CBES
Center for BioEnergy Sustainability

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

THE UNIVERSITY of TENNESSEE

Bioenergy Sustainability Assessment

Image: http://news.illinois.edu/news/08/0730miscanthus.html

Mathematical Approaches to protocol development

Nathan L. Pollesch

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Overview

- How is sustainability measured within the context of bioenergy?
- What are the challenges in bioenergy sustainability assessment?
- Can introducing mathematics contribute to meeting those challenges and achieving assessment goals?

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- ~~Can introducing mathematics contribute to meeting those challenges and achieving assessment goals?~~

  What types of mathematics can be introduced?

Indicators for Bioenergy Sustainability

Nathan L. Pollesch :: University of Tennessee, Department of Mathematics

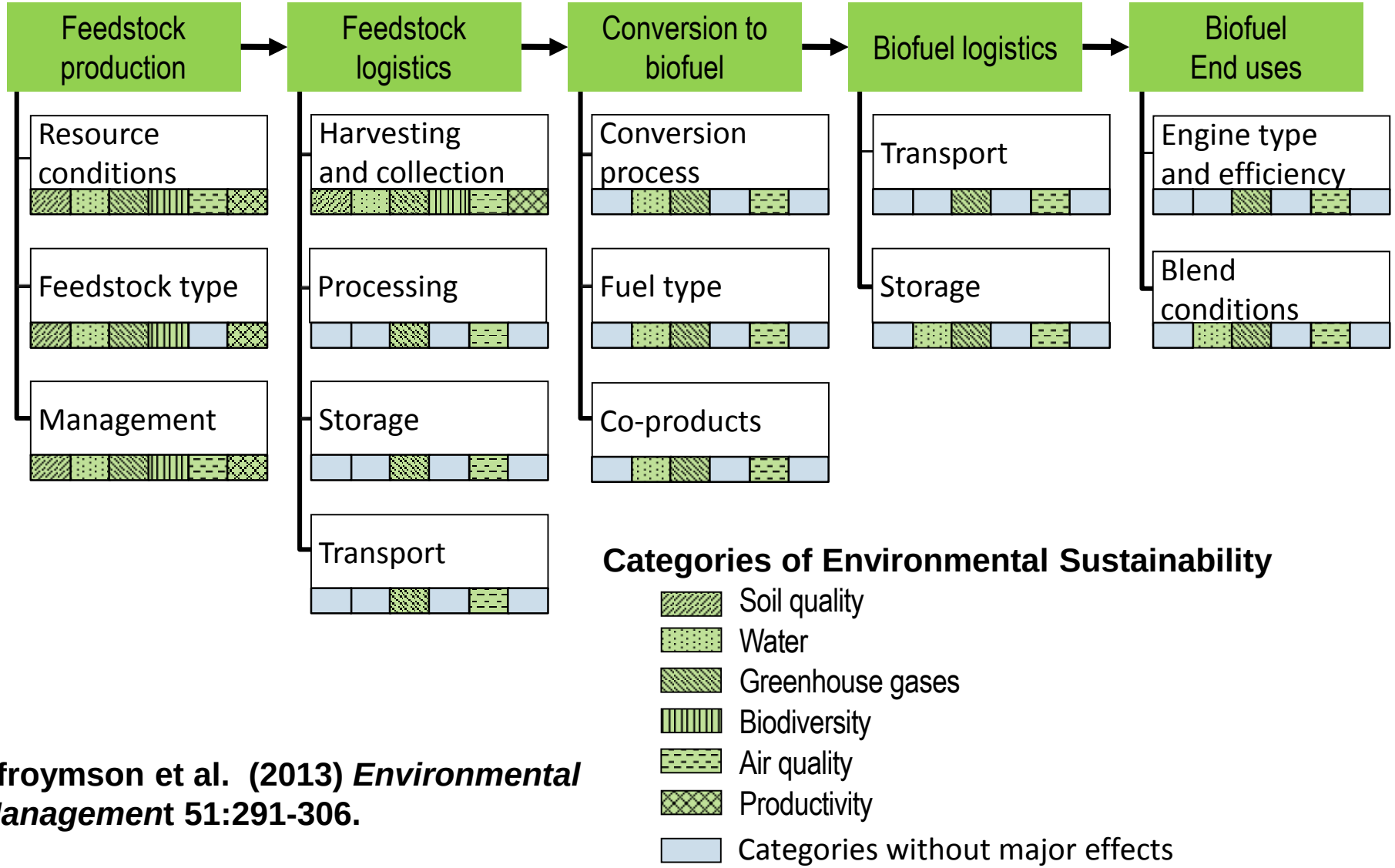
Categories of environmental sustainability indicators

Environment	Indicator	Units
Soil quality	1. Total organic carbon (TOC)	Mg/ha
	2. Total nitrogen (N)	Mg/ha
	3. Extractable phosphorus (P)	Mg/ha
	4. Bulk density	g/cm^3
Water quality and quantity	5. Nitrate concentration in streams (and export)	concentration: mg/L; export: kg/ha/yr
	6. Total phosphorus (P) concentration in streams (and export)	concentration: mg/L; export: kg/ha/yr
	7. Suspended sediment concentration in streams (and export)	concentration: mg/L; export: kg/ha/yr
	8. Herbicide concentration in streams (and export)	concentration: mg/L; export: kg/ha/yr
	9. Storm flow	L/s
	10. Minimum base flow	L/s
	11. Consumptive water use (incorporates base flow)	feedstock production: m^3/ha/day; biorefinery: m^3/day

Environment	Indicator	Units
Greenhouse gases	12. CO_2 equivalent emissions (CO_2 and N_2O)	kgC_{eq}/GJ
Biodiversity	13. Presence of taxa of special concern	Presence
	14. Habitat area of taxa of special concern	ha
Air quality	15. Tropospheric ozone	ppb
	16. Carbon monoxide	ppm
	17. Total particulate matter less than 2.5µm diameter ($PM_{2.5}$)	$\mu g/m^3$
	18. Total particulate matter less than 10µm diameter (PM_{10})	$\mu g/m^3$
Productivity	19. Aboveground net primary productivity (ANPP) / Yield	gC/m^2/year

McBride et al. (2011) *Ecological Indicators* 11:1277-1289

Looking at the biofuel supply chain in terms of environmental sustainability indicators



Efroymson et al. (2013) *Environmental Management* 51:291-306.

