Max-Planck-Institut für Bildungsforschung

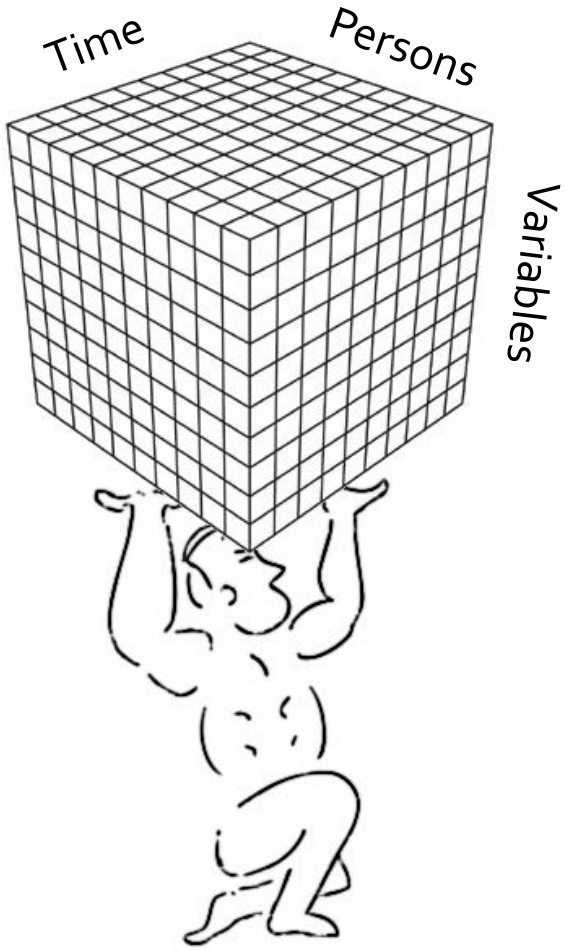
50 Years of Research on Human Development

Center for Lifespan Psychology

The best of both worlds: Towards a synthesis of theory-based and data-driven modeling

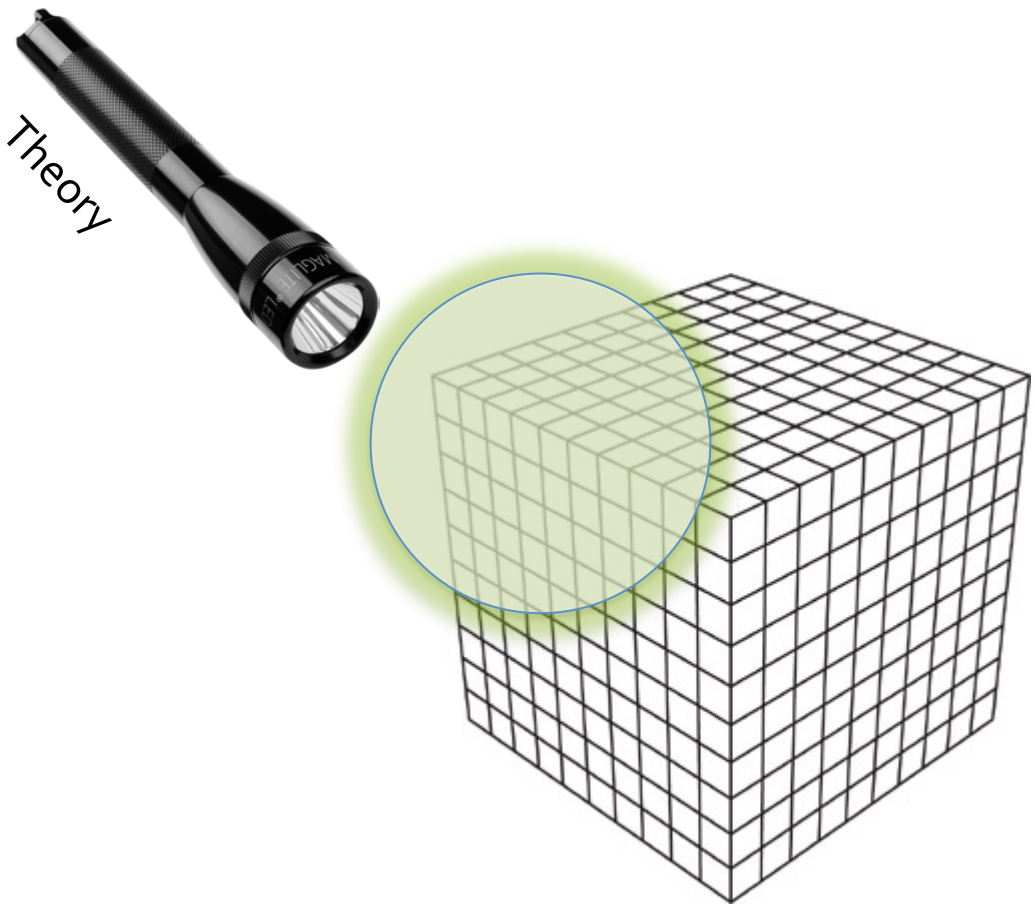
Andreas Brandmaier

Big Data: Volume, Velocity, Variety

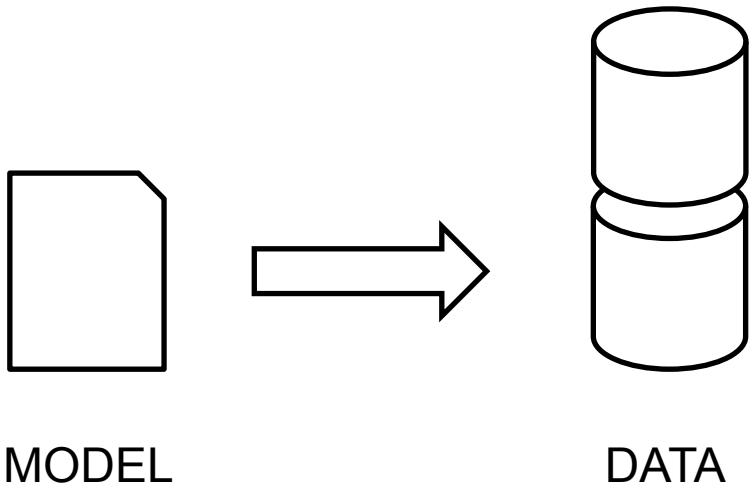


Cattell's
Big Data Cube

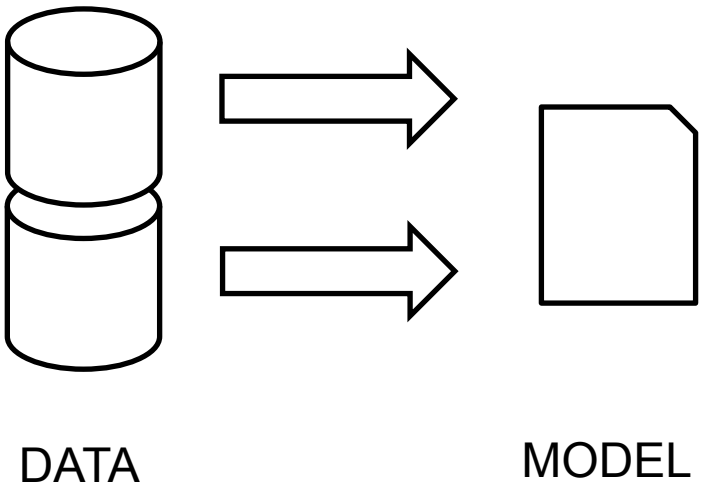
Big Data: Surprise



Theory-Based Modeling



Data-Driven Modeling



Two Cultures

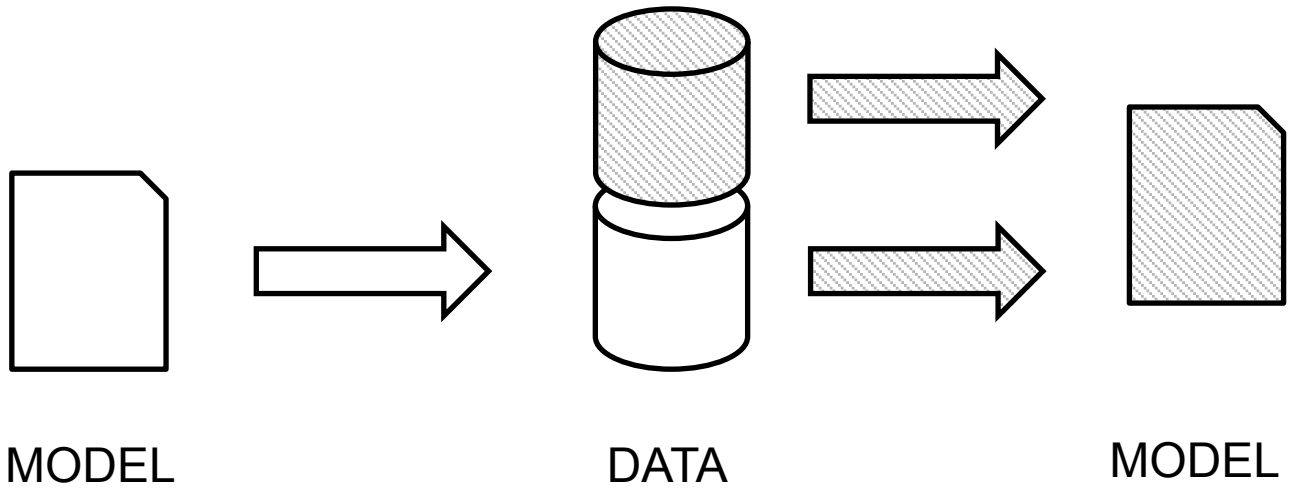
There are two cultures in the use of statistical modelling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown.

[...]

If our goal as a field is to use data to solve problems, then we need to move away from exclusive dependence on data models and adopt a more diverse set of tools.

-- Breiman, 2001

The Best of Both Worlds? Theory-Guided Exploration

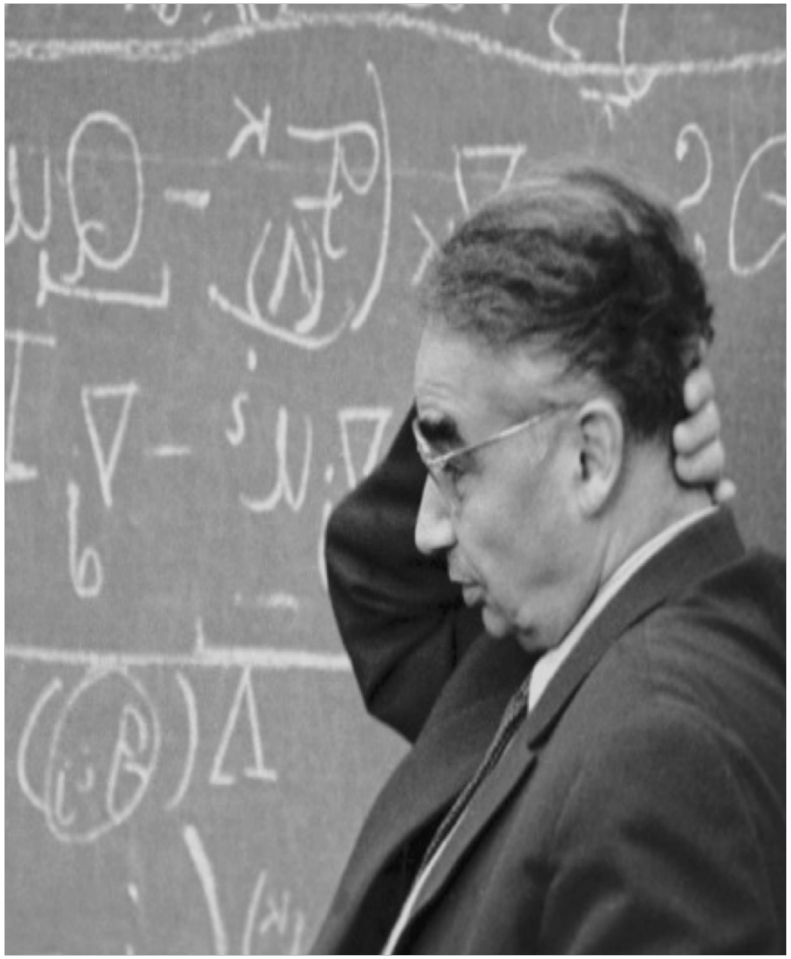


Can we use machine-learning-inspired approaches to modify our initial theory? Would ML allow us to select among variables those who are most "important"?

