min\{x_j^*, T\}}{\max\{x_j^*, T\}}$	DTI		✓
Z-Score Normalization			
$Z_j(\boldsymbol{x}^*) = \frac{x_j^* - \bar{x}^*}{S_N(\boldsymbol{x}^*)}$ where $\bar{x}^* = \frac{1}{n}\sum_{j=1}^{n} x_j^*$, $S_N = \left(\frac{1}{n}\sum_{j=1}^{n}(x_j^* - \bar{x}^*)^2\right)^{1/2}$	n/a	✓	✓
Unit Equivalence			
$C_j(x_j^*, c_f) = x_j^* c_f$ where c_f is a *conversion factor* from x_j^*'s to desired units	n/a		
Target Normalization to Interval [0, 1]			
$T_{L,j}(x_j^*, T, B) = \begin{cases} 0, & x_j^* \leq B \\ 1 - \frac{T - x_j^*}{T - B}, & B < x_j^* < T \\ 1, & x_j^* \geq T \end{cases}$	LTB		✓
$T_{S,j}(x_j^*, T, B) = \begin{cases} 1, & x_j^* \leq T \\ 1 - \frac{x_j^* - T}{B - T}, & T < x_j^* < B \\ 0, & x_j^* \geq B \end{cases}$	STB		✓
$T_{D,j}(x_j^*, T, B_l, B_u) = \begin{cases} 1 - \frac{T - x_j^*}{T - B_l}, & B_l < x_j^* < T \\ 1, & x_j^* = T \\ 1 - \frac{x_j^* - T}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$	DTI		✓

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Change in normalized value with respect to change in x_j^*
Ratio Normalization
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Z-Score Normalization
$\frac{\partial}{\partial x_j^*}(Z_j(\boldsymbol{x}^*)) = \frac{\left((\frac{1}{n}\sum_{j=1}^{n}(x_j^* - \bar{x}^*)^2)^{\frac{1}{2}}(1 - \frac{1}{n})\right) - \left(\frac{n^{-1/2}(x_j^* - \bar{x}^*)^2}{(\sum_{j=1}^{n}(x_j^* - \bar{x}^*)^2)^{1/2}}\right)\left(\frac{\sum_{k \neq j}(x_k^* - \bar{x}^*)}{-n(x_j^* - \bar{x}^*)} + (1 - \frac{1}{n})\right)}{\frac{1}{n}\sum_{j=1}^{n}(x_j^* - \bar{x}^*)^2}$
Unit Equivalence Normalization
$\frac{\partial}{\partial x_j^*}(C(x_j^*, c_f)) = c_f$
Target Normalization to Interval [0,1]
$\frac{\partial}{\partial x_j^*}(T_{L,j}(x_j^*, T, B)) = \begin{cases} \frac{1}{T - B}, & B < x_j^* < T \\ 0, & \text{else} \end{cases}$
$\frac{\partial}{\partial x_j^*}(T_{S,j}(x_j^*, T, B)) = \begin{cases} \frac{-1}{B - T}, & T < x_j^* < B \\ 0, & \text{else} \end{cases}$
$\frac{\partial}{\partial x_j^*}(T_{D,j}(x_j^*, T, B_l, B_u)) = \begin{cases} \frac{1}{T - B_l}, & B_l < x_j^* < T \\ \frac{-1}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$

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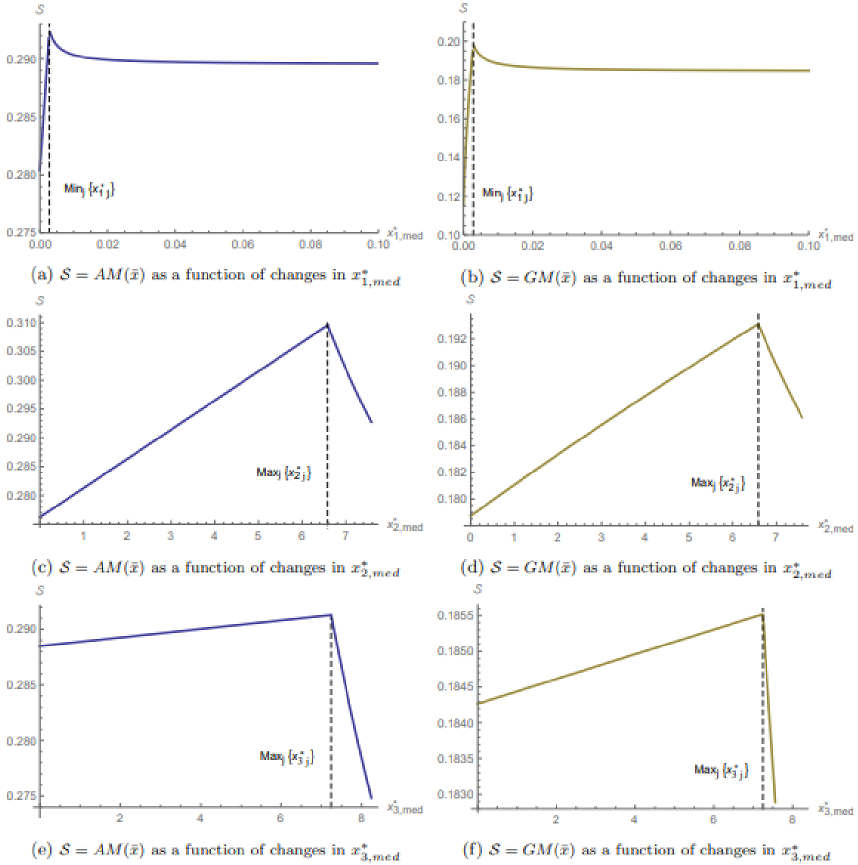

Figure 2.2: Changes in S in response to changes in median values of from the data sets for phosphorus ($x^*_{1,med}$), yield ($x^*_{2,med}$), and %OM ($x^*_{3,med}$) under ratio normalization scheme. Dashed lines show $\min_j x^*_{ij}$ and $\max_j x^*_{ij}$ values from Table 2.5. In all cases, the median value from each data set was varied in order to show the effect that changing non-normalized indicator measures has on S. Notice the behavior of S when the median value becomes the $\min_j x^*_{ij}$ in (a,b) and the $\max_j x^*_{ij}$ in (c,d,e,f). This dramatic change is due to the fact that ratio normalization is an internal normalization process, and the dependence of all normalized values in the data set on the minimum or maximum value of that data set. All functions depicted correspond to functions presented in Table 2.7

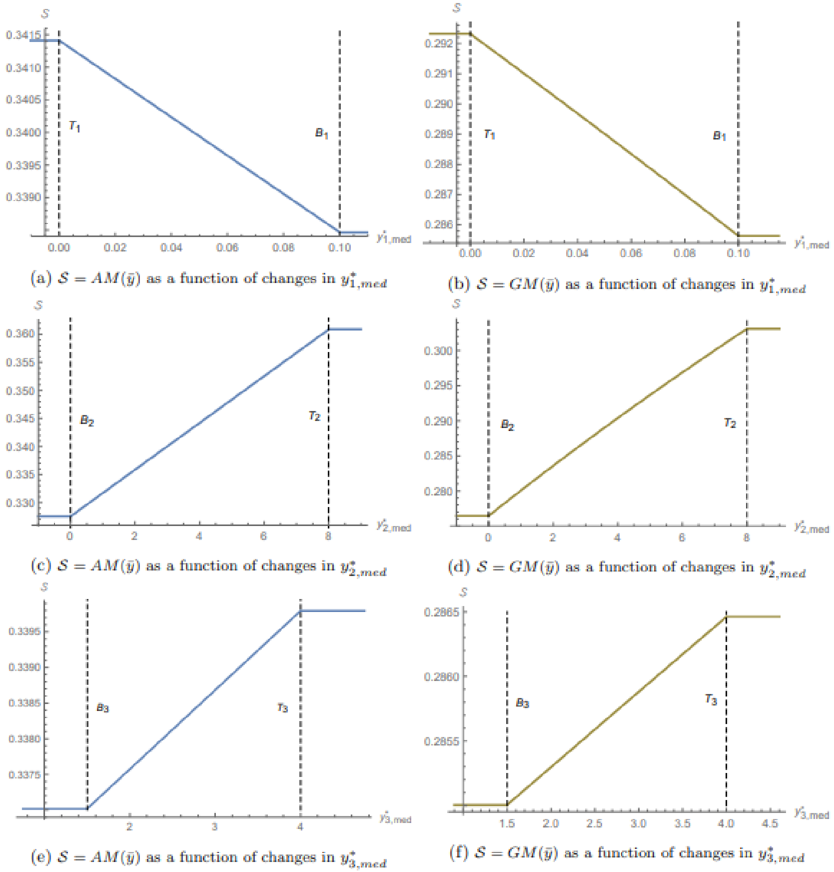

Figure 2.3: Changes in S in response to changes in median values of from the data sets for Phosphorus ($y^*_{1,med}$), Yield ($y^*_{2,med}$), and %OM ($y^*_{3,med}$) under target normalization scheme. In all cases, the median value from each data set was varied in order to show the effect that changing non-normalized indicator measures has on S. Dashed lines show normalization parameters from Table 2.6. When the median value is changed to values outside the baseline and target intervals, there is no response in S to further changes due to the normalized value becoming a constant 0 or 1. All functions depicted correspond to functions presented in Table 2.8

Normalization in sustainability assessment: Methods and implicatio

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Z-Score Normalization			
$Z_j(\boldsymbol{x}^*) = \frac{x_j^* - \bar{x}^*}{S_N(\boldsymbol{x}^*)}$ where $\bar{x}^* = \frac{1}{n}\sum_{j=1}^n x_j^*$, $S_N = \left(\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2\right)^{1/2}$	n/a	✓	✓
Unit Equivalence			
$C_j(x_j^*, c_f) = x_j^* c_f$ where c_f is a *conversion factor* from x_j^*'s to desired units	n/a		
Target Normalization to Interval [0, 1]			
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$T_{S,j}(x_j^*, T, B) = \begin{cases} 1, & x_j^* \leq T \\ 1 - \frac{x_j^* - T}{B - T}, & T < x_j^* < B \\ 0, & x_j^* \geq B \end{cases}$	STB		✓
$T_{D,j}(x_j^*, T, B_l, B_u) = \begin{cases} 1 - \frac{T - x_j^*}{T - B_l}, & B_l < x_j^* < T \\ 1, & x_j^* = T \\ 1 - \frac{x_j^* - T}{B_u - T}, & T < x_j^* < B_u \\ 0, & \text{else} \end{cases}$	DTI		✓

Note: LTB: Larger-the-better, STB: Smaller-the-better, DTI: Distance-to-ideal, $\boldsymbol{x}^* = \{x_1^*, x_2^*, ..., x_n^*\}$, T is a target or ideal value for a given indicator, B is a baseline or non-ideal value for a given indicator (B_l and B_u used when an upper and lower baseline are required), $\bar{x}^*$ is the sample mean, S_N is the sample standard deviation, and c_f is a conversion factor to change units of $\boldsymbol{x}^*$ to alternate units (ex. dollars or greenhouse gas equivalents).