Challenges in bioenergy sustainability assessment

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Diverse production pathways

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Research and data collection infrastructure also vary by region and feedstock choice

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Bioenergy sustainability is context dependent

Virginia Dale, ORNL

Goals in for bioenergy sustainability assessments

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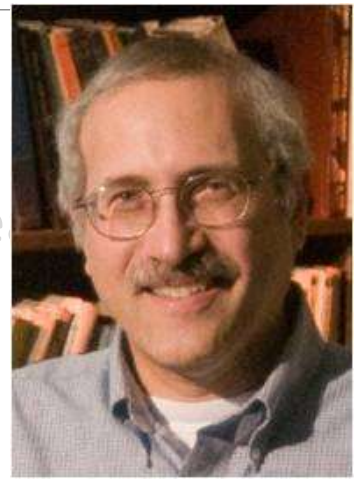
Robustness of assessment protocols



Lou Gross
University of Tennessee

7 Key Components for Sustainability Assessment

Identification of goals and boundaries for analysis

Indicator selection and categorization

Normalization and weighting

Aggregation

Analysis of data quality

Evaluation of assessment results

Visualization and reporting

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Aggregation: → Research focused on studying mathematical properties of aggregation functions and how they can be utilized to develop flexible, adaptable, and robust assessment protocols

Analysis of data quality

Evaluation of assessment results

Visualization and reporting

Applying mathematics to develop aggregation strategies

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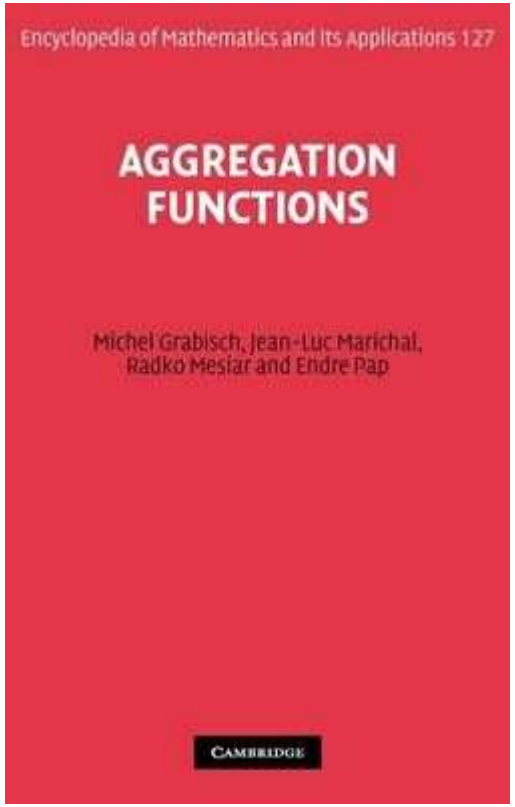
Mathematical study of aggregation functions

Aggregation Functions by Grabisch, Marichal, Mesiar, and Pap (2009) provides a formal framework for the study of aggregation functions and their application.



Two important factors for determining appropriate aggregation strategies:

- Desired assessment goals
- Characteristics of indicator data

Concerns in assessment can be addressed by appropriate selection of aggregation functions

Sustainability assessments are context dependent. Fostering consistent assessment valuations under varying contexts is critical

- Compensatory behavior of index/aggregation function
  - ex. Should a low environmental indicator value be able to offset a high economic indicator in the total aggregate value? (Weak vs. strong sustainability argument)

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  - Admissible transformations by scale of measurability (ratio, interval, ordinal, …) lead to invariant functions with respect to those scales

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- A simple change in units of measurement can change assessment outputs
  - Admissible transformations by scale of measurability (ratio, interval, ordinal, …) lead to invariant functions with respect to those scales
- Aggregation can take place at many steps within an assessment
  - Inconsistencies can arise if aggregate values are used in further aggregations and if the input ordering is varied

Example: Meaningfulness of Aggregation Function on a Measurability Scale

Meaningfulness of aggregation functions on independent ratio scales

A researcher is interested in tracking nitrogen and phosphorus concentration in a stream adjacent to a bioenergy production site. Measurements are taken in consecutive years.

- Year 1: nitrogen concentration is 0.97 mg/L and phosphorus concentration is 0.051 mg/L
- Year 2: nitrogen concentration is 0.95 mg/L and phosphorus concentration is 0.082 mg/L

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Alternatively, consider the researcher recording phosphorus measurements in cg/L instead of mg/L. This would yield values of 0.0051 cg/L year 1 and 0.0082 cg/L year 2. The aggregate value of indicators is then (0.970+0.0051)/2=0.48755 for the first year and (0.95+0.0082)/2=0.4791 the second year.

-- The researcher *now* finds that the aggregate value has **decreased** from year 1 to year 2 –

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Both mg/L and cg/L are ratio scale measurement units. In order to consistently allow changes between different ratio scale units, the aggregation function must be <u>meaningful on independent ratio scales</u>. Notably, use of the geometric mean would resolve this issue.

Quick Summary on Meaningfulness

Meaningfulness of a function is related to the ability of the function to maintain the information contained in the data.

Meaningfulness is with respect to *scales of measurability*

- Example scales are Ordinal, Interval, and Ratio

Category	Indicator	Units	Measurability Scale
Soil quality	1. Total organic carbon (TOC)	Mg/ha	Ratio scale
	2. Total nitrogen (N)	Mg/ha	Ratio scale
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	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
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	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
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Productivity	19. Aboveground net primary productivity (ANPP)/yield	g C/m^2/year	Ratio scale

*** Due to variation of habitat for species of special concern in different contexts, this indicator does not have specified units of measurement (McBride et al., 2011).*

Example: Aggregation and *Associativity* of the Aggregation Function

Soil Quality Indicators

- TOC
- N
- P
- Bulk Density

Water Quality Indicators

- Nitrate Conc.
- Total P
- Susp. Sediment
- Herbicide
- Storm Flow
- Min. Base Flow
- Consumptive Use

Greenhouse Gases Indicator

- CO_2 Equiv Emiss.