Typical Questions Asked

Given a theory/model:

- "How can we best explain the heterogeneity/ uncertainty in our data?"
- "What subset of variables is most predictive about my outcome(s)?"

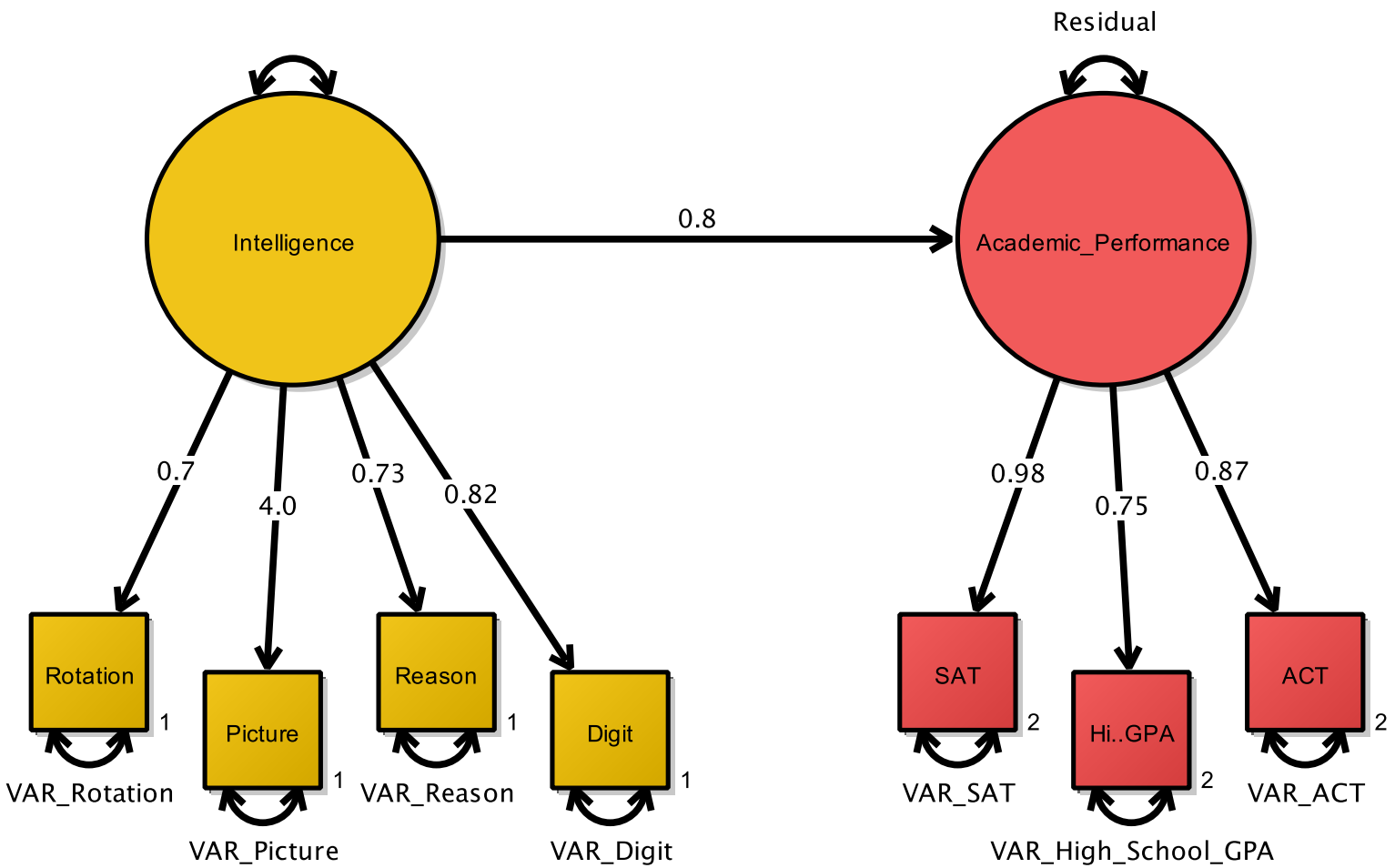


THEORY-DRIVEN MODELING

Structural Equation Modeling

- Express relationships among observed and latent variables
- Encompass a variety of linear models:
  - t Test
  - Regression
  - (repeated measures) ANOVA
  - Mixed-effect models
  - Mediation models
  - Multilevel models

SEM = Measurement + Structure

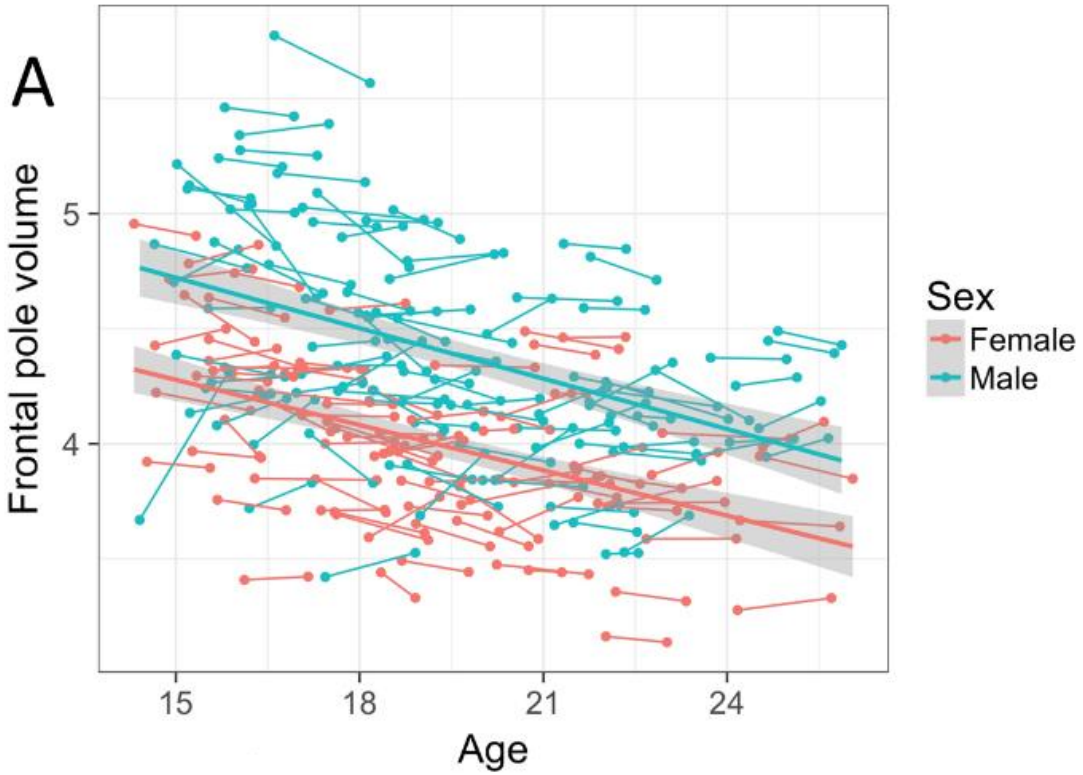


What can SEM do for you? (the practical description)

- A universal language to formalize your natural language hypotheses
- Moving your hypotheses from an item to a construct level
- A framework to specify and also test models of your hypotheses (model comparison)
- A one-to-one mapping between formal languages of SEM (matrix algebra, sets of equations, computer programs) to diagrams

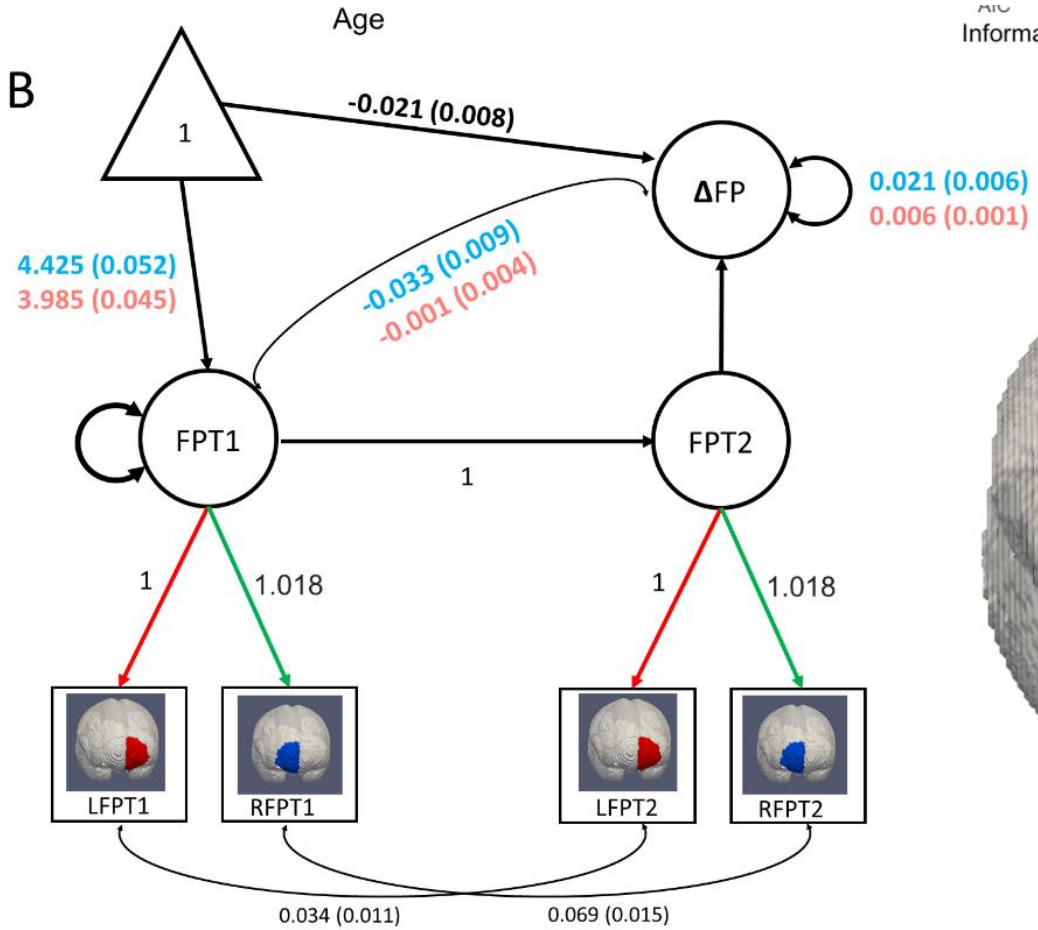
Example: Frontal Lobe Thinning

- Neuroscience in Psychiatry Network Data
- 176 participants
- Mean age = 18.84, range 14.3-24.9
- Outcome: Frontal pole volume
- Q: Are there sex differences in cortical development?