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Z-Score Normalization
$\frac{\partial}{\partial x_j^*}(Z_j(\boldsymbol{x}^*)) = \frac{\left((\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2)^{\frac{1}{2}}(1 - \frac{1}{n})\right) - \left(\frac{n^{-1/2}(x_j^* - x^*)^2}{(\sum_{j=1}^n (x_j^* - x^*)^2)^{1/2}}\right)\left(\frac{\sum_{k \neq j}(x_k^* - x^*)}{-n(x_j^* - x^*)} + (1 - \frac{1}{n})\right)}{\frac{1}{n}\sum_{j=1}^n (x_j^* - \bar{x}^*)^2}$
Unit Equivalence Normalization
$\frac{\partial}{\partial x_j^*}(C(x_j^*, c_f)) = c_f$
Target Normalization to Interval [0,1]
$\frac{\partial}{\partial x_j^*}(T_{L,j}(x_j^*, T, B)) = \begin{cases} \frac{1}{T - B}, & B < x_j^* < T \\ 0, & \text{else} \end{cases}$
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Normalization in sustainability assessment: Methods and implicatio

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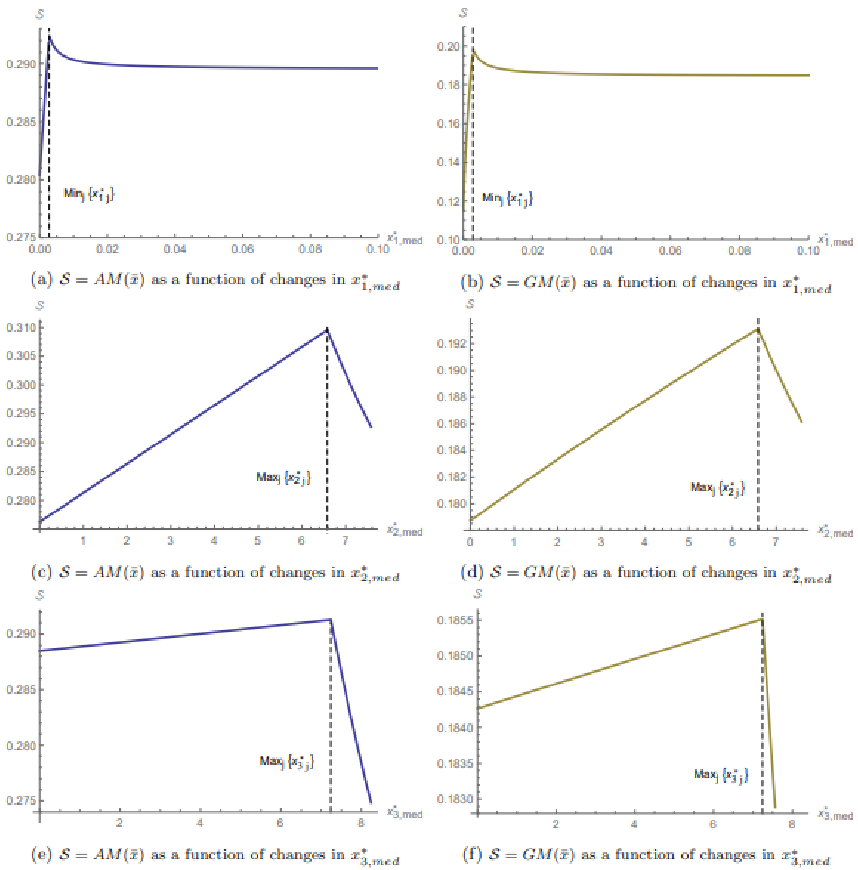

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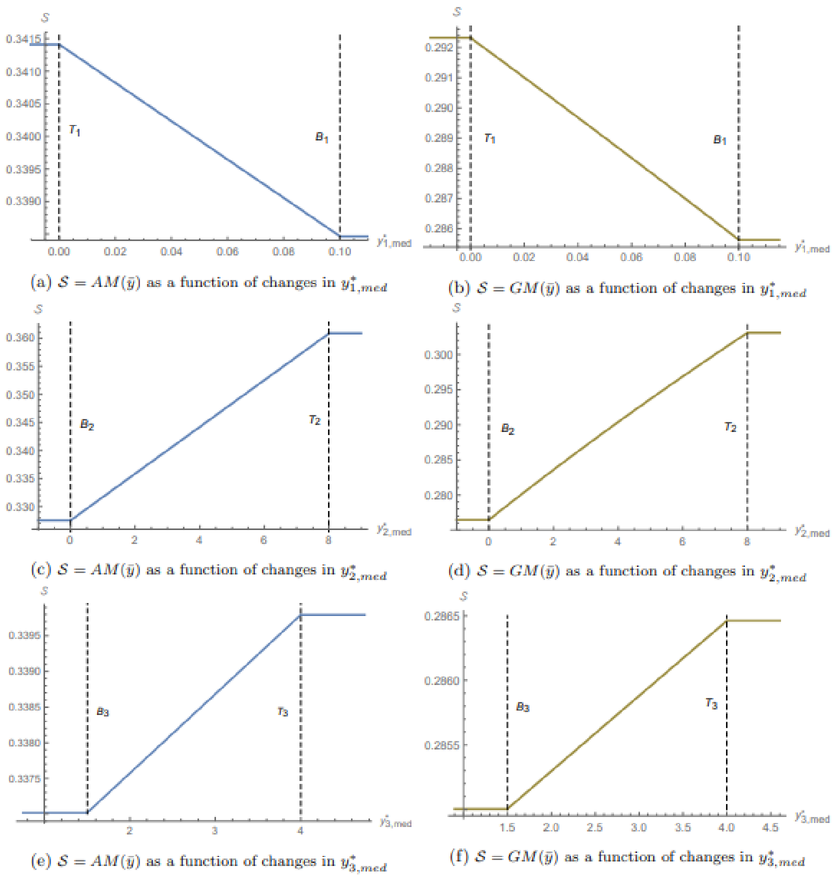
(f) $\mathcal{S} = GM(\bar{x})$ as a function of changes in $x^*_{3,med}$

Figure 2.2: Changes in $\mathcal{S}$ in response to changes in median values of from the data sets for phosphorus ($x^*_{1,med}$), yield ($x^*_{2,med}$), and %OM ($x^*_{3,med}$) under ratio normalization scheme. Dashed lines show $\min_j x^*_{ij}$ and $\max_j x^*_{ij}$ values from Table 2.5. In all cases, the median value from each data set was varied in order to show the effect that changing non-normalized indicator measures has on $\mathcal{S}$. Notice the behavior of $\mathcal{S}$ when the median value becomes the $\min_j x^*_{ij}$ in (a,b) and the $\max_j x^*_{ij}$ in (c,d,e,f). This dramatic change is due to the fact that ratio normalization is an internal normalization process, and the dependence of all normalized values in the data set on the minimum or maximum value of that data set. All functions depicted correspond to functions presented in Table 2.7



(a) $\mathcal{S} = AM(\bar{y})$ as a function of changes in $y^*_{1,med}$

(b) $\mathcal{S} = GM(\bar{y})$ as a function of changes in $y^*_{1,med}$

(c) $\mathcal{S} = AM(\bar{y})$ as a function of changes in $y^*_{2,med}$

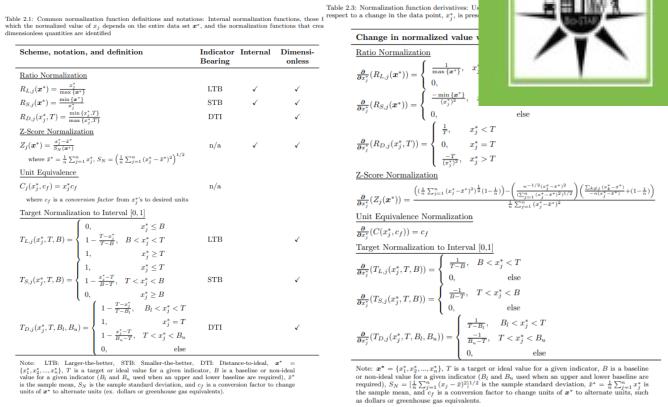
(d) $\mathcal{S} = GM(\bar{y})$ as a function of changes in $y^*_{2,med}$