Biodiversity Indicators

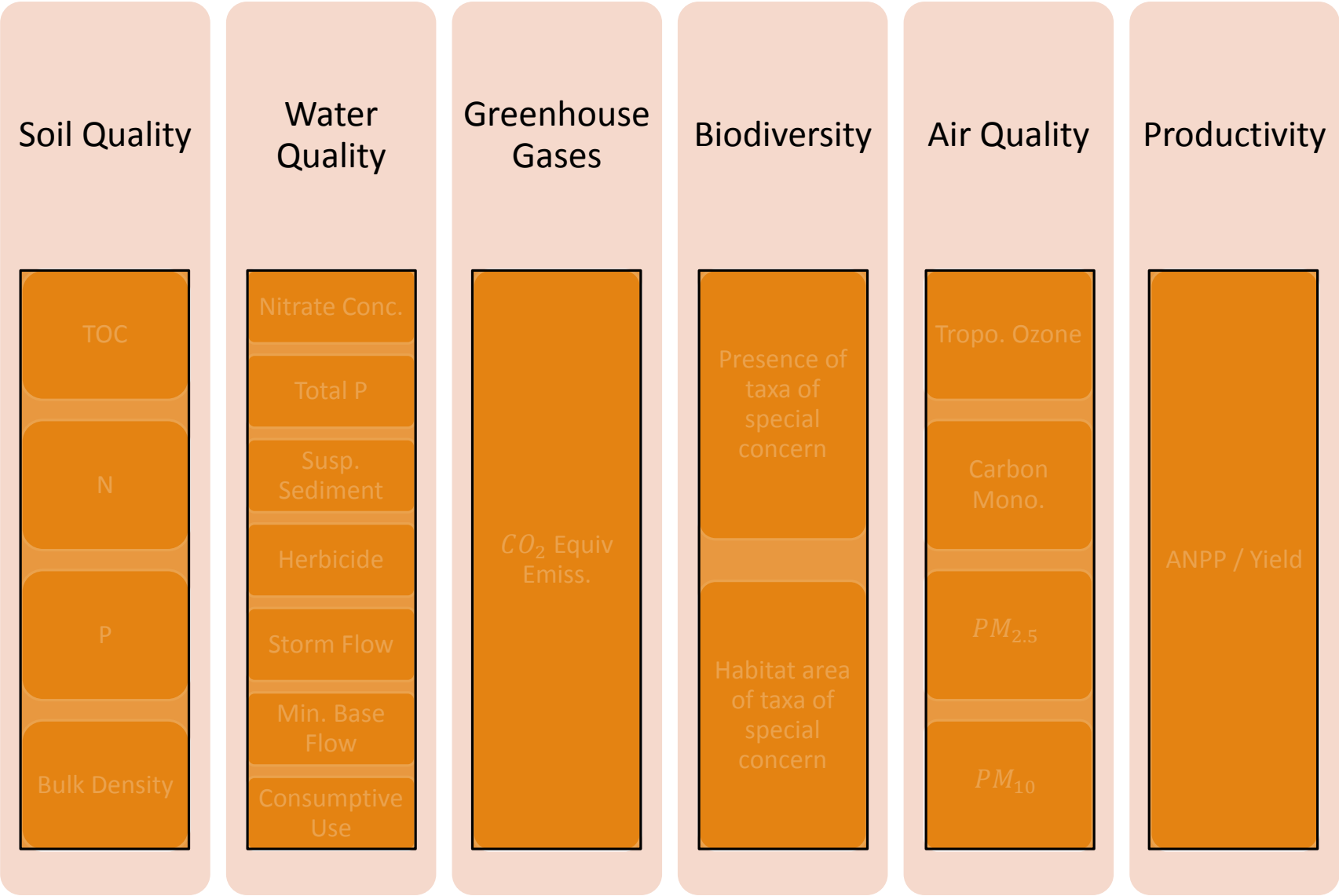
- Presence of taxa of special concern
- Habitat area of taxa of special concern

Air Quality Indicators

- Tropo. Ozone
- Carbon Mono.
- $PM_{2.5}$
- PM_{10}

Productivity Indicator

- ANPP / Yield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Soil Quality
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Environmental Sustainability

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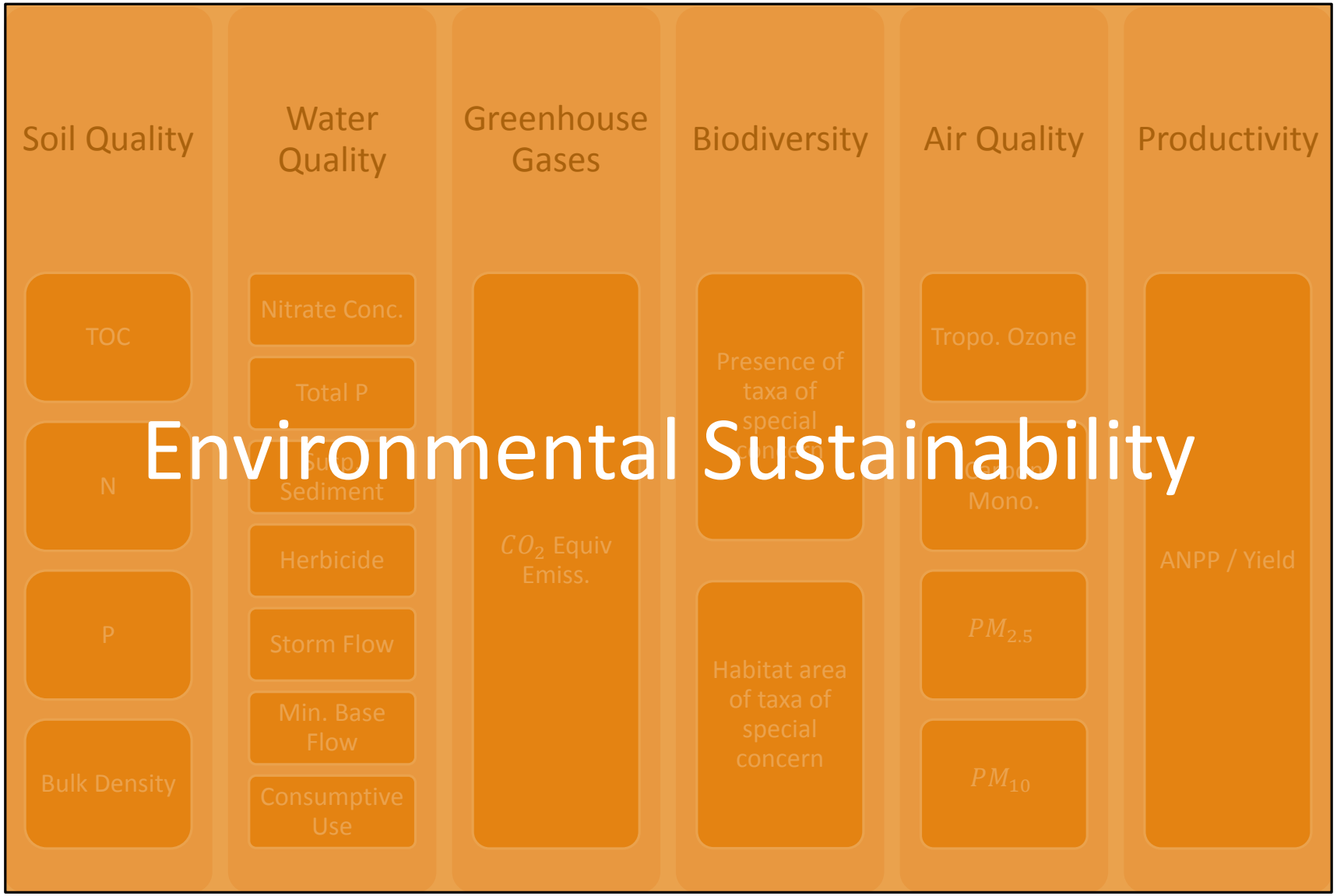