Kievit et al.,Dev Cog Neuro, 2018

Example: Frontal Lobe Thinning



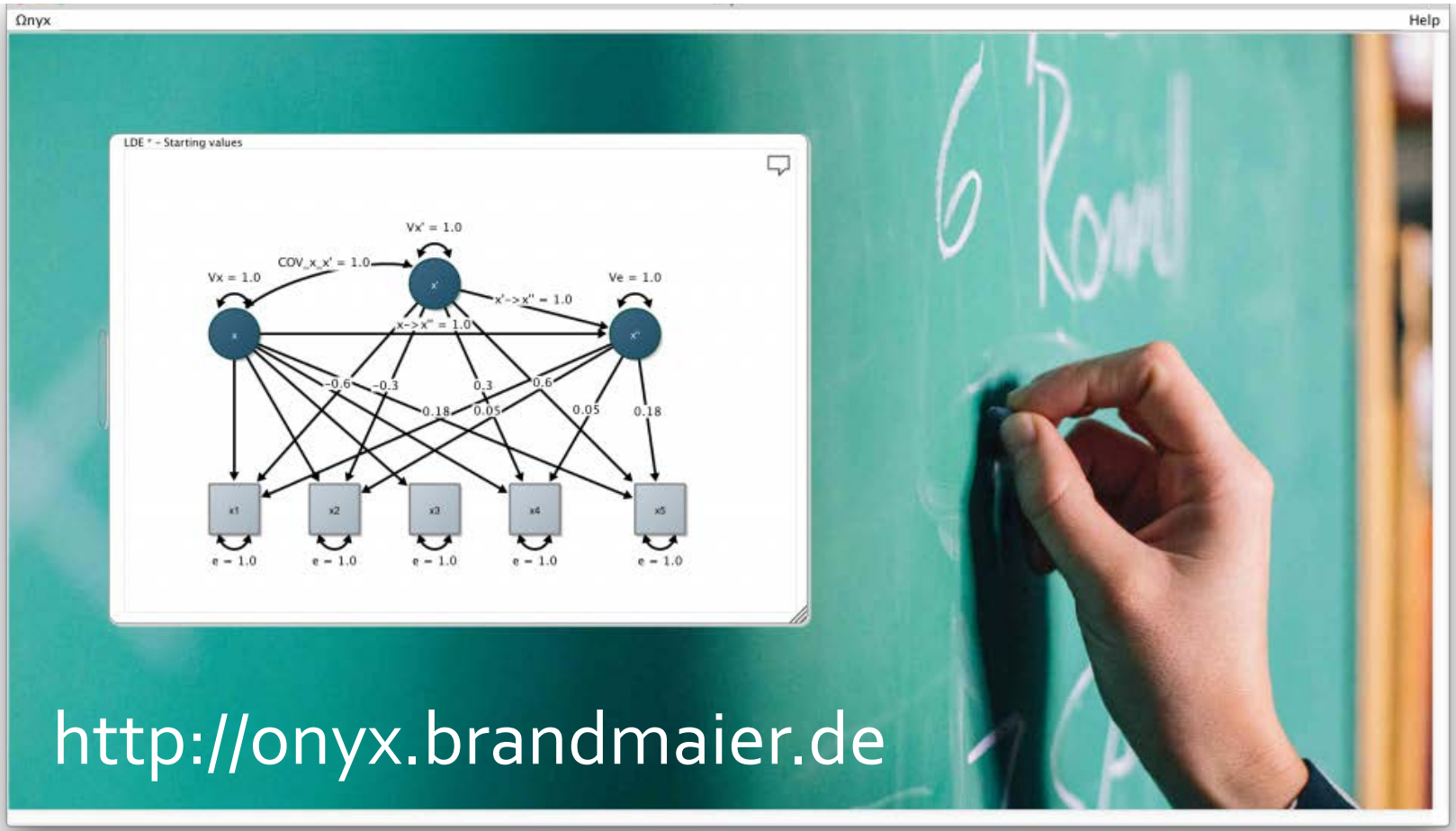
McArdle & Hamagami 2001,Kievit et al.,Dev Cog Neuro, 2018

Surprise in Theory-Based Modeling

- Likelihood of data given model = surprise under data from the true distribution („cross-entropy“)
- A well-fitting data set is not surprising (most published results are not surprising in an information-theoretic sense)
- In theory-based modeling, we hope for low surprise!

Kievit et al.,Dev Cog Neuro, 2018

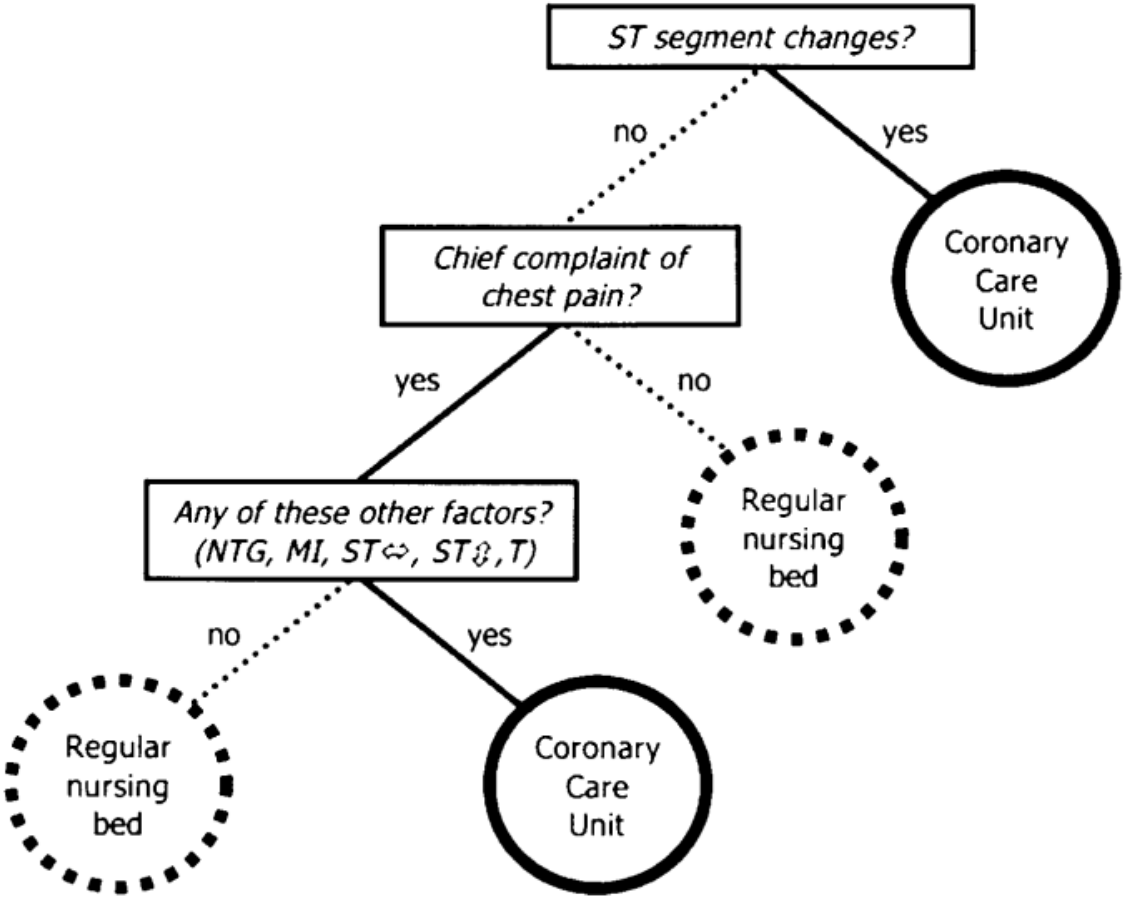
Commercial Break: Ωnyx



Von Oertzen, Brandmaier, & Tsang, 2013

DATA-DRIVEN MODELING

The Decision Tree



Gigerenzer & Kurzenhäuser 2005, Green & Mehr 1997

Example: Should I go to this conference?

Food quality	Scient. quality	Fees	Mood
low	high	high	happy
high	low	low	happy
high	high	high	happy
low	low	high	sad
high	low	high	happy
high	high	low	happy
low	low	low	sad
high	low	high	happy

Total Entropy=0.56

Big Data in Ψ 2018

Example: Should I go to this conference?

Food quality	Scient. quality	Fees	Mood
low	high	high	happy
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high	low	high	happy
high	high	low	happy
low	low	low	sad
high	low	high	happy

Fees

Total Entropy=0.56

Entropy | high fees =0.50

Entropy | low fees =0.64

Entropy | fees=**0.55**

Example: Should I go to this conference?

Food quality	Scient. quality	Fees	Mood
low	high	high	happy
high	low	low	happy
high	high	high	happy
low	low	high	sad
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high	high	low	happy
low	low	low	sad
high	low	high	happy