(e) $\mathcal{S} = AM(\bar{y})$ as a function of changes in $y^*_{3,med}$

(f) $\mathcal{S} = GM(\bar{y})$ as a function of changes in $y^*_{3,med}$

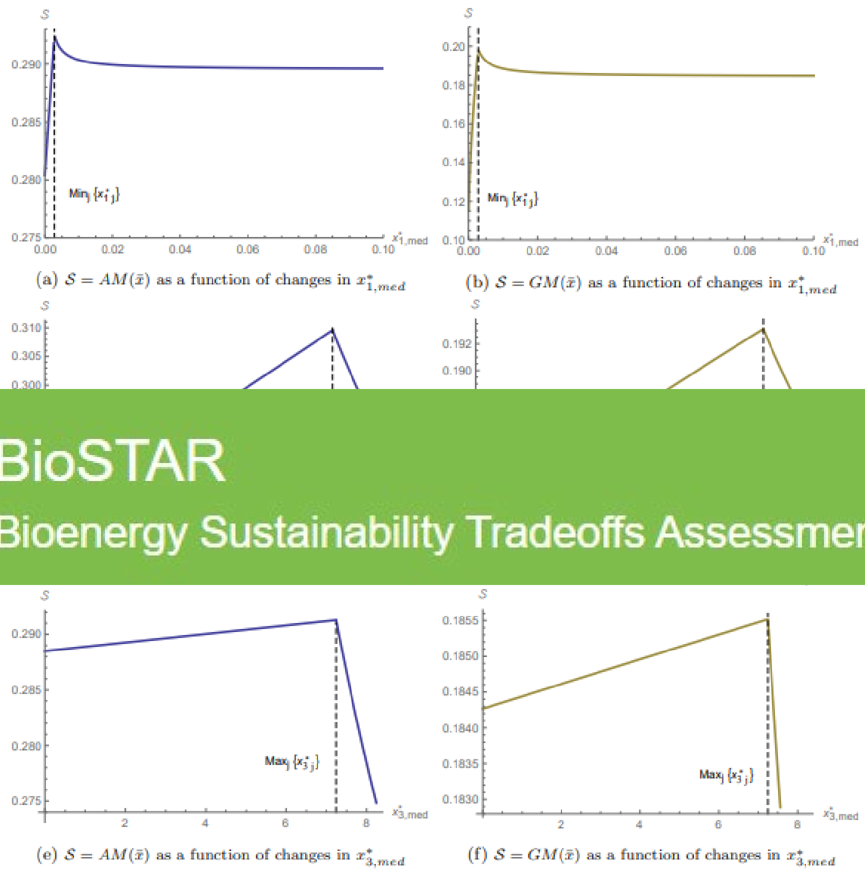
Figure 2.3: Changes in $\mathcal{S}$ in response to changes in median values of from the data sets for Phosphorus ($y^*_{1,med}$), Yield ($y^*_{2,med}$), and %OM ($y^*_{3,med}$) under target normalization scheme. In all cases, the median value from each data set was varied in order to show the effect that changing non-normalized indicator measures has on $\mathcal{S}$. Dashed lines show normalization parameters from Table 2.6. When the median value is changed to values outside the baseline and target intervals, there is no response in $\mathcal{S}$ to further changes due to the normalized value becoming a constant 0 or 1. All functions depicted correspond to functions presented in Table 2.8

Distance to target normalization is often preferable



Normalization in sustainability assessment: Methods and implicatio

Ecol Econ Pollesch and Dale, 2016



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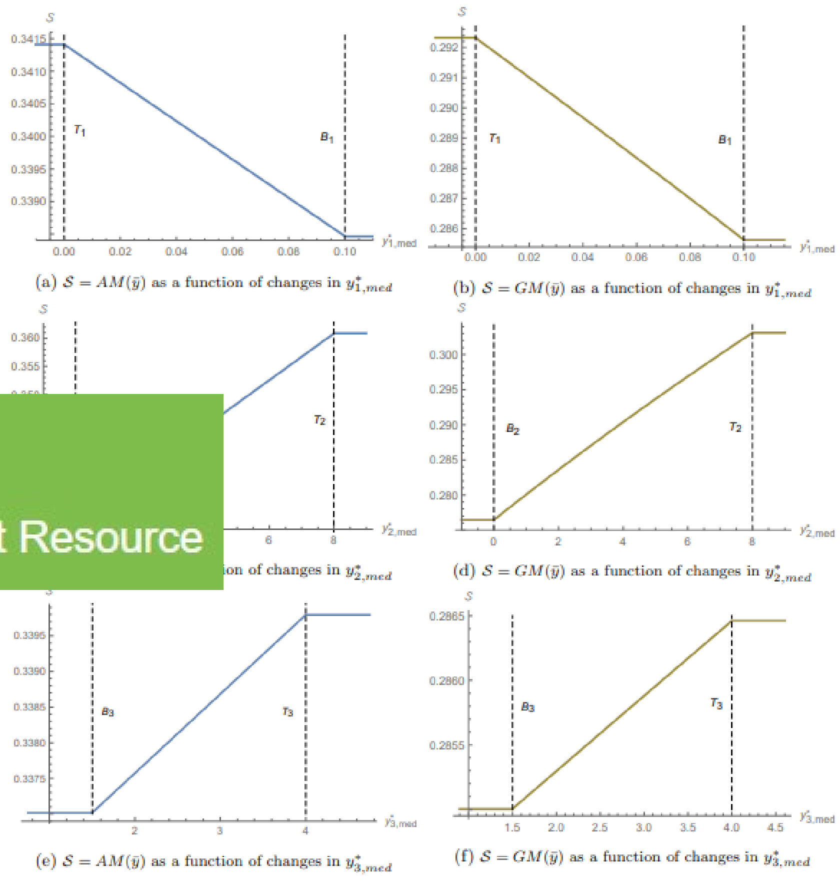

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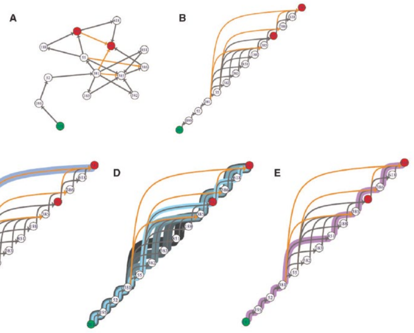
BioSTAR

Bioenergy Sustainability Tradeoffs Assessment Resource

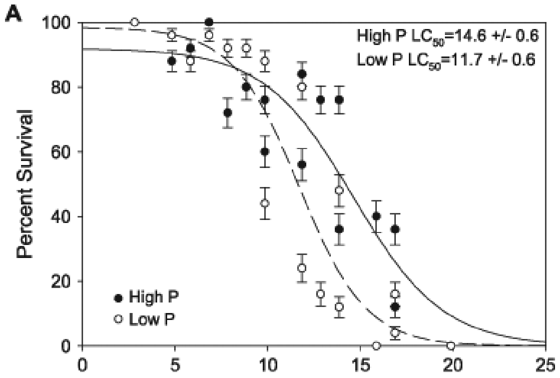
Distance to target normalization is often preferable

$$IS_i = (1-\lambda)\left[\min_j\left(W_j\bar{R}_{ij}\right)\right] + \lambda\sum_{j=1}^{m} W_j\bar{R}_{ij}$$

Applications of aggregation theory to sustainability assessment
Ecol Econ Pollesch and Dale, 2015

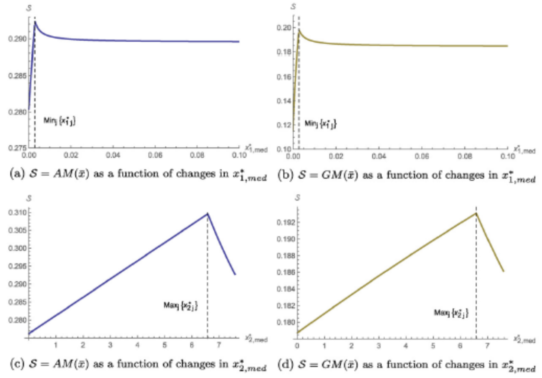


Extracting and benchmarking emerging adverse outcome pathway knowledge
Toxsci Pollesch et al., 2019



Frost et al., 2017

Stoichiometric ecotoxicology for a multi-substance world
Bioscience Peace et al., 2021



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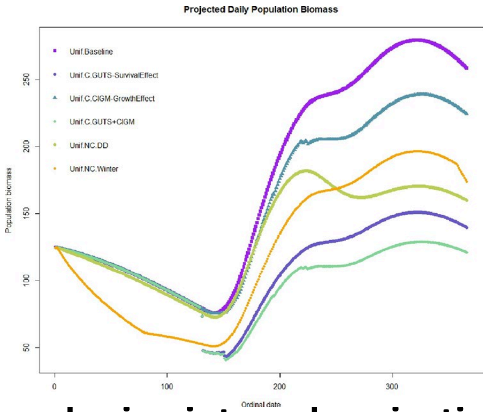
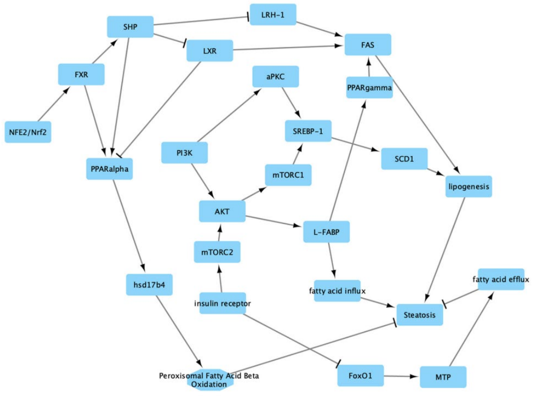
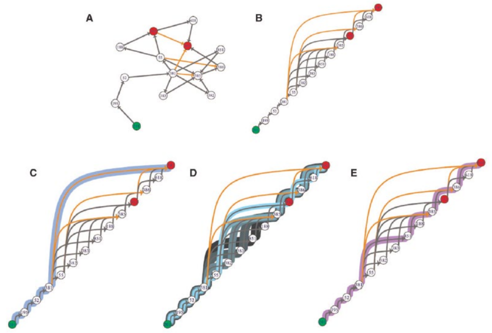


Developing integral projection models for ecotoxicology
Eco Mod Pollesch et al., 2022



Predicting the Probability that a Chemical Causes Steatosis using adverse outcome pathway Bayesian Networks
Risk Anal. Burgoon et al., 2020