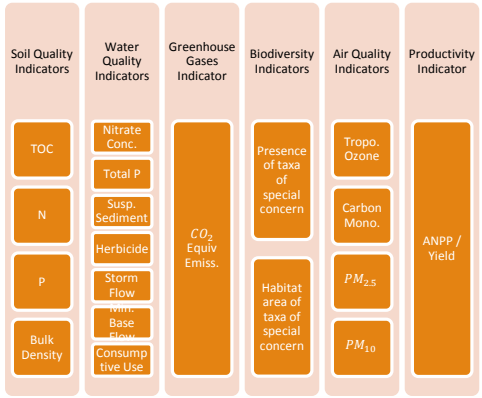
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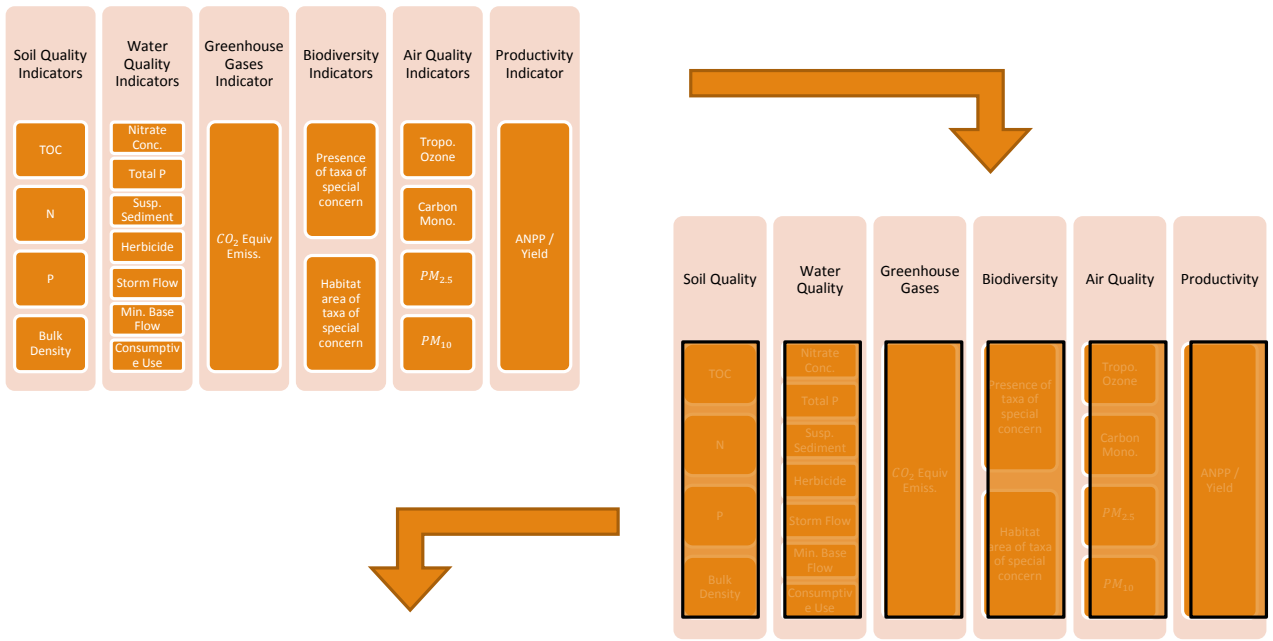
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Example: Discrepancies of aggregate values and associativity of arithmetic mean

Consider two indicators that have been normalized to values between 0 and 1. Let 1 represent some ideal value and 0 represent the non-ideal value.

Indicator A has 5 observations $(0.5, 0.4, 0.6, 0.5, 0.5)$

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This discrepancy is due to the fact that the arithmetic mean is <u>not associative</u>.

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A function F, such that $F{:}\cup_{n\in\mathbb{N}} \mathbb{I}^n \to \mathbb{I}$ is ***associative*** if

$$F(x) = x \;\forall\, x \in \mathbb{I}$$

$$F(\boldsymbol{x}, \boldsymbol{x}') = F(F(\boldsymbol{x}), F(\boldsymbol{x}'))$$

for all $\boldsymbol{x}, \boldsymbol{x}' \in \cup_{n\in\mathbb{N}} \mathbb{I}^n$

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Associativity relates to the consistency of sub-aggregates (or aggregates of subsets of indicator variables) to the aggregate value for the entire set of variables under the same aggregation function.