Food

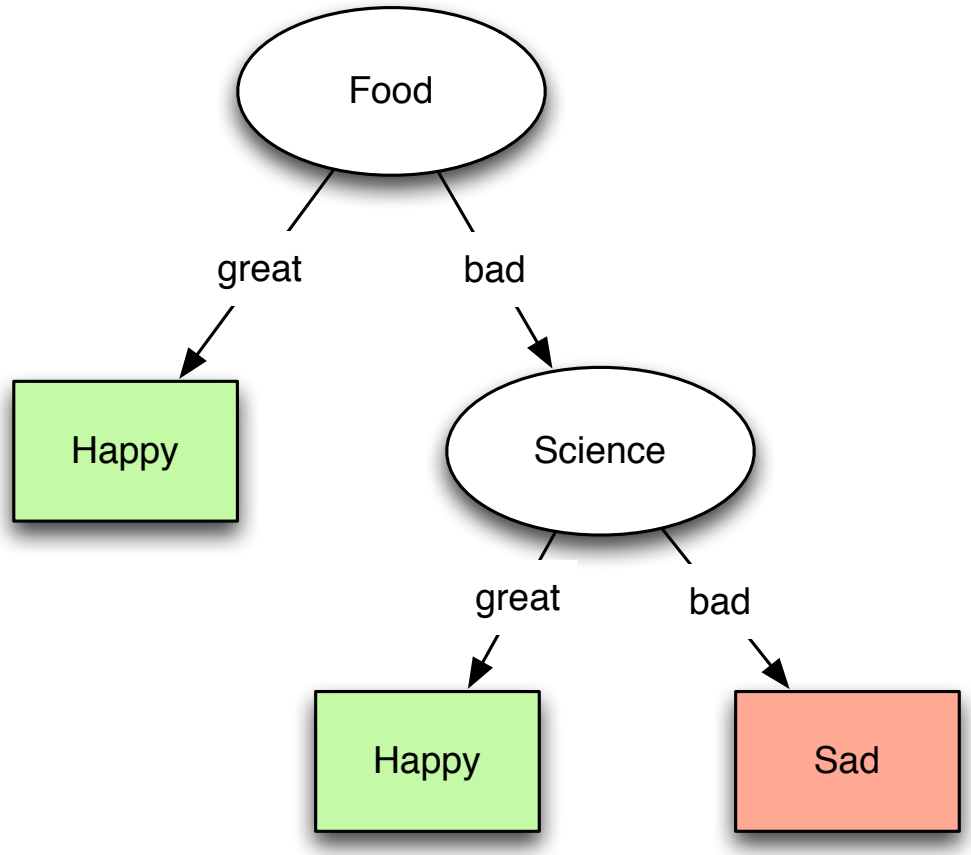
Entropy=0.56

Entropy | nice food=0

Entropy | bad food=0.64

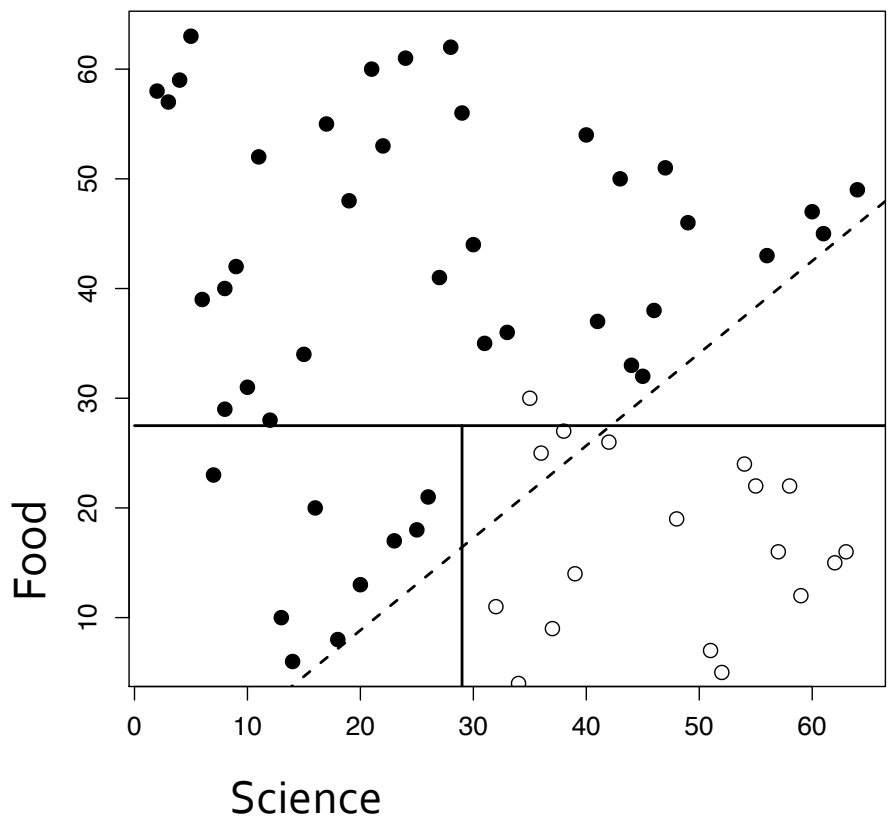
Entropy | food=**0.24**

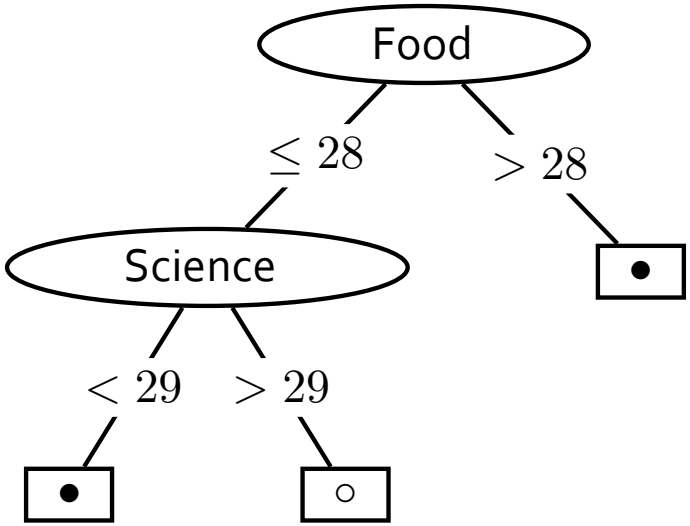
Decision Tree



A Geometric Perspective (Toy Example)

Prediction of Happiness





Adapted from Brandmaier et al., book chapter, 2013

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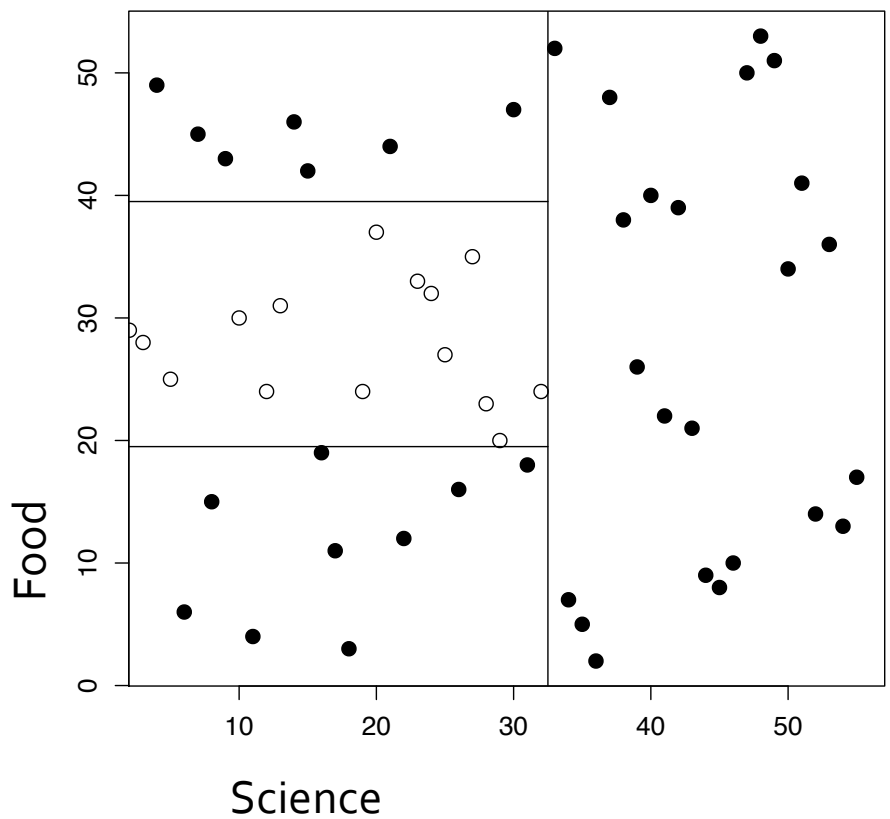
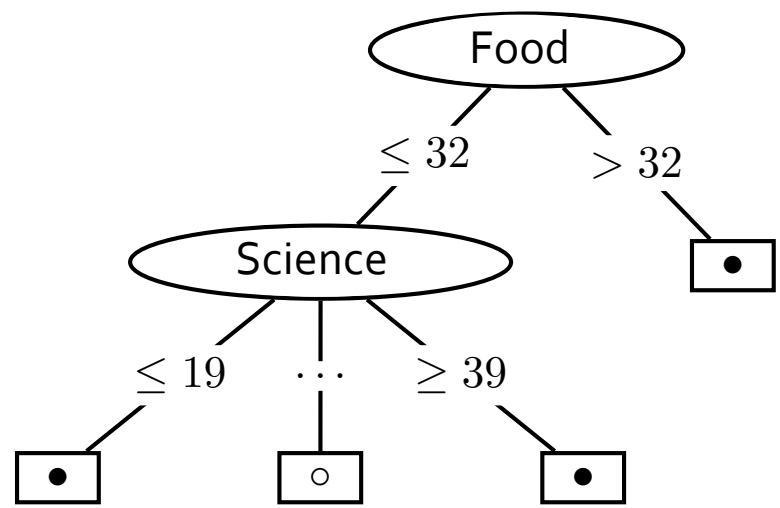




Adapted from Brandmaier et al., book chapter, 2013

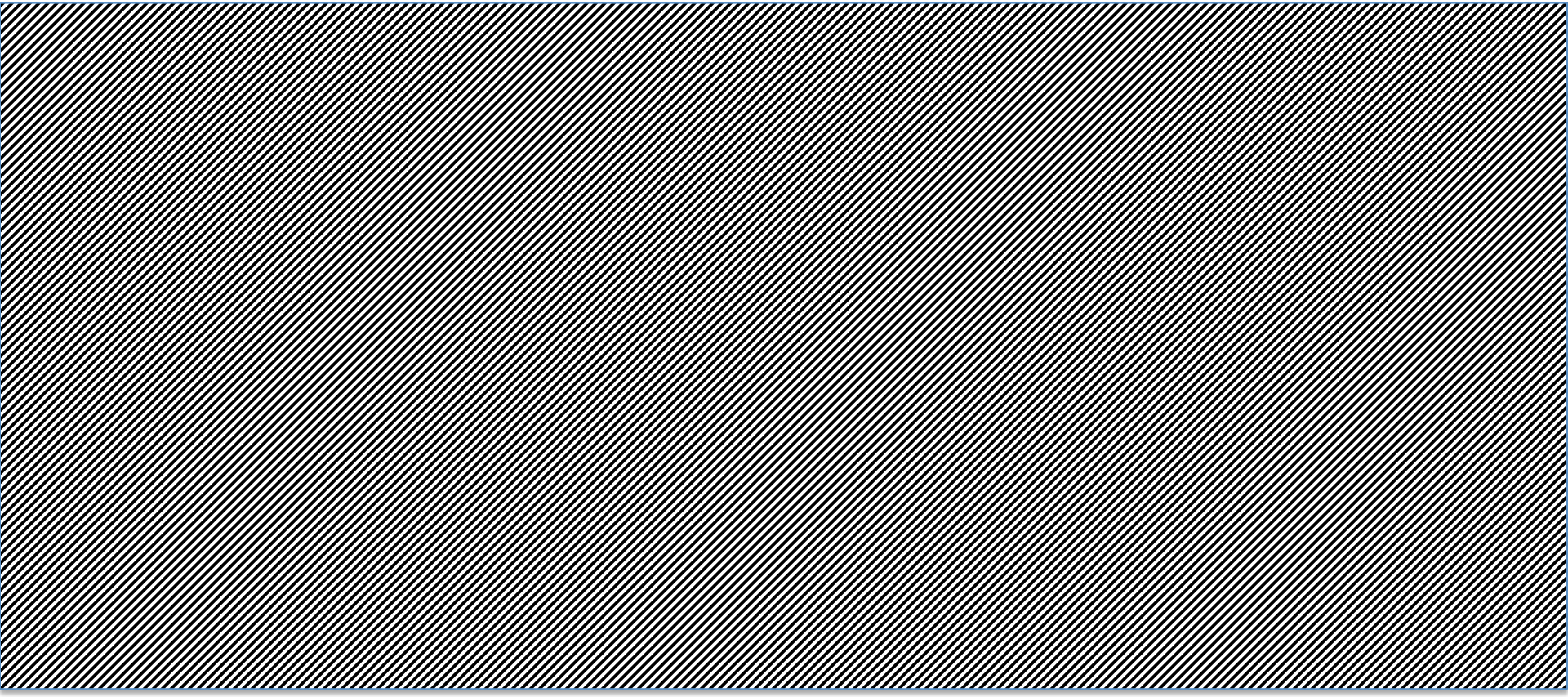
Interim Summary: Decision Trees

- **Reduce surprise** (by maximizing information gain)
- Using a greedy **heuristic**
- No distributional assumptions
- **Straightforward to understand** (equivalent to IF-THEN rules)
- Complexity depends on the data
- Uncover **non-linear** influences of predictors
- **Invariant to scaling** of predictors
- Detection of **complex interactions**

Why Predictive Modeling?

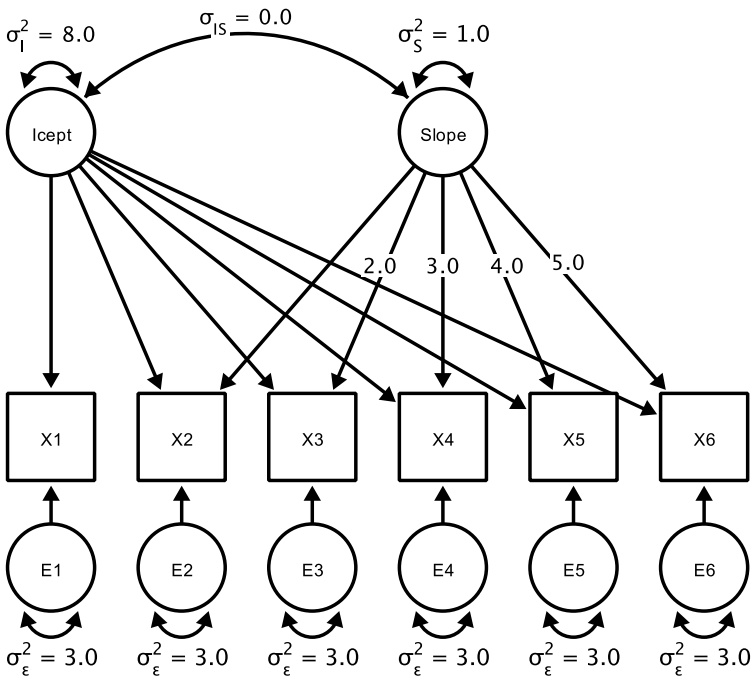
1) Uncover **surprising** causal/correlational associations and lead to the **generation of new hypotheses**.
2) Predictive models may serve as a **reference point** to existing explanatory models.
3) Predictive modeling can **suggest improvements** to existing explanatory models.