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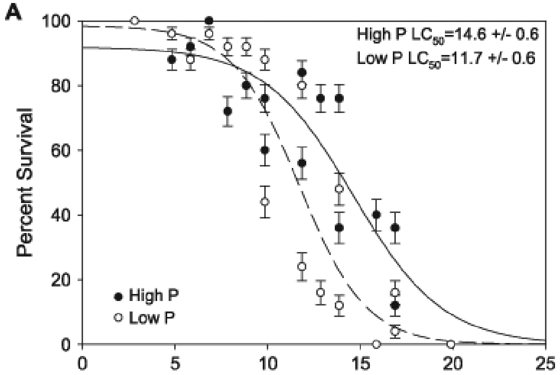

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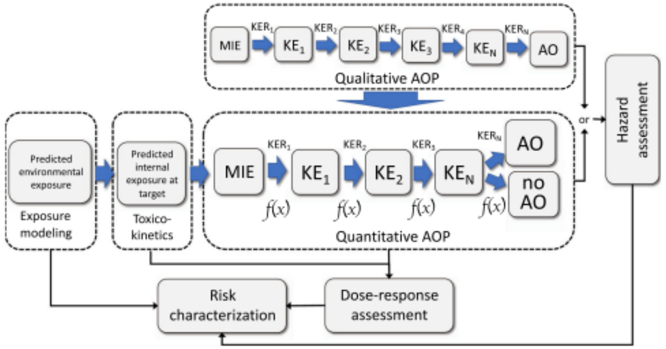
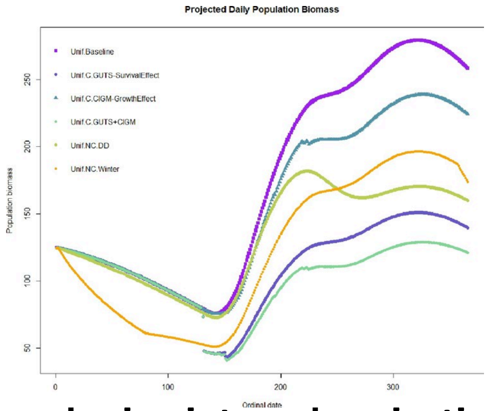


Building and applying quantitative adverse outcome pathway models for chemical hazard and risk assessment
ET&C Perkins et al., 2019



Developing integral projection models for ecotoxicology
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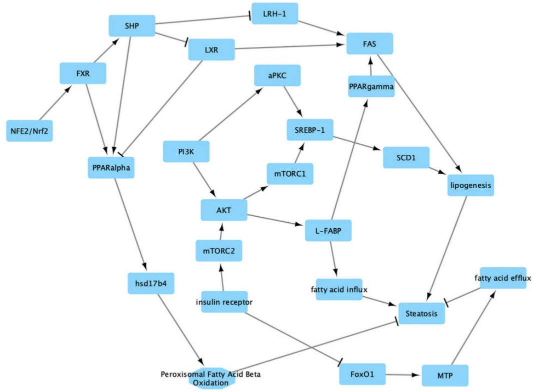

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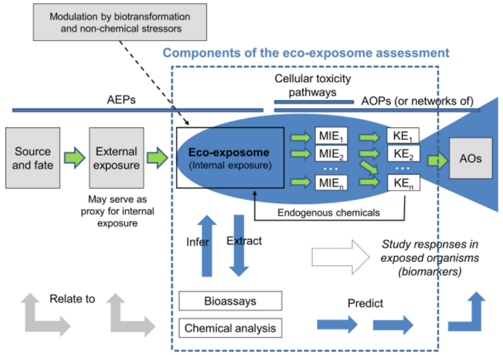
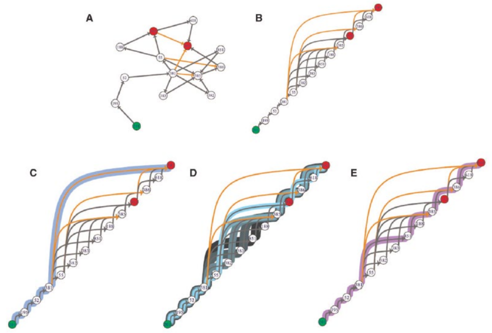
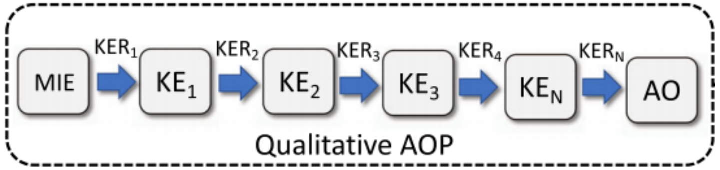


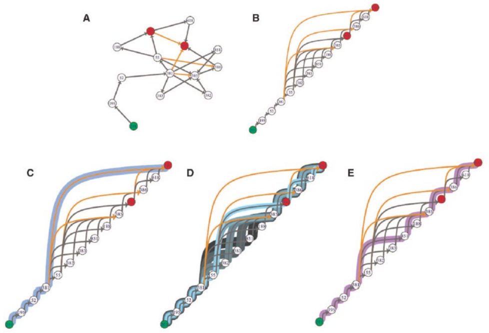
The Eco-Exposome Concept: Supporting an integrated Assessment of Mixtures of Environmental Chemicals
ET&C Scholz et al., 2022



Extracting and benchmarking emerging adverse outcome pathway knowledge
Toxsci Pollesch et al., 2019

Adverse Outcome Pathways are models of measurable, causal, toxicological relationships





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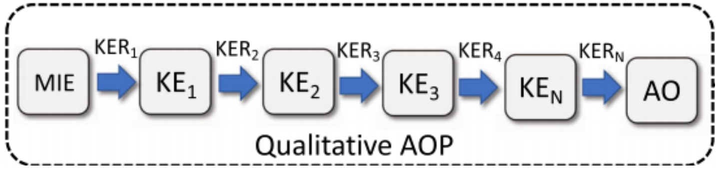
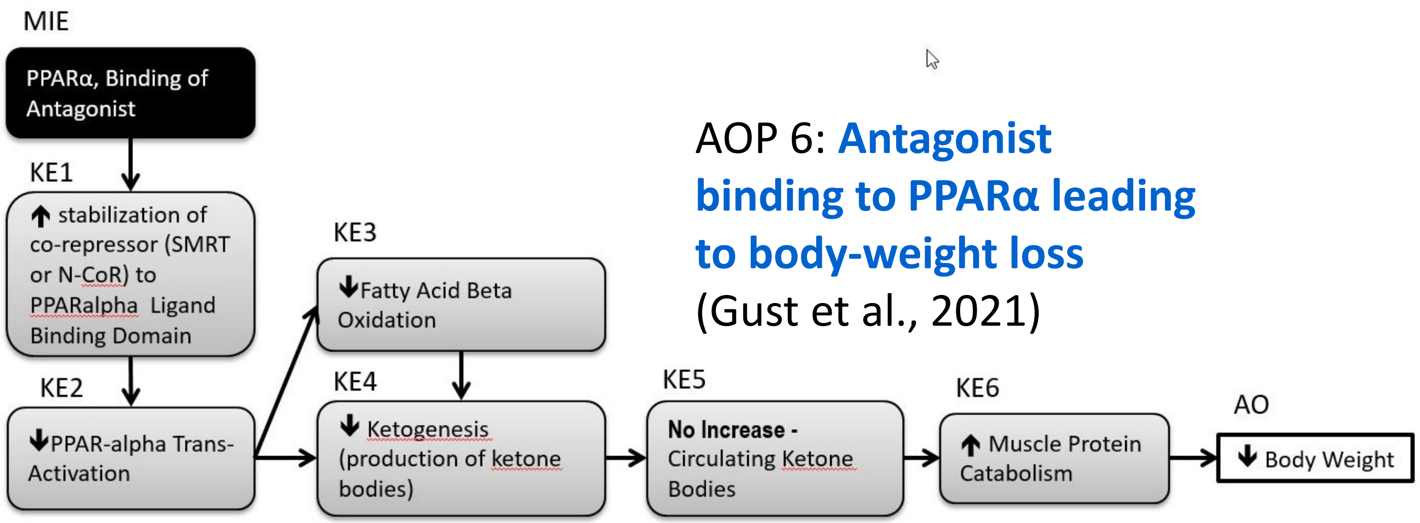
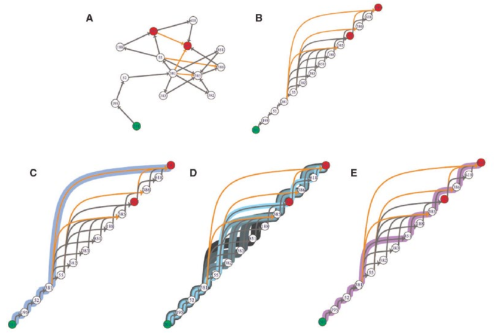




AOP 6: **Antagonist binding to PPARα leading to body-weight loss**
(Gust et al., 2021)

(Many of these AOPs are DAGs)