Normalization

Z-Score Standardization

Distance-to-target (distance from baseline)

Monetization or Energy/emergy

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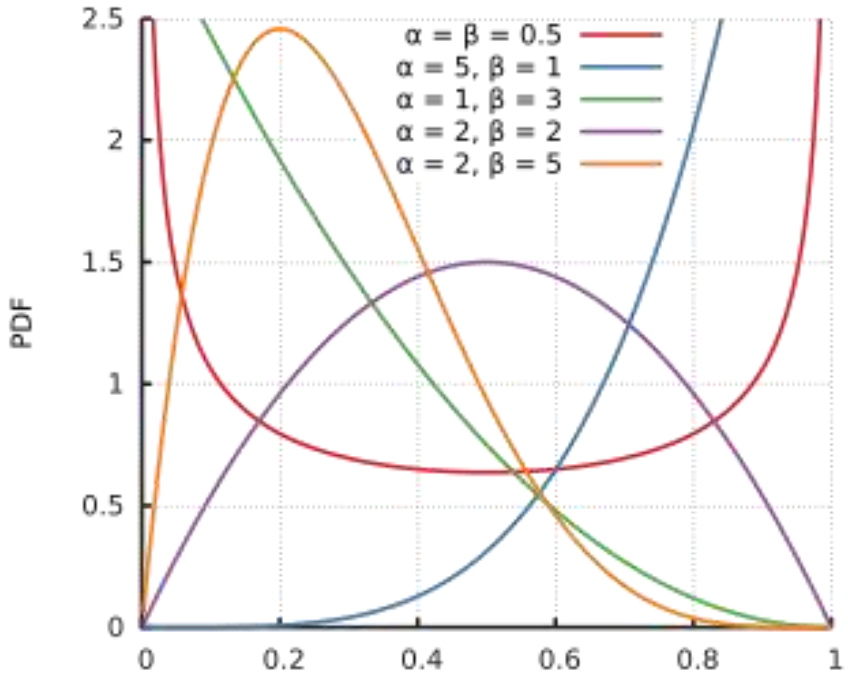
Distributions of Normalized Indicator Data

Distributions communicate not only mean values of indicators, but also uncertainty.

Furthermore, moving from data points to distributions of data allows for the utilization statistical and probabilistic techniques.

Using distance to target normalization, indicator measures will be mapped to values between 0 and 1, where 0 is a baseline value (non-ideal value) and 1 represents a target or (ideal value).

An ideal distribution to describe data that is on the interval between 0 and 1 is the *Beta Distribution.*



Mixture Modeling using Beta Distributions

- Mixture modeling refers to the combination of random variables using weights to generate distributions that fit multi-modal data.
- Beta distributions offer flexible behavior through various parameterization.
- Mixture models and model selection using information criteria provide a framework to pursue *information theoretic aggregation strategies*

Image from: http://en.wikipedia.org/wiki/Beta_distribution

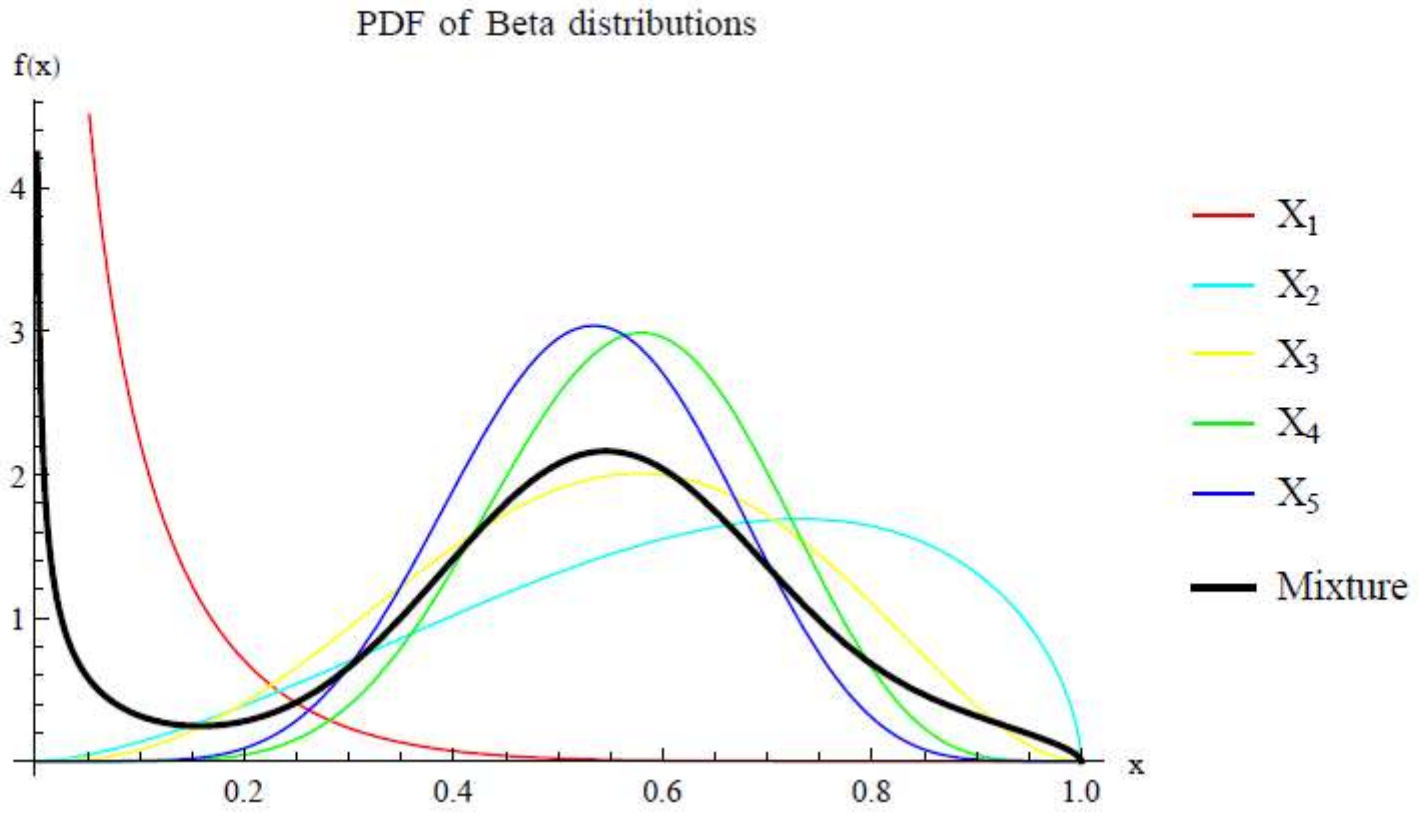
Information Theoretic Approach to Aggregation of Distributions

- How can one aggregate the information from multiple distributions for indicators in such a way that ***reduces complexity*** and ***maintains the most information***
- Various information criteria can be used for model selection
  - Akaike Information Criteria (AIC)
  - Schwarz Bayesian Information Criteria (SBIC or BIC)
- Both of these information criteria balance a maximized likelihood of a distribution given the data and a penalty for overfitting (i.e. introduction of unnecessary parameters and complexity)