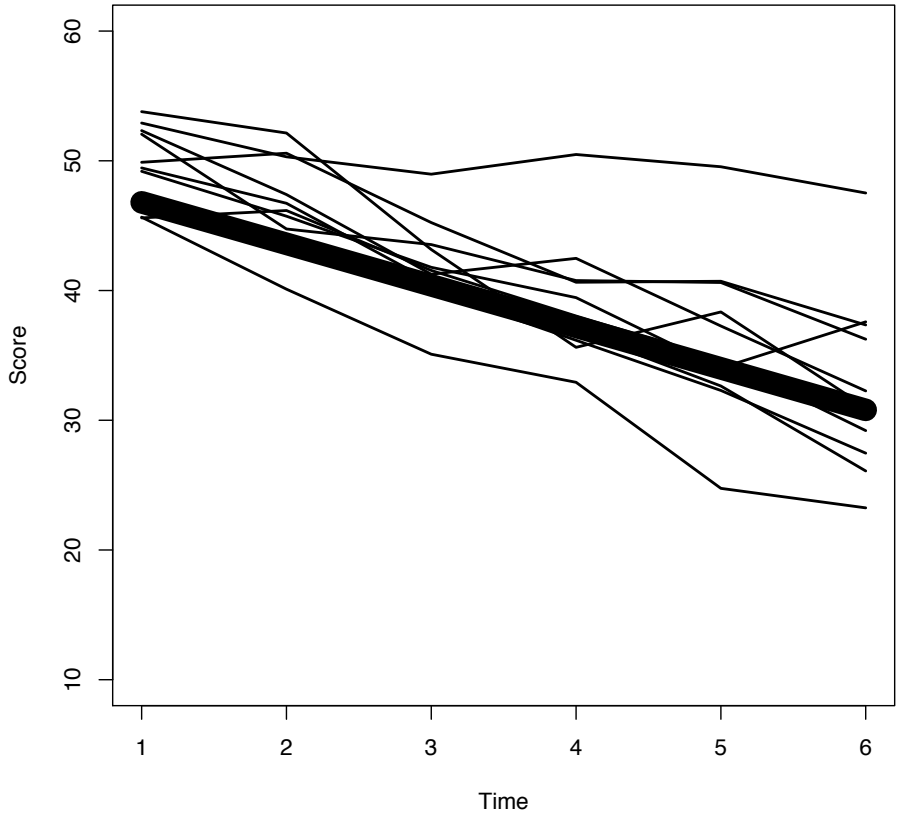
What if…



..we combined SEM and decision trees?

A Simple Example: Wechsler Intelligence Scale for Children





Brandmaier et al., Psychol Methods, 2013

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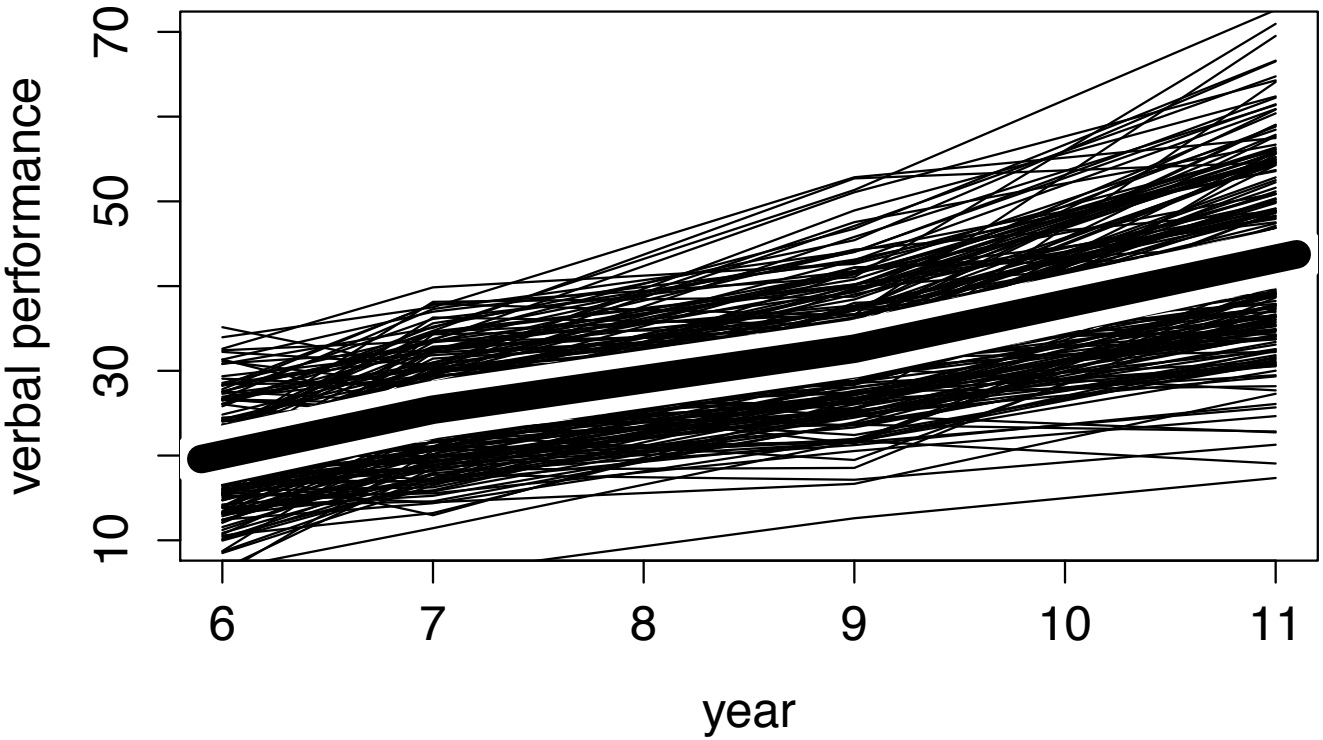
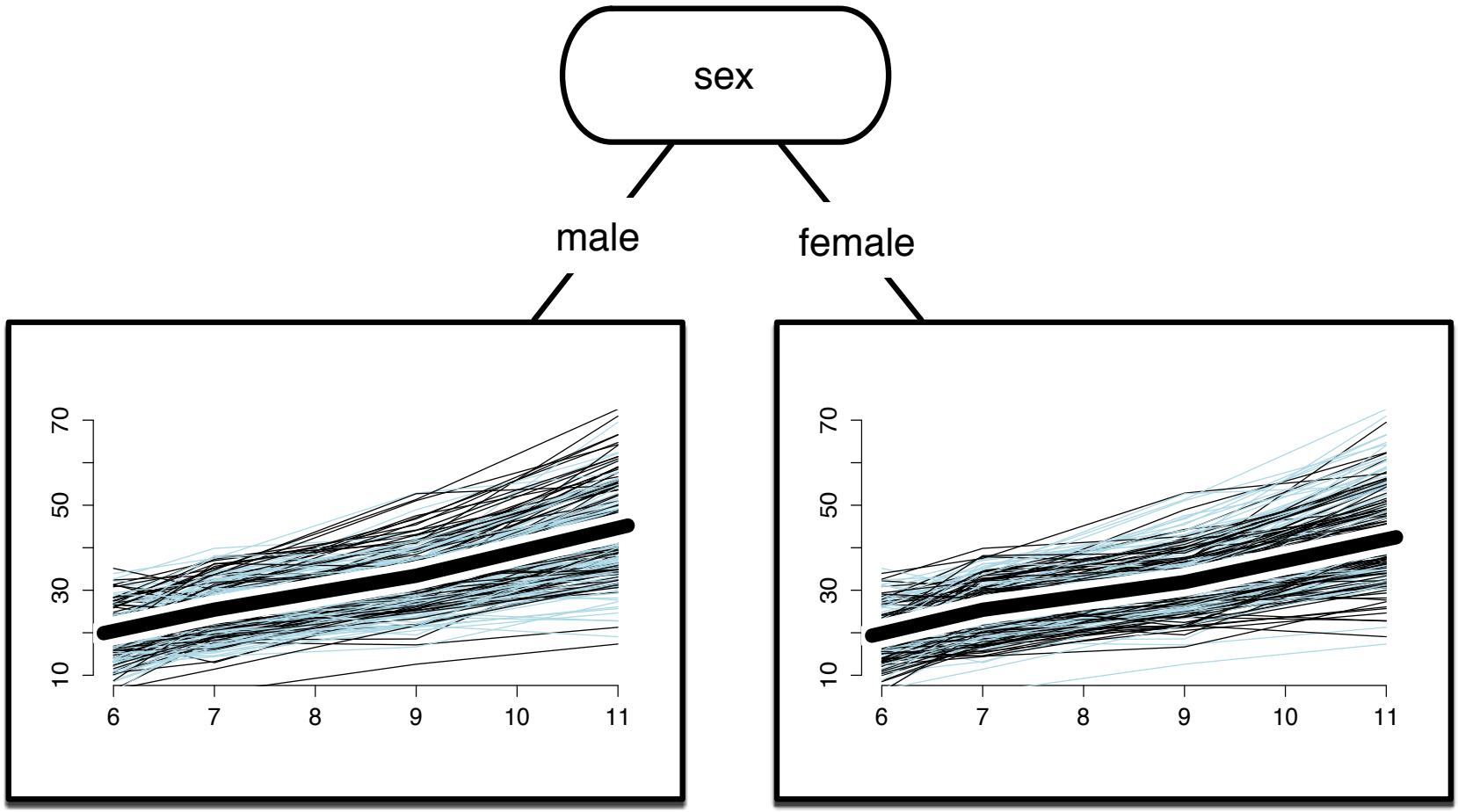