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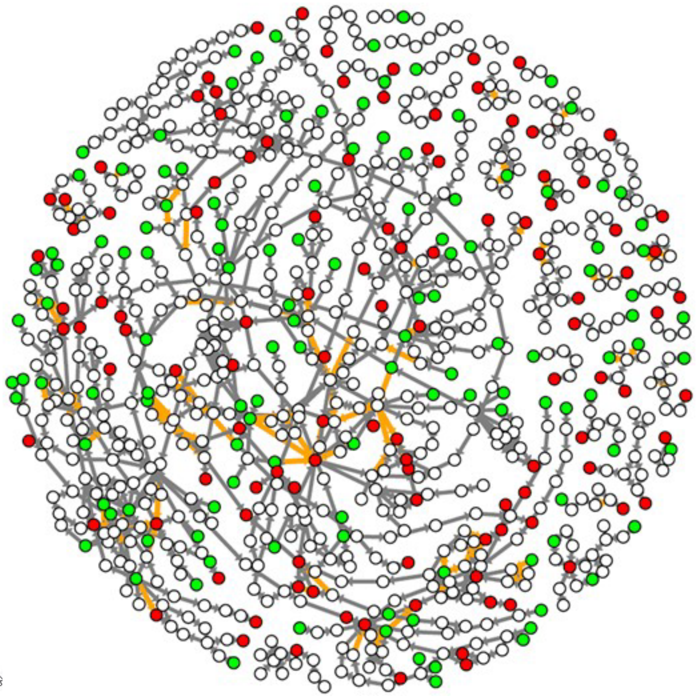
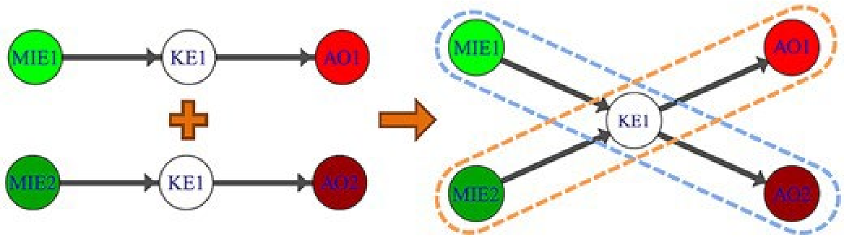
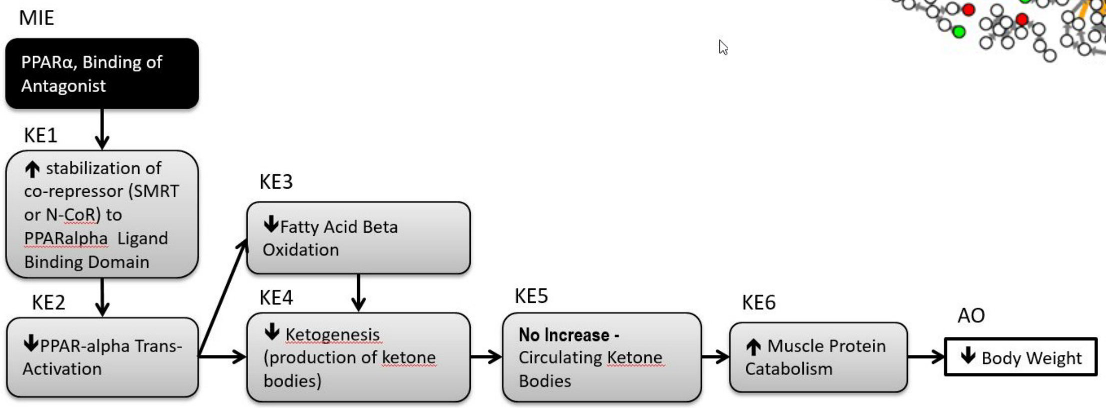
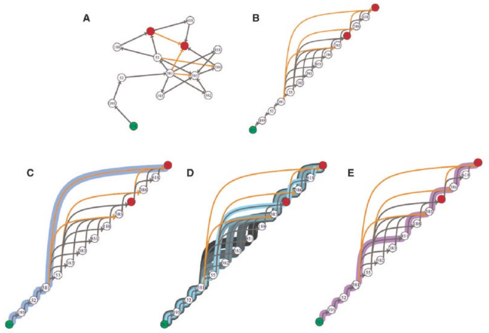






- We identified all unique linear AOPs in the network.
- We then categorized them as expert-specified versus “emergent” AOPs



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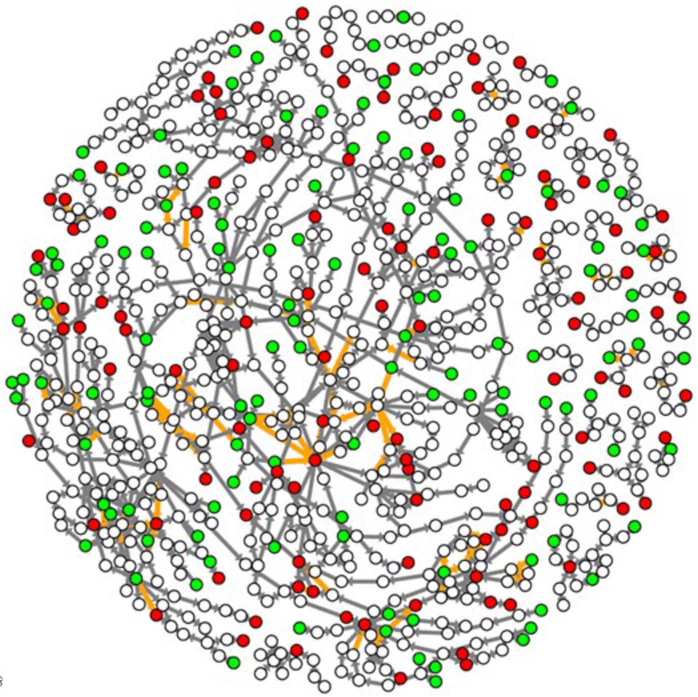
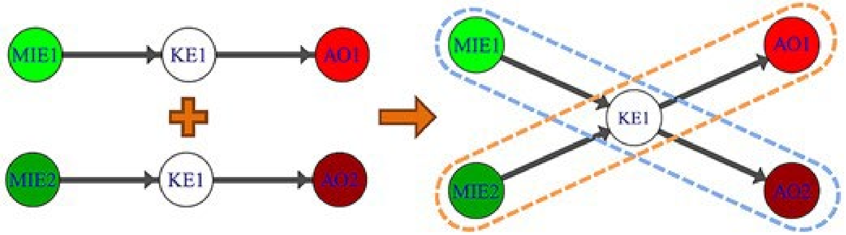
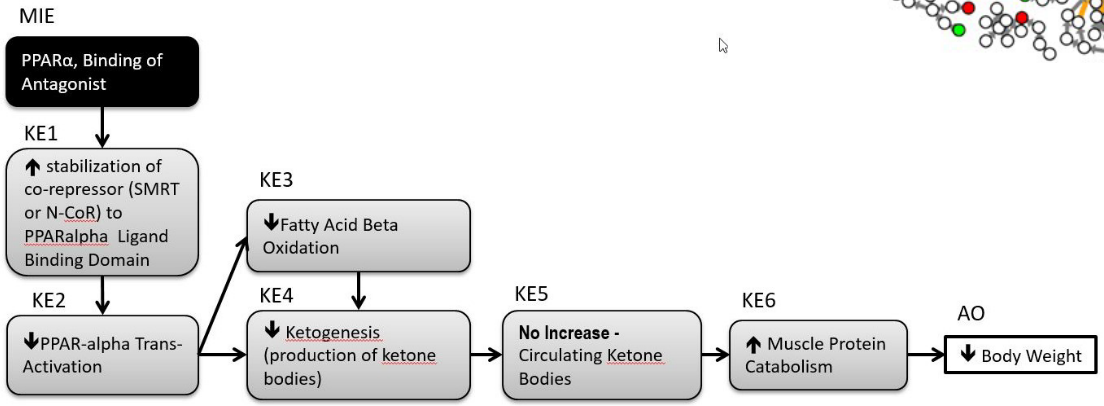
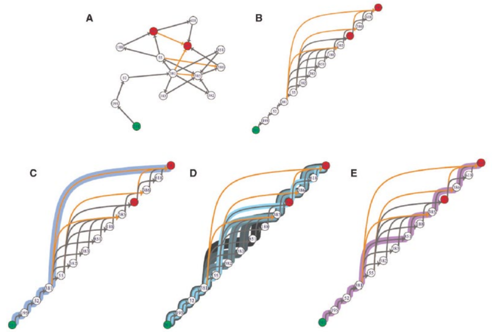






- We identified all unique linear AOPs in the network.
- We then categorized them as expert-specified versus “emergent” AOPs

- We found that there were 187 expert-specified AOPs, and **9405** emergent AOPs
- Are these emergent AOPs novel toxicological information? Or are the computational artifacts? (We are working on that now)



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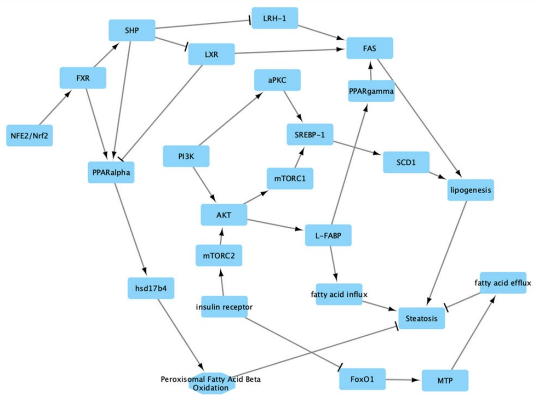