Example: Model Selection for Aggregate Probability Distribution

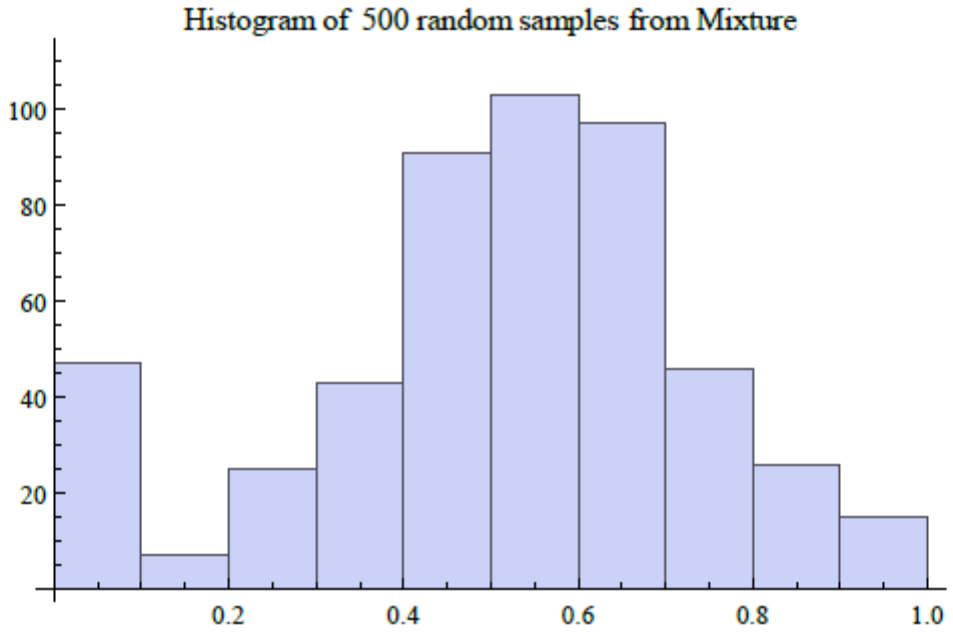
Example: Model Selection for Aggregate Distribution

Figure 1: Probability distribution functions of individual mixture components, $f(X|\theta_i)$, and complete mixture distribution $f(X|\Theta) = \sum_{i=1}^{S} \pi_i f(X|\theta_i)$



Example: Model Selection for Aggregate Distribution

Figure 2: 500 random samples from complete mixture distribution $f(X|\Theta) = \sum_{i=1}^{S} \pi_i f(X|\theta_i)$



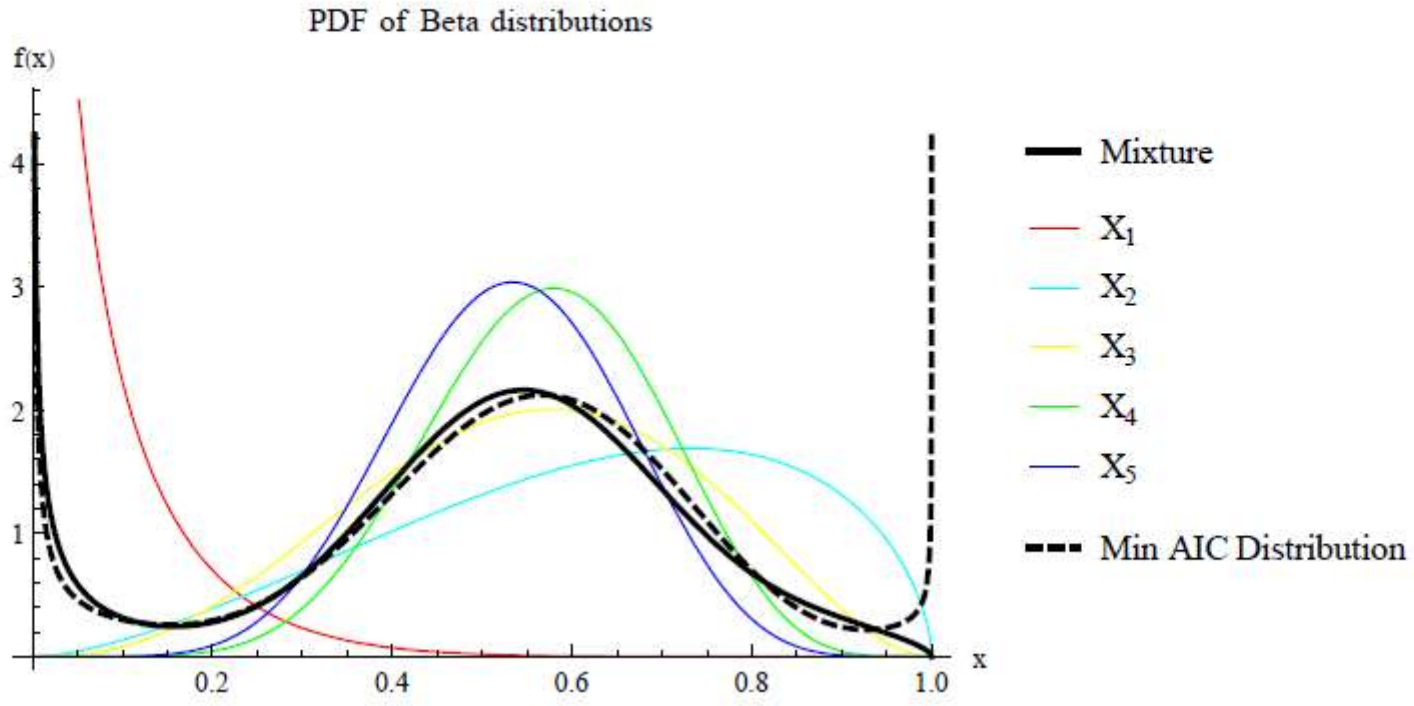
Example: Model Selection for Aggregate Distribution