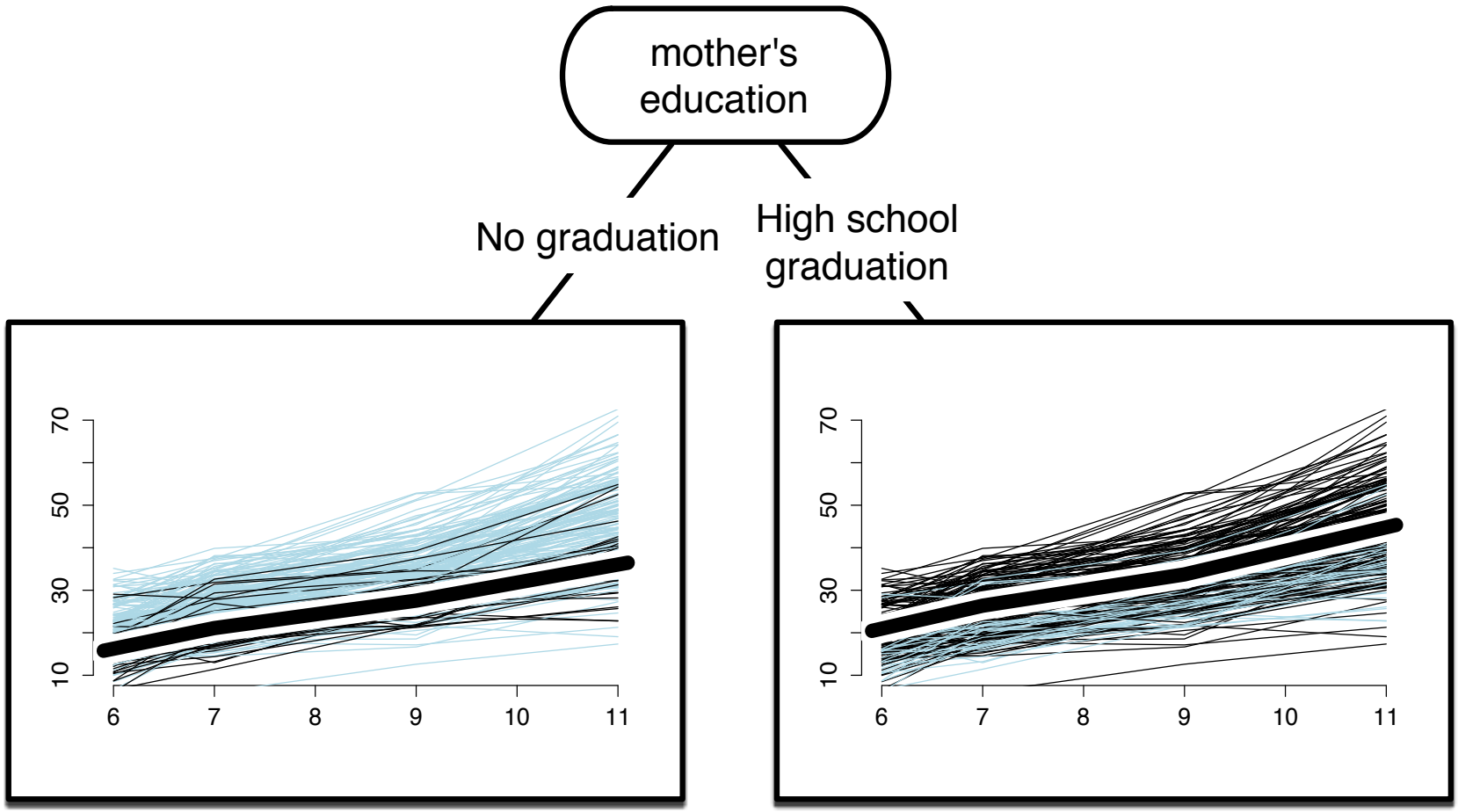
Brandmaier et al., Psychol Methods, 2013

Split Candidate: Sex



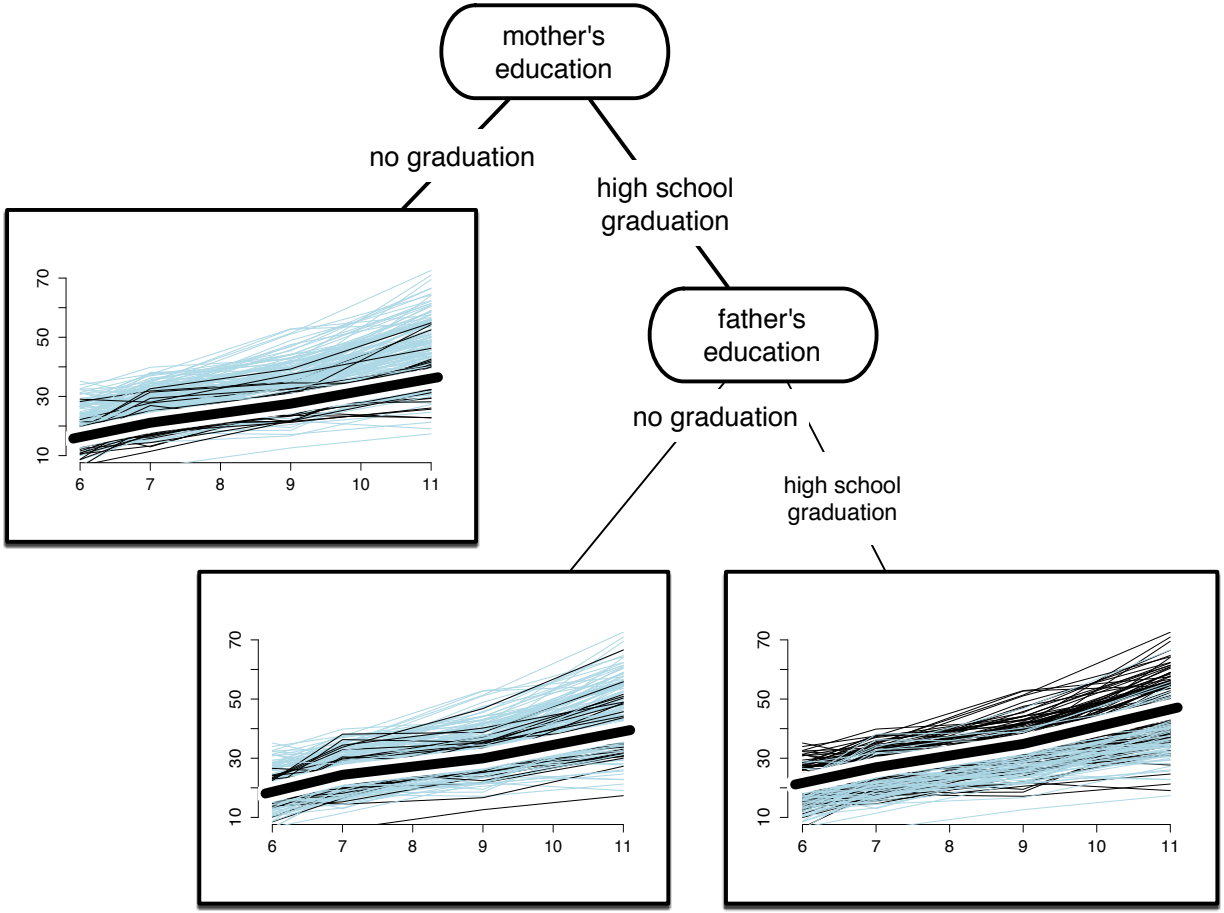
Brandmaier et al., Psychol Methods, 2013

Split Candidate: Mother's Education



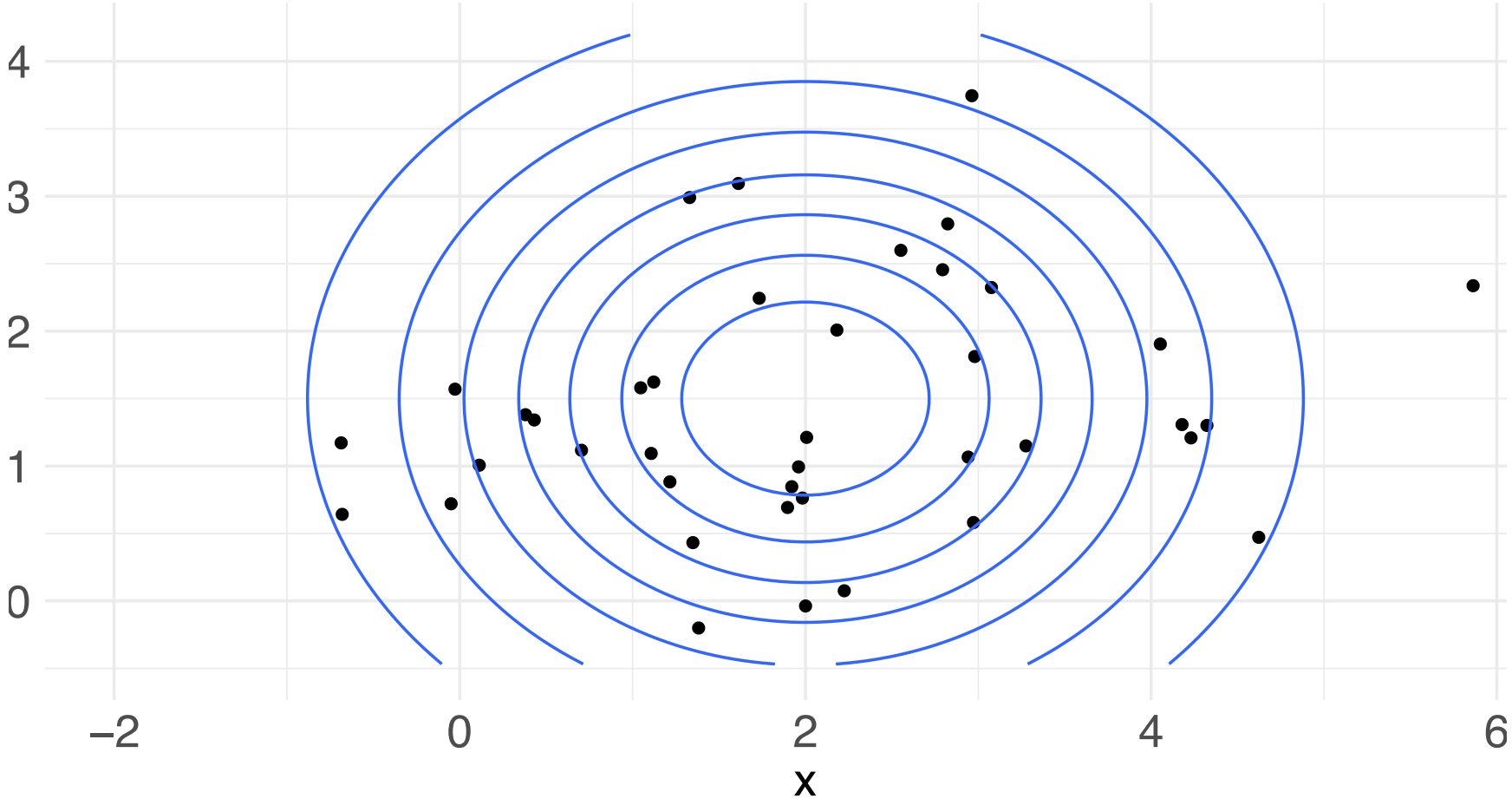
Brandmaier et al., Psychol Methods, 2013