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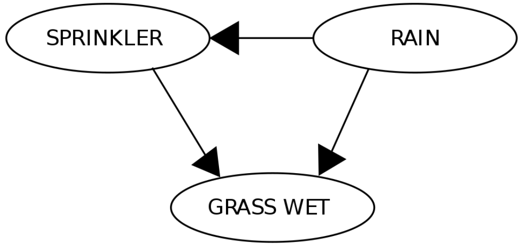
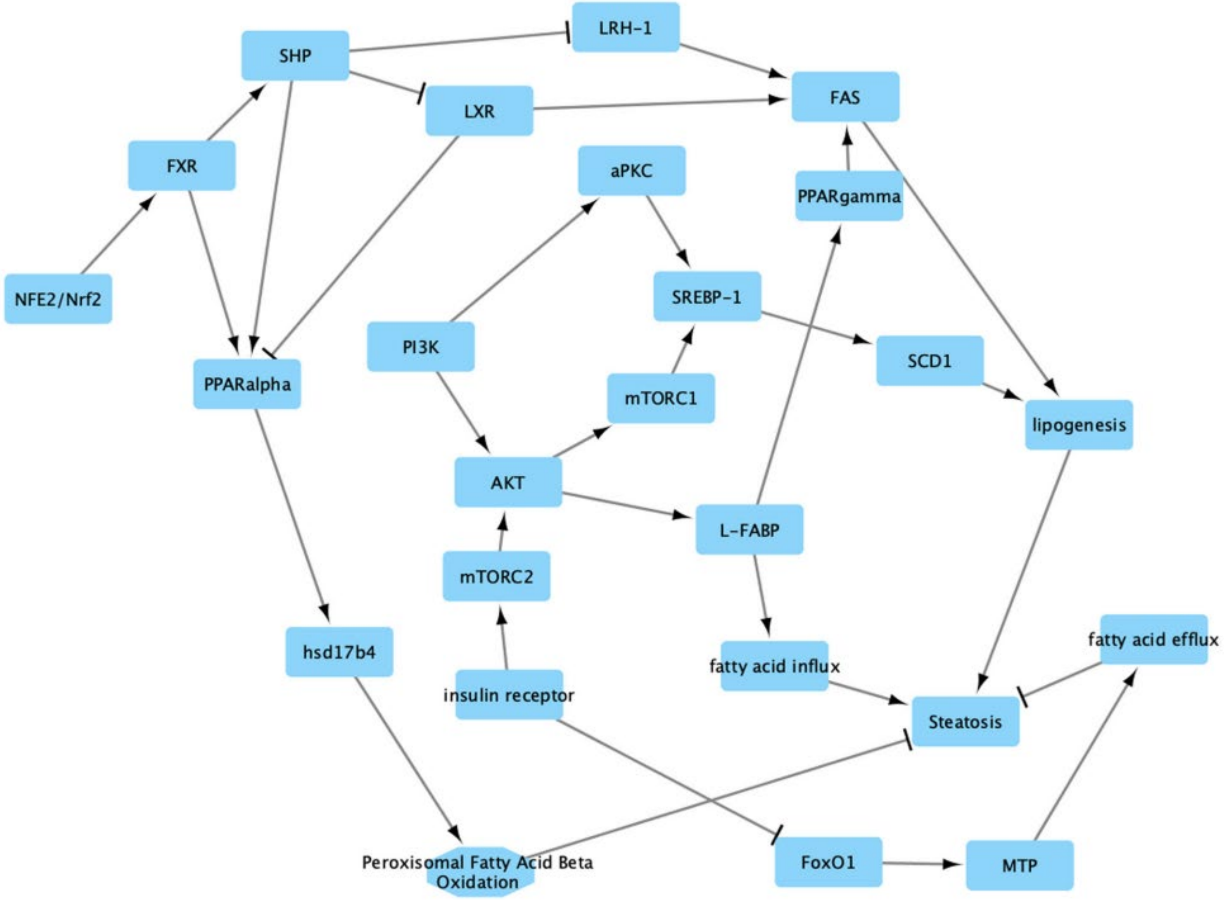
Simple Bayesian Network

	SPRINKLER	
RAIN	T	F
F	0.4	0.6
T	0.01	0.99



RAIN	
T	F
0.2	0.8

		GRASS WET	
SPRINKLER	RAIN	T	F
F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01



While we are on the topic of networks

"Can you come to my office? I have a question about networking"

While we are on the topic of networks

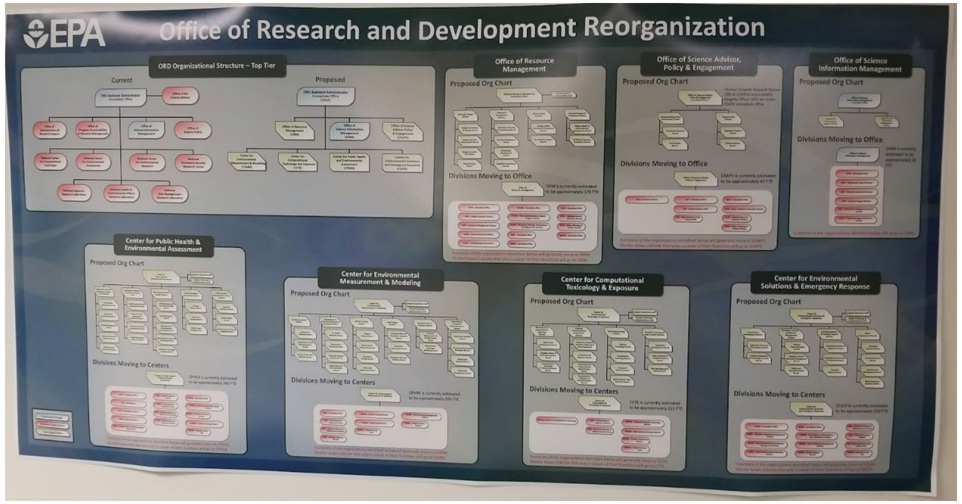
“Can you come to my office? I have a question about networking”

“Have you ever heard of the six degrees of Kevin Bacon?”

“I have to plan a meeting where I break the managers into small groups, and I want to make it so everyone gets to know everyone the best.”*

*Not exact quotes, but close enough

While we are on the topic of networks



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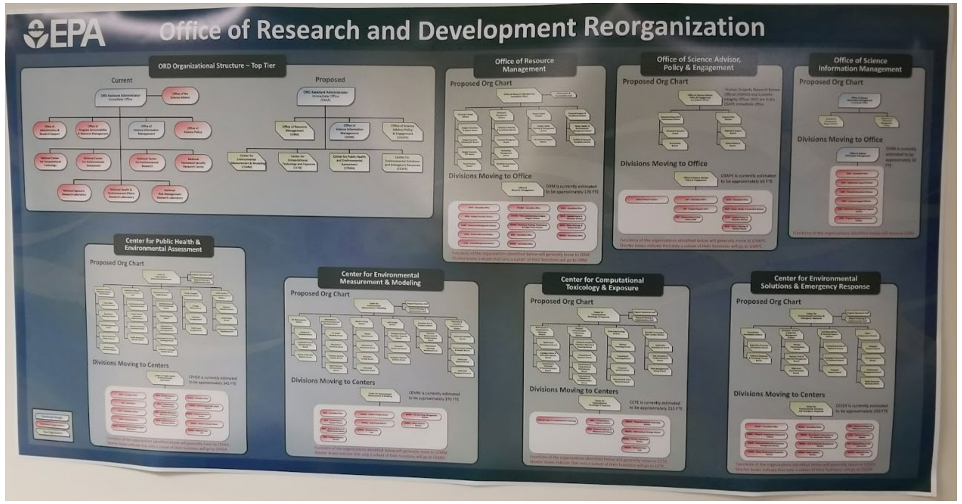
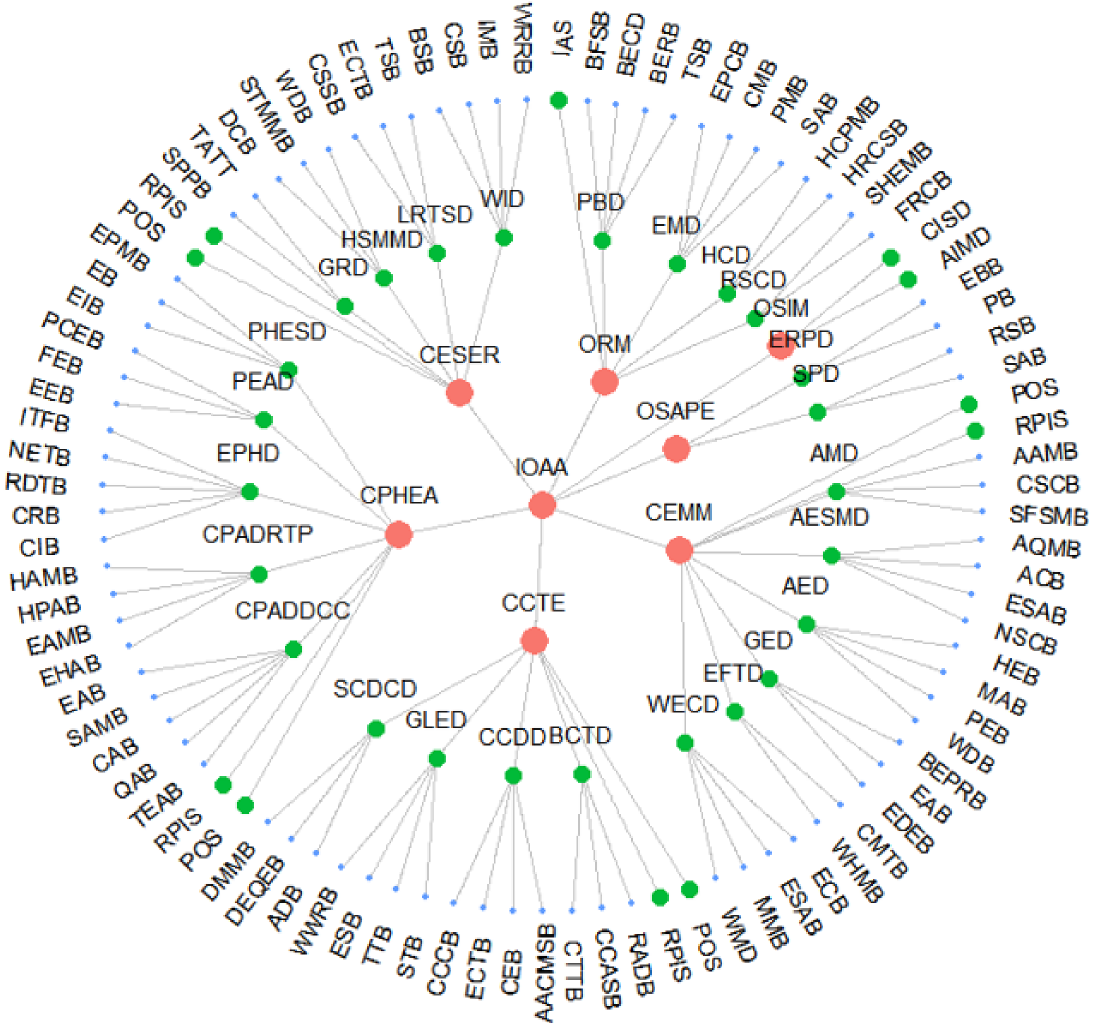
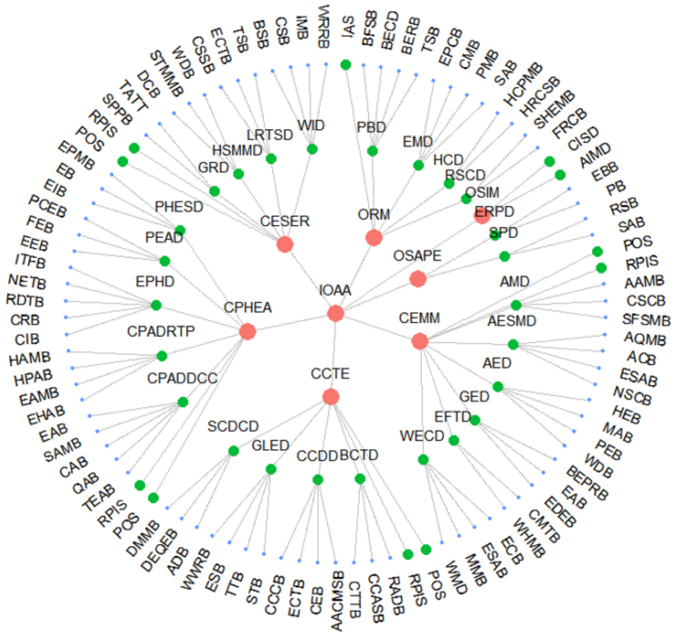
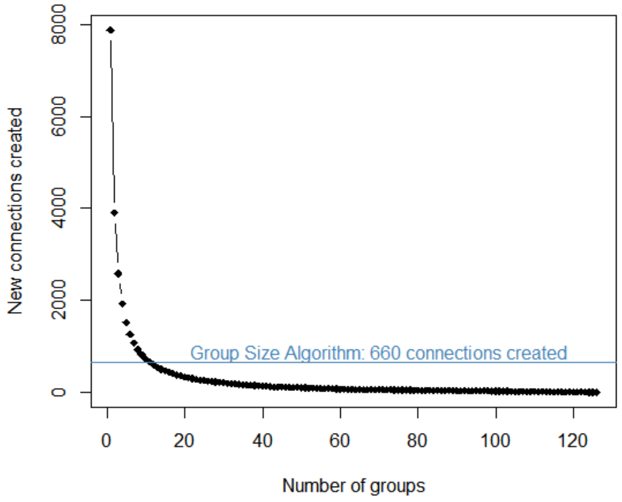
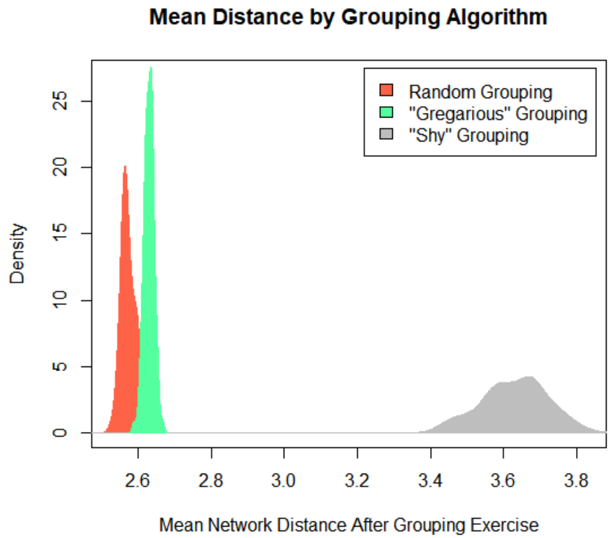