Table 2: Results of Model Selection using EM algorithm and AIC and SBIC scoring

Model	Resulting Best Fit Distribution	AIC	SBIC
True	$0.1235 * Beta(0.4578, 7.6471) + 0.1777 * Beta(2.6379, 1.6001)$ $+ 0.1956 * Beta(3.6942, 2.9778) + 0.0439 * Beta(8.0519, 6.1129)$ $+ 0.4593 * Beta(7.8943, 7.0184)$	-265.587	-202.367
5	$0.1190 * Beta(0.2936, 4.1697) + 0.1862 * Beta(12.4762, 10.0026)$ $+ 0.0290 * Beta(22.2633, 13.0948) + 0.5067 * Beta(5.3001, 4.9414)$ $+ 0.1593 * Beta(4.1007, 1.4631)$	-270.52	-207.301
4	$0.3583 * Beta(10.4648, 8.323) + 0.2571 * Beta(5.4156, 5.4778)$ $+ 0.2071 * Beta(3.5420, 1.7887) + 0.1774 * Beta(0.2400, 0.7294)$	-275.782	-225.207
3	$0.1950 * Beta(0.2757, 0.7540) + 0.1040 * Beta(6.8493, 2.0416)$ $+ 0.7010 * Beta(7.1216, 6.1327)$	-281.716	-243.784
2	$0.7588 * Beta(6.2147, 4.9760) + 0.2412 * Beta(0.3163, 0.5550)$	-283.587	-258.299

Example: Model Selection for Aggregate Distribution

Figure 6: Comparison of PDF for *true* Beta components and Beta mixture distribution with 2-component, minimum information mixture model, selected through EM algorithm



Summary: Issues and Solutions

Issues

Correct and Incorrect aggregation functions don't exist

- Tradeoffs
- Appropriate aggregation function choice depends on implementation and **data**

Solutions

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- Utilize theoretical results to understand when inconsistency can arise and anticipate issues

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- Explicit weighting of indicators before aggregation introduces bias
- Normalization weights indicators implicitly before aggregation

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Normalization and Weighting

- Bias cannot be avoided, pin normalized values and weights to targets and baselines
- Quantify implicit weights and impact of implicit weights on aggregate outputs.

Future Research Directions

- Aggregation can take place over space and/or time, which may lead to different aggregation strategies
  - ex. Does the assessment compare multiple sites for the same period of time or does it compare a site to itself over some time period?
- Upon development of aggregation strategy, create complementary statistical methods for the assessment of data variability and uncertainty
  - Preliminary work to quantify uncertainty utilizing the geometric mean as the aggregation function has yielded positive results
- Sensitivity testing and analysis of assessment results
  - Issues of comparability arise often in assessment of multiple sites
- Develop visualization and communication tool utilizing assessment protocols

Thank you.

INTERESTED?

Check in for results at the

Center for bioenergy sustainability:

http://web.ornl.gov/sci/ees/cbes/

Email:

npollesc@utk.edu

RESOURCES

Ebert, U. and Welsch, H. (2004). Meaningful environmental indices: A social choice approach. *J. Environmental Econ. Manage.,* 47(2): 270-283

Dale, V.H., Efroymson, R.A., Kline, K.L., Langholtz, M.H., Leiby, P.N., Oldosu, G.A., Davis, M.R., Downing, M.E., and Hilliard, M.R., (2013). Indicators for assessing socioeconomic sustainability of bioenergy systems: a short list of practical measures. *Ecological Indicators,* 26: 87-102.

Grabisch, M., Marichal, J-L., Mesiar, R., and Pap, E. (2009). *Aggregation Functions.* Cambridge University Press, New York, 1 edition.

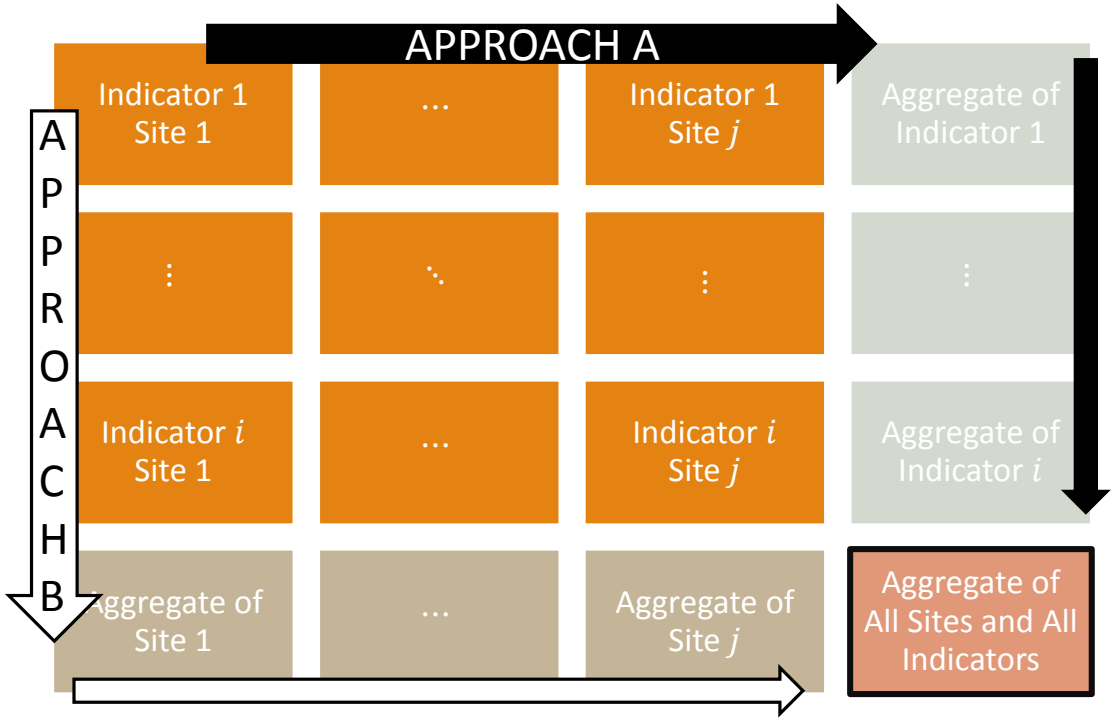
McBride, A.C., Dale, V.H., Baskaran, L.M., Downing, M.E., Eaton, L.M., Efroymson, R.A., Garten, C.T., Kline, K.L., Jager, H.I., Mulholland, P.J., Parish, E.S., Schweizer, P.E., and Storey, J.M. (2011). Indicators to support environmental sustainability of bioenergy systems. *Ecological Indicators,* 11(5):1277-1289.