Two-Level Tree



Brandmaier et al., Psychol Methods, 2013

A Probabilistic Perspective



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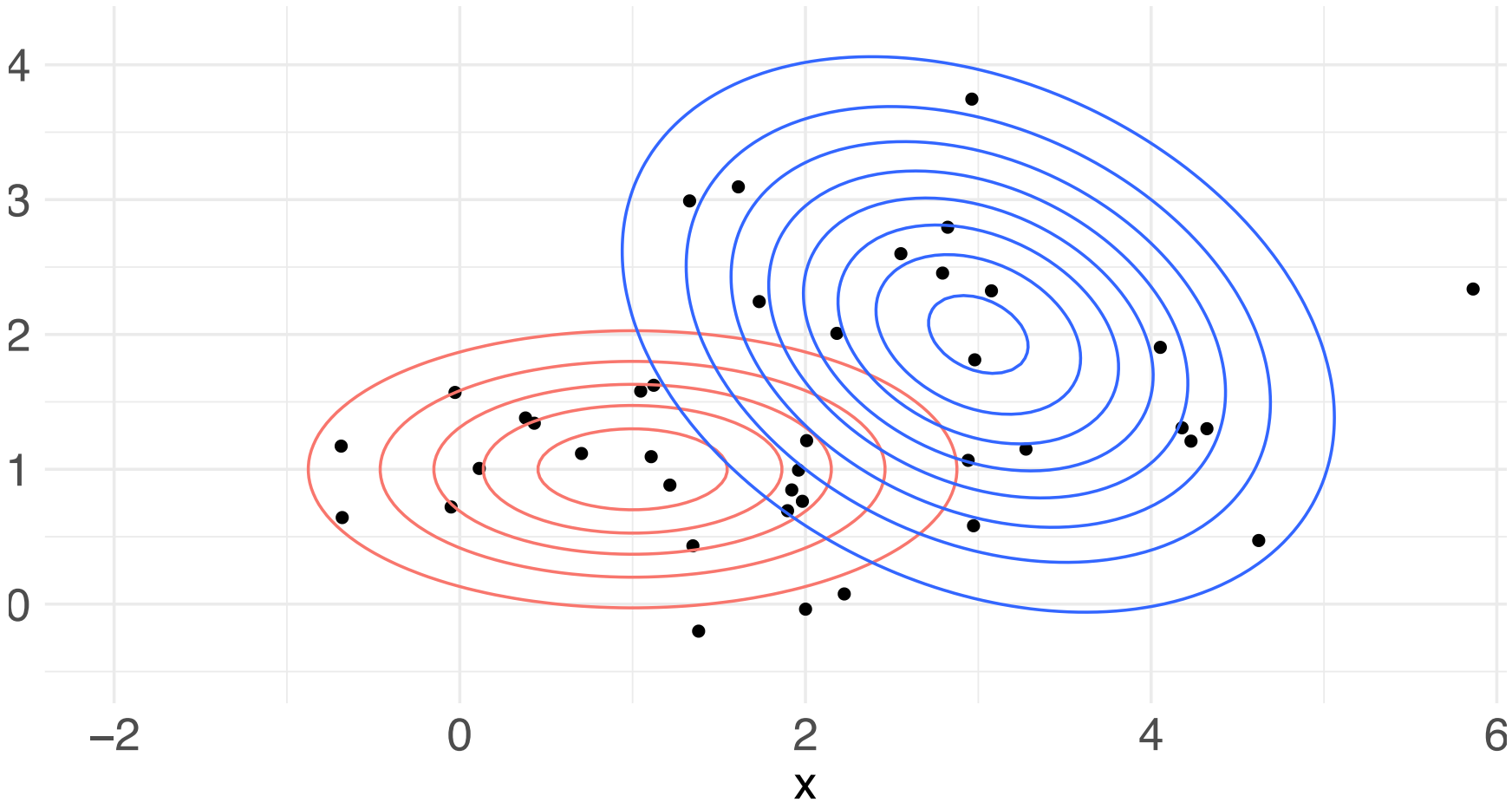
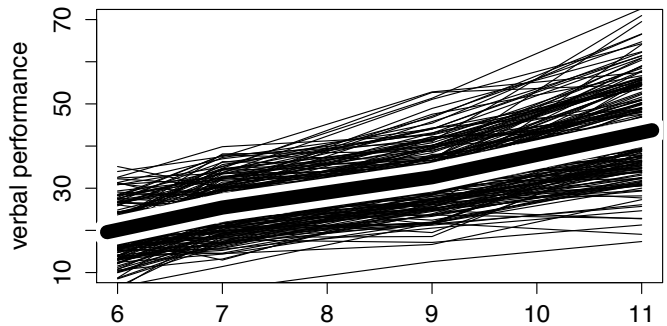
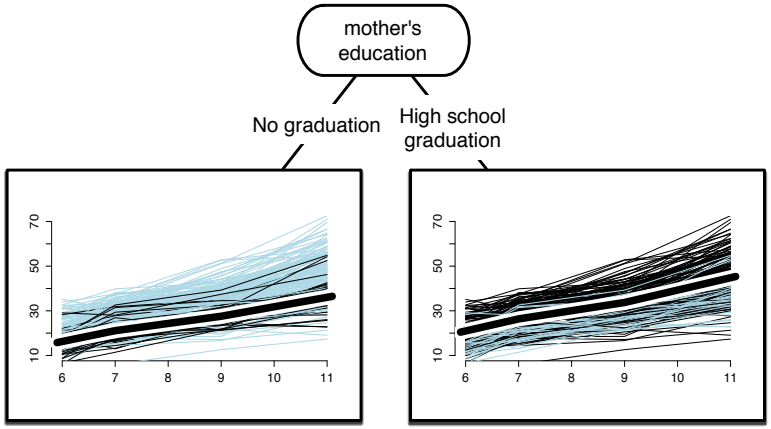
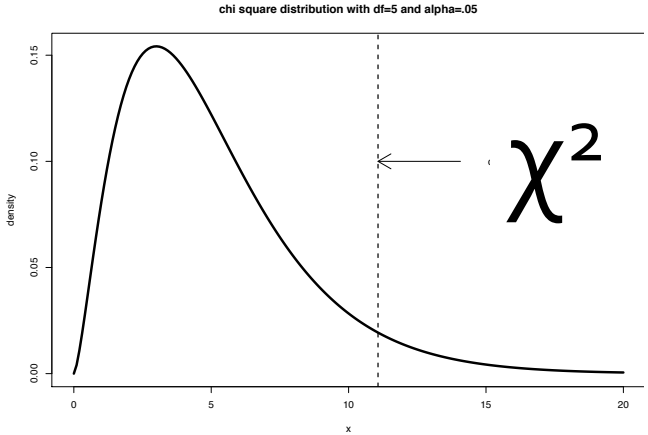


Likelihood Ratio Splitting = Surprise Minimization



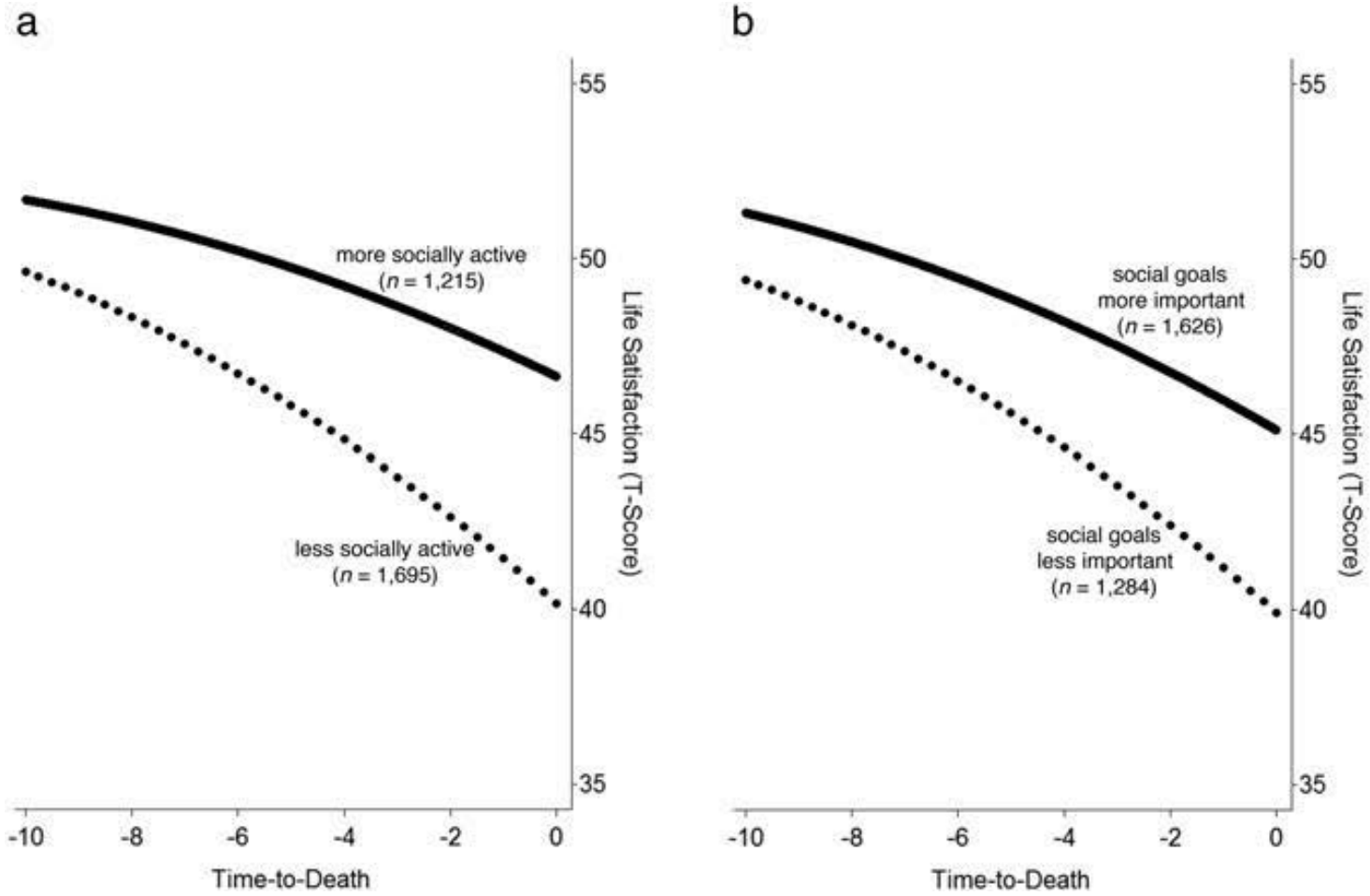


Ho: "Split is uninformative. Information gain is zero"