Minimizing total distance by sub-grouping in a hierarchical organization







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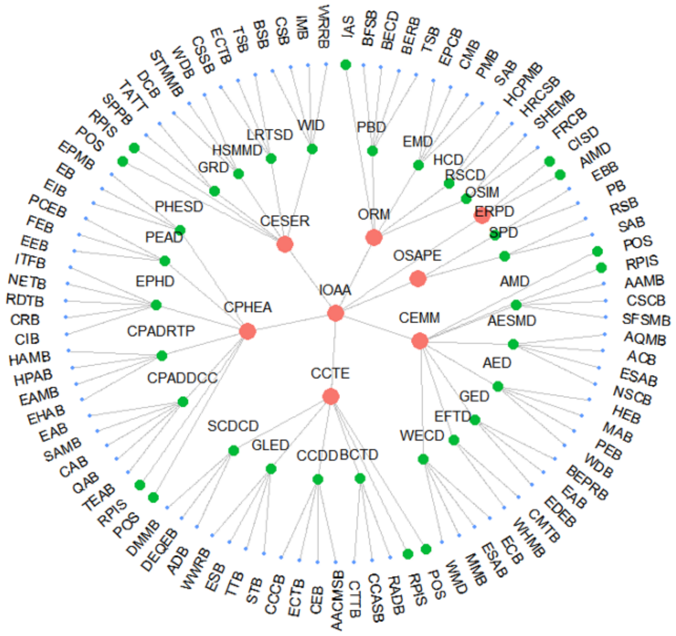

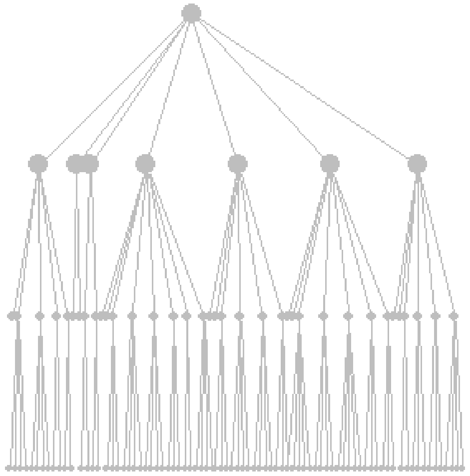

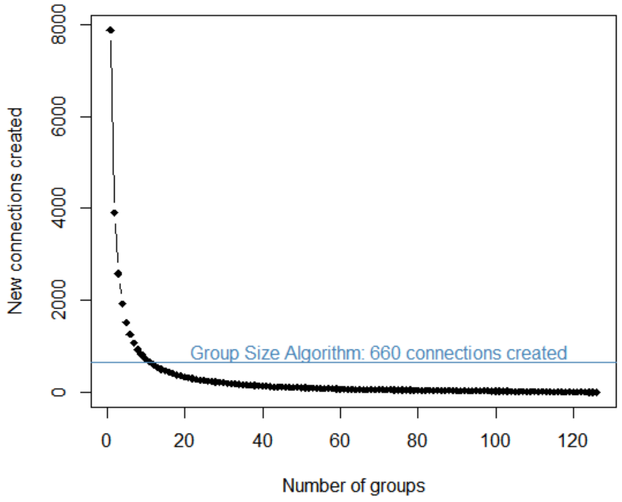

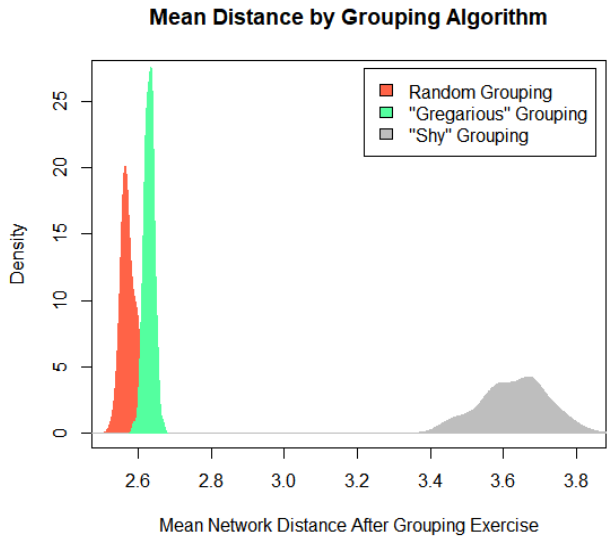

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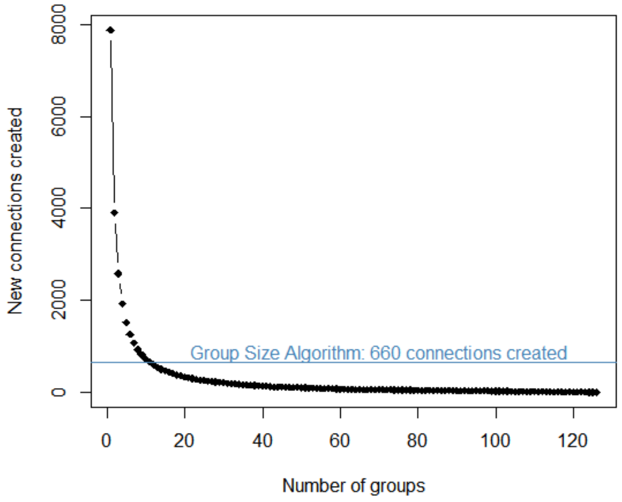