Additional slides if time allows

Multiple site-multiple indicator assessment

Consistency of aggregate output where assessments treat multiple sites and with multiple indicators is related to the properties of **bisymmetry and strong bi-symmetry**

- *Example: Bisymmetry ensures that aggregating rows and then columns of data, is equivalent to aggregating columns and then rows. Thus approach A and approach B yield the same total aggregate value for all sites and all indicators. (see diagram on right)*



Multiple site-multiple indicator assessment: Strong Bisymmetry

$F{:}\cup_{n\in\mathbb{N}} \mathbb{I}^n \to \mathbb{I}$ is *strongly bisymmetric* if $F(x) = x \ \forall\, x \in \mathbb{I}$ and if for any $n, p \in \mathbb{N}$ we have

$$F\left(F(x_{11}, \dots, x_{1n}), \dots, F\left(x_{p1}, \dots, x_{pn}\right)\right) = F(F\left(x_{11}, \dots, x_{p1}\right), \dots, F\left(x_{1n}, \dots, x_{pn}\right))$$

for all $p \times n$ matrices

$$\begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{p1} & \cdots & x_{pn} \end{pmatrix} \in \mathbb{I}^{p\times n}$$

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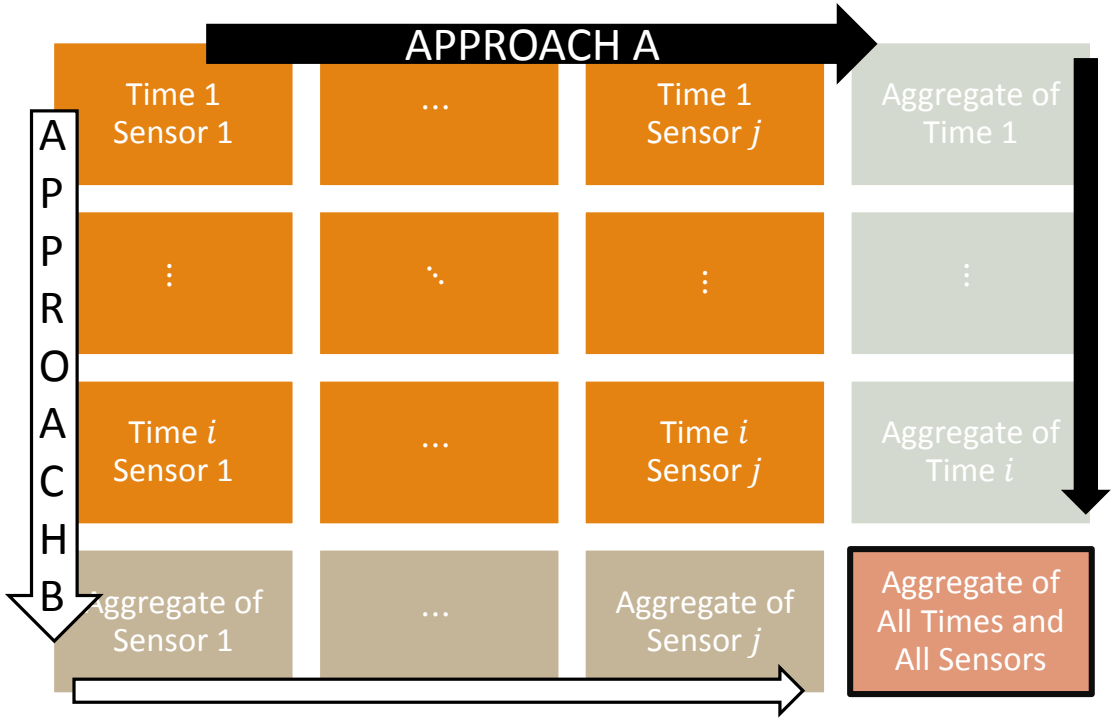

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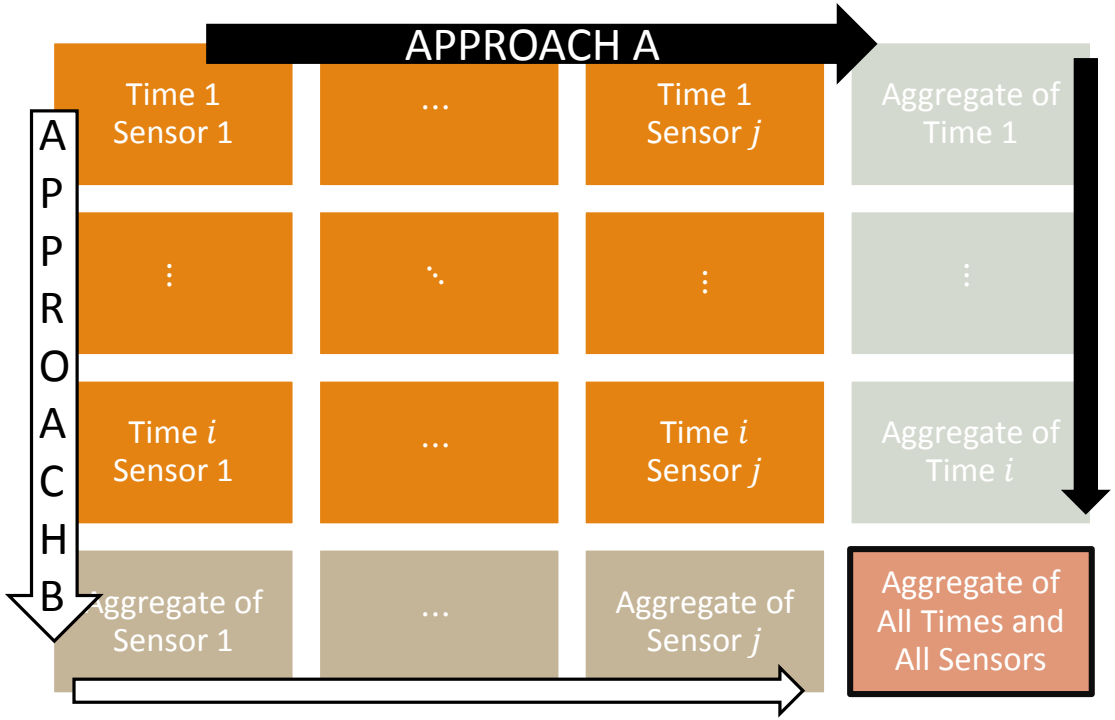
- *Fortunately, many common aggregation functions have the property of bisymmetry.*
  - *Ex. Arithmetic and Geometric means, Min, Max, Product, Sum*