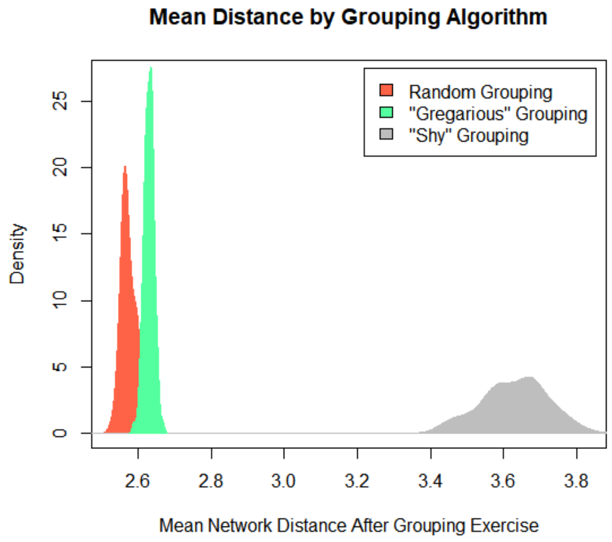

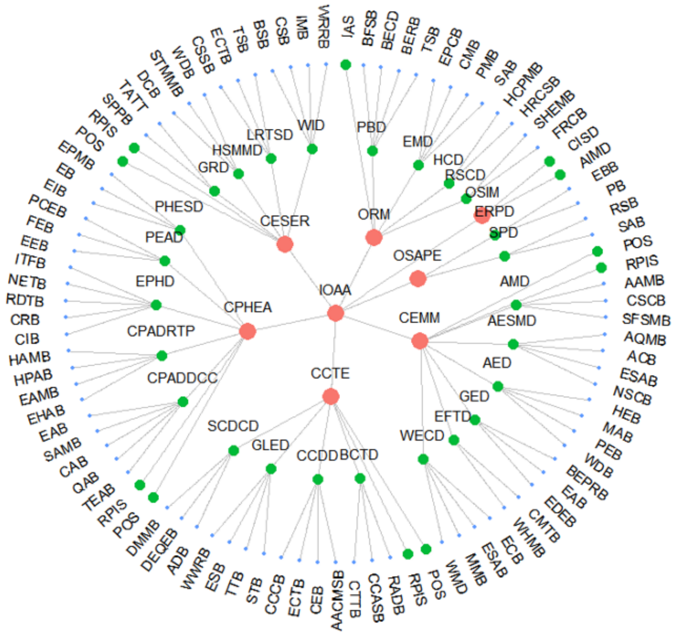

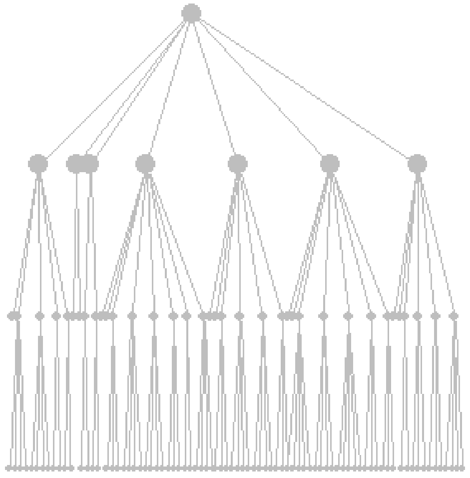

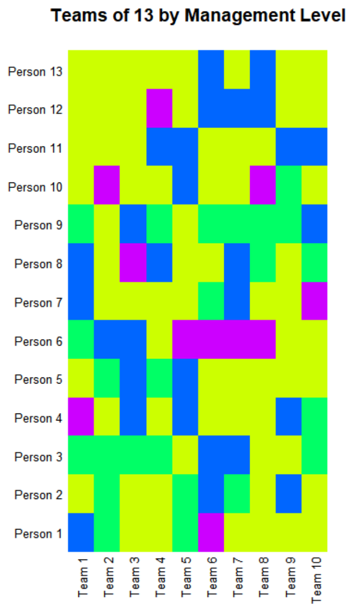

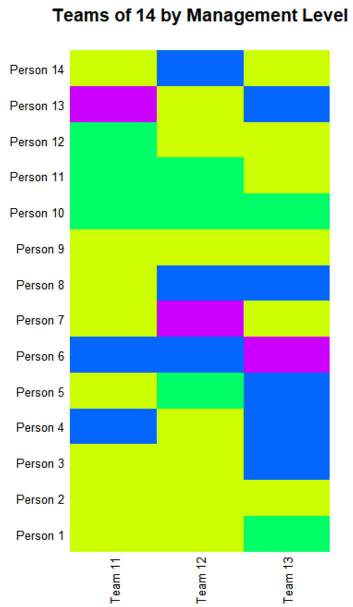

In summary:

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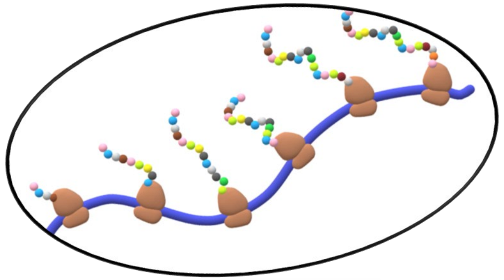
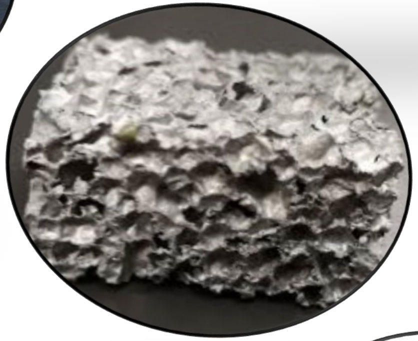
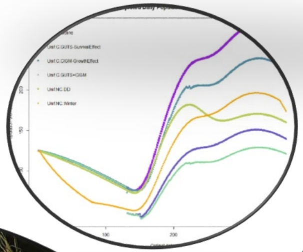
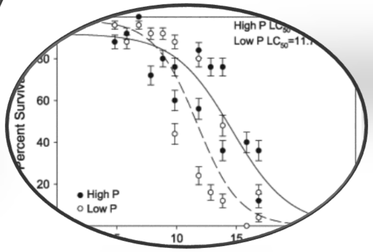
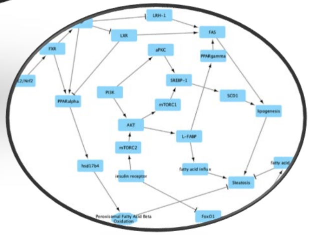
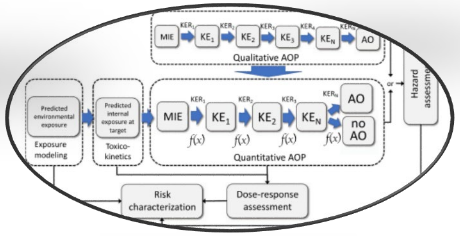


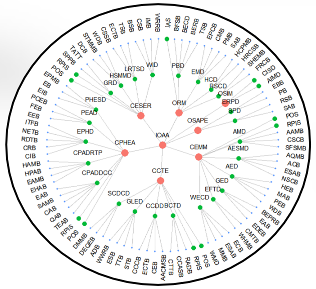




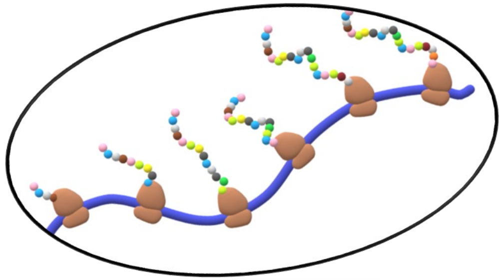

High P
Low P
Percent Survival
60
40
20
10
15

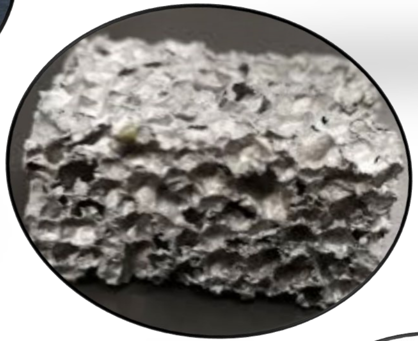


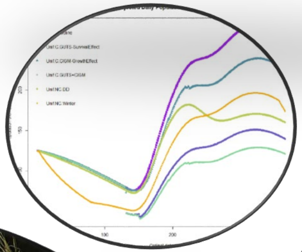

MIE
Qualitative AOP
Predicted environmental exposure
Exposure modeling
Predicted internal exposure at target
Toxico-kinetics
AO
no AO
Quantitative AOP
Risk characterization
Dose-response assessment

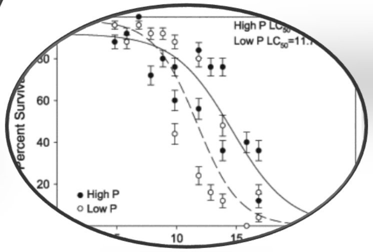


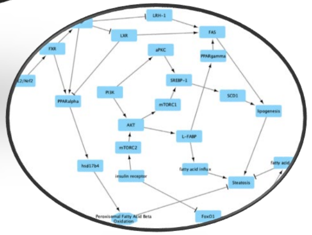
In summary:

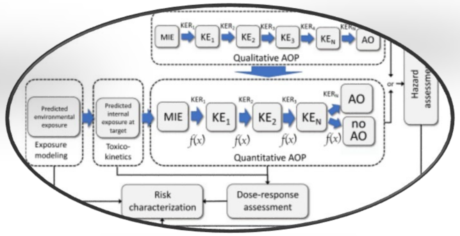


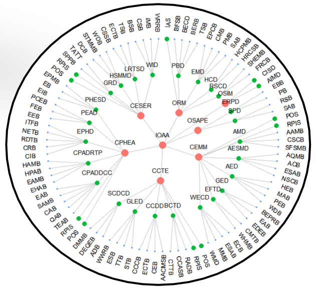












UMD

OAK RIDGE National Laboratory

Center for Bioenergy Sustainability

Mathematics of Planet Earth

NIMBioS
National Institute for Mathematical and Biological Synthesis

SETAC

Society of Environmental Toxicology and Chemistry

Aquatic Sciences Center
UNIVERSITY OF WISCONSIN–MADISON

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WATERBORNE ENVIRONMENTAL

CENTER FOR COMPUTATIONAL TOXICOLOGY AND EXPOSURE

What's next?

Current EPA Collaborations

- Toxicity Translation and Ecological Modeling
  - "What is Tox Translation?"
    - Theoretical model development stuff
  - Fish Toxicity Translator v2.0 Model/GUI
    - IPMs and coding
- Adverse Outcome Pathways
  - Data Mining/Knowledge Discovery
  - Quality assessment

Exciting New Research Areas and Ideas

- Supporting Literature/Text Mining
- Adverse Outcome Pathways
  - qAOPs using Petri nets
  - Network Analysis Continued
- Toxicity Translation
  - Computational Workflow Development

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More Exciting New Research Areas and Ideas

- Information Theory
- Bayesian Network Research
  - Sensitivity analysis
- Ecological Model Development Theory
- Aggregation Theory for EPA's multi-criteria assessments
- Graph Theory/Network Analysis
  - Optimal subgrouping in trees!

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Even More Exciting New Research Areas and Ideas

- Chronic Effects Modeling Approaches
  - Add on from Acute effects
- Stoichiometric Ecotoxicology
- Quantitative Justice SIAM Working Group

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http://Pollesch.dev

Please reach out if you want to chat about any of this work