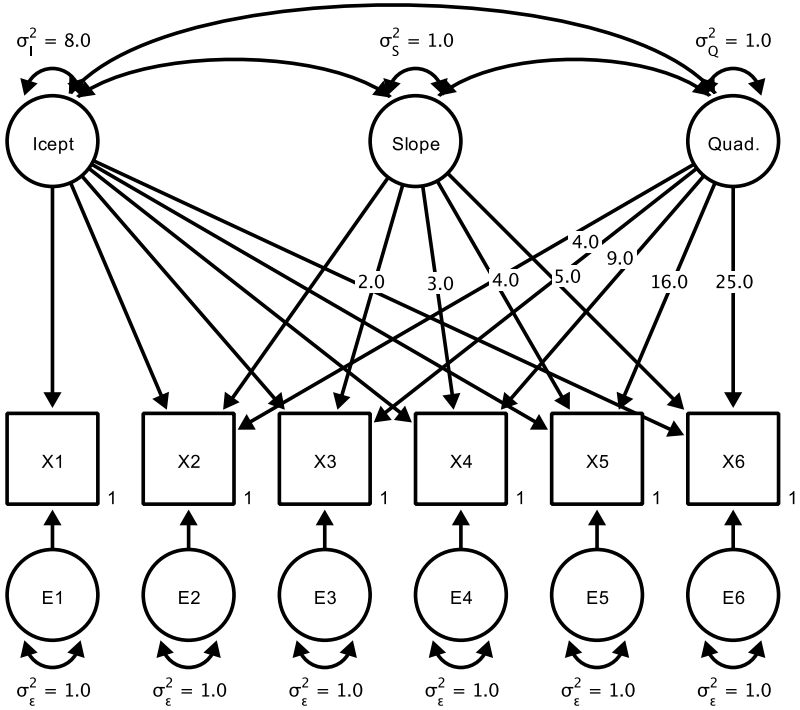
TERMINAL DECLINE IN WELL-BEING

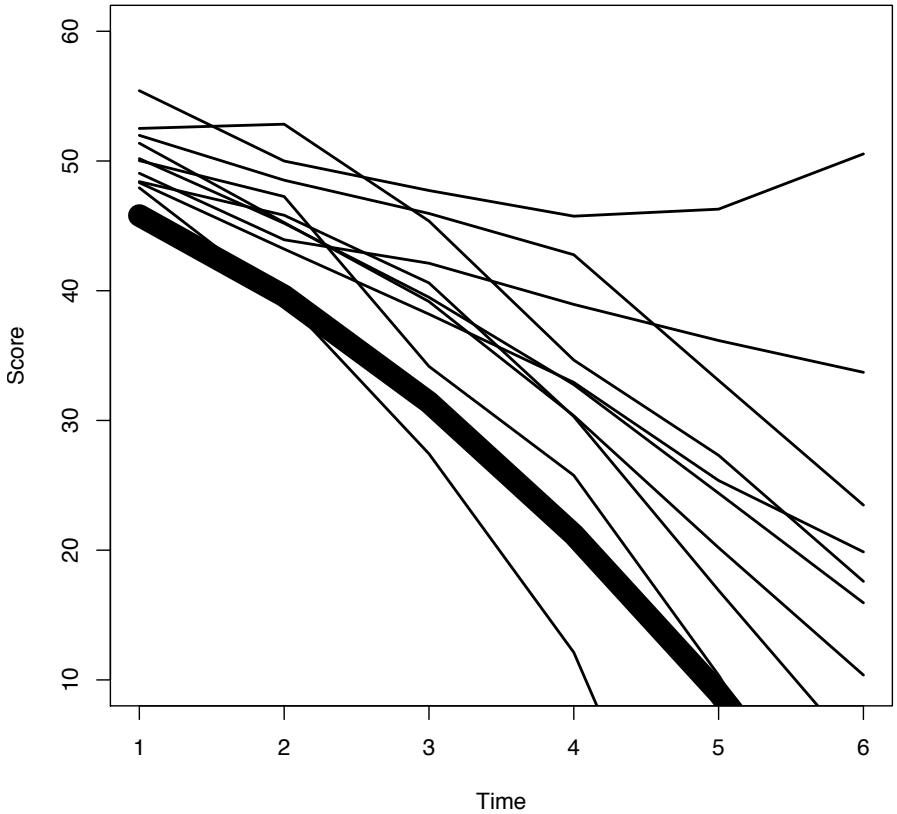
Terminal Decline in Well-Being



Gerstorf et al., Psychol Aging, 2016

Quadratic Growth Curve Models

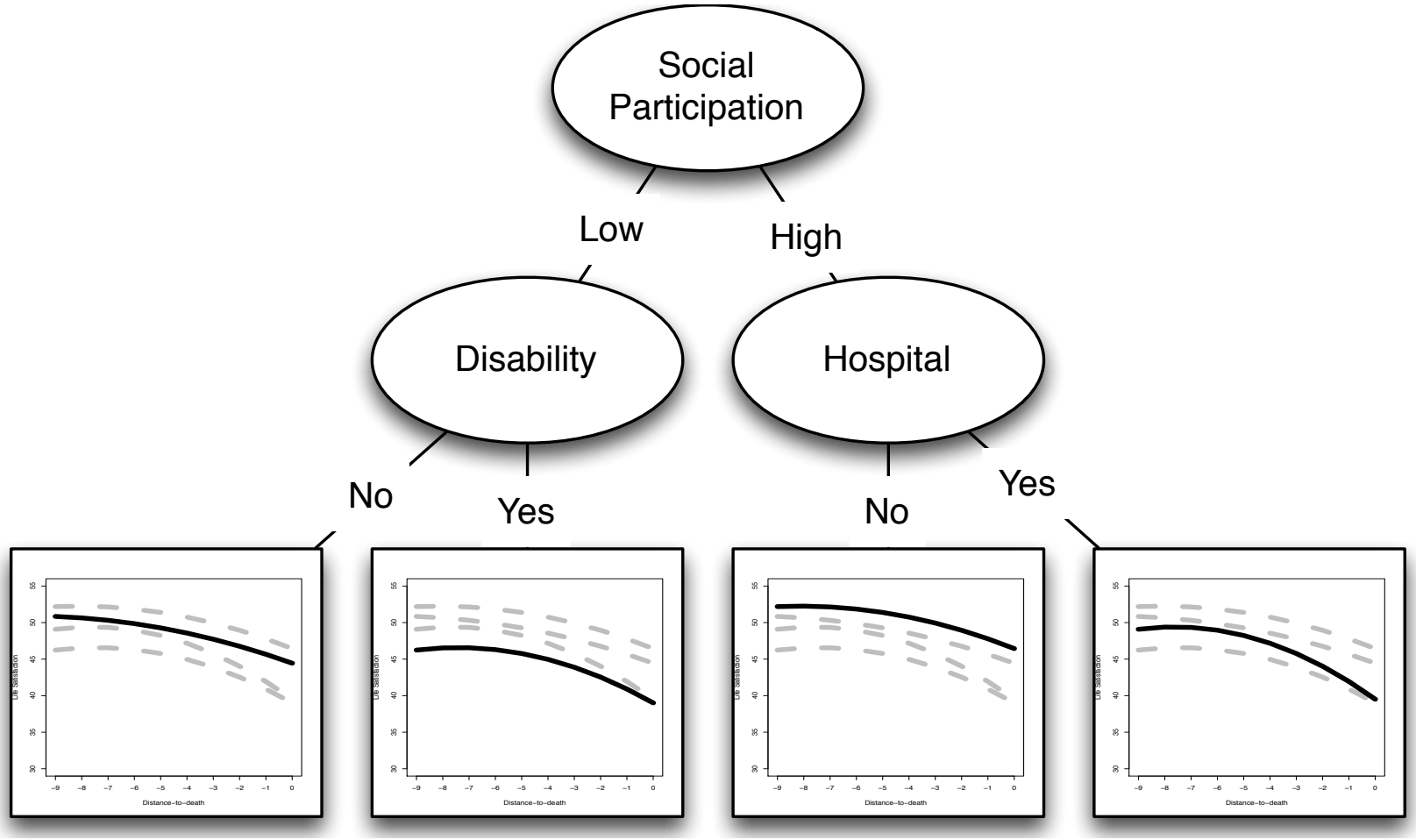




Example: Terminal Decline in Well-being using SOEP

- 4,404 now-deceased participants of the nationwide German SOEP (age at death: M = 73.2 years; 17-102 years; SD = 14.3 years; 52% women)
- Terminal decline, all available observations obtained in the last 10 years of life realigned along a time-to-death time metric
- Outcome: "How satisfied are you currently with your life, all things considered?", 11-point scale
- Predictors: socio-demographic (e.g., age at death, education, religion), health and burden (e.g., disability, unemployment, divorce), psychosocial (e.g., social participation, perceived control, life goals).

First Two Levels of the Well-Being Tree

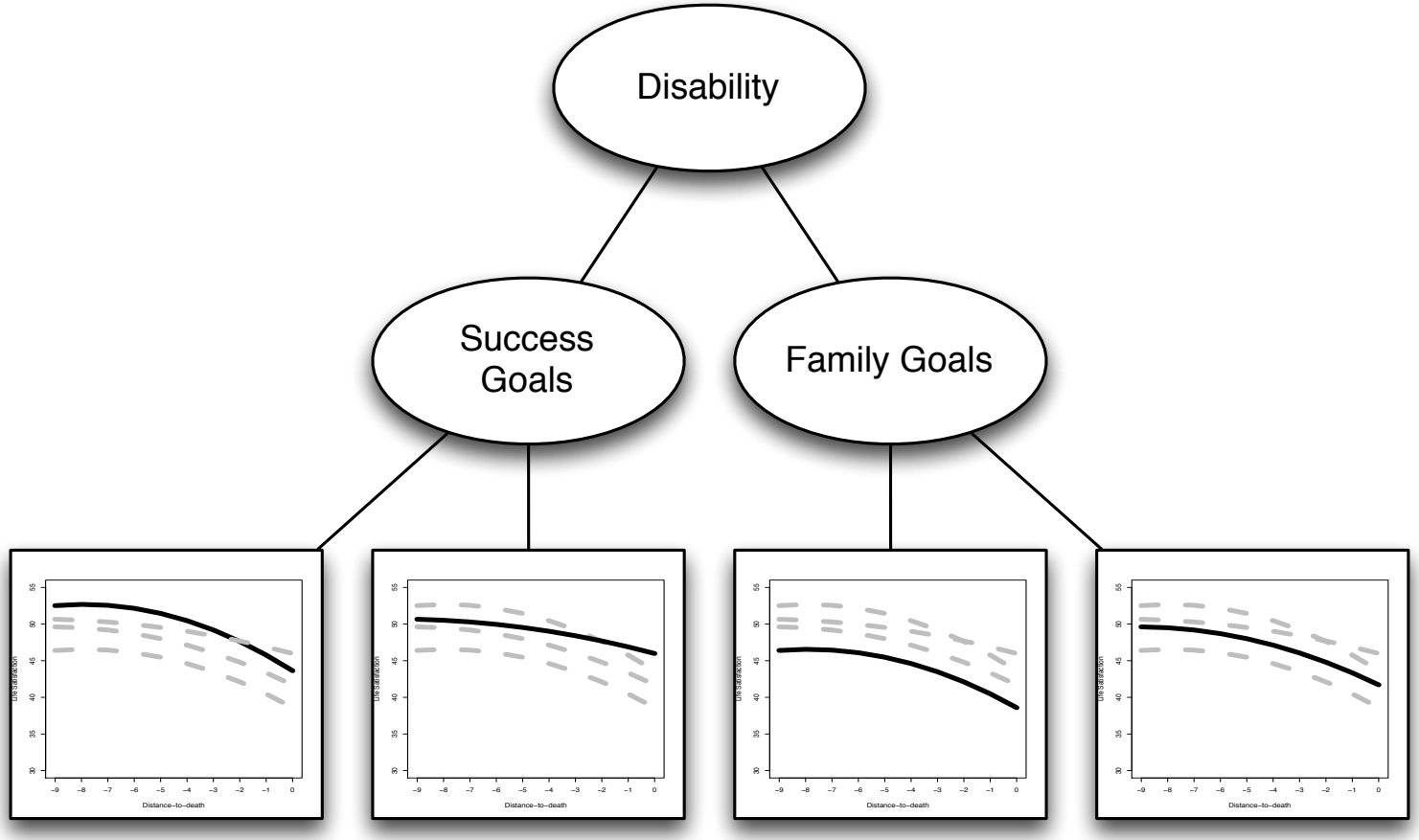


Brandmaier et al., Dev. Psychol., 2017

Problems in Interpretation

- What about variables not in the tree? Important or unimportant?
- Single trees may be unstable. Slight changes may drastically change their structure

A Resampled Well-Being Tree



SEM Forests

- Interpretation of variables in a tree as "important" is impeded by instability of trees (small changes in the sample may lead to different trees, e.g., two almost equally strong predictors)
- How to assess predictors left out (e.g., when strongly correlated with in-tree predictors)?

Remedy (SEM Tree + Random Forests):

- Draw bootstrap or subsamples from original datasets
- Fit a SEM Tree to each sub sample
- Draw subset of predictors when determining the next splitting variable

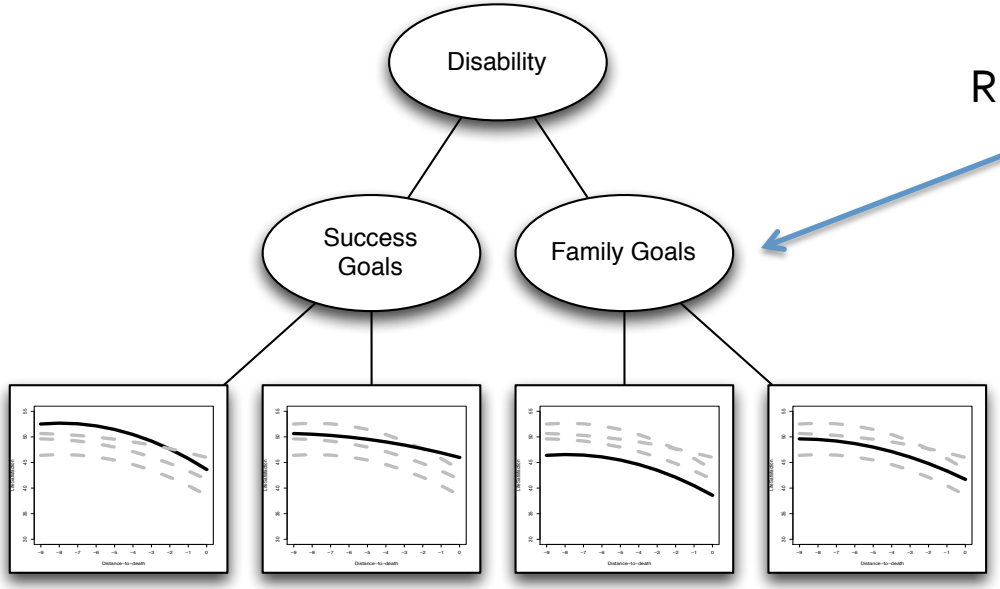
Brandmaier, Prindle, McArdle, & Lindenberger, 2016

Permutation Importance

A simple scheme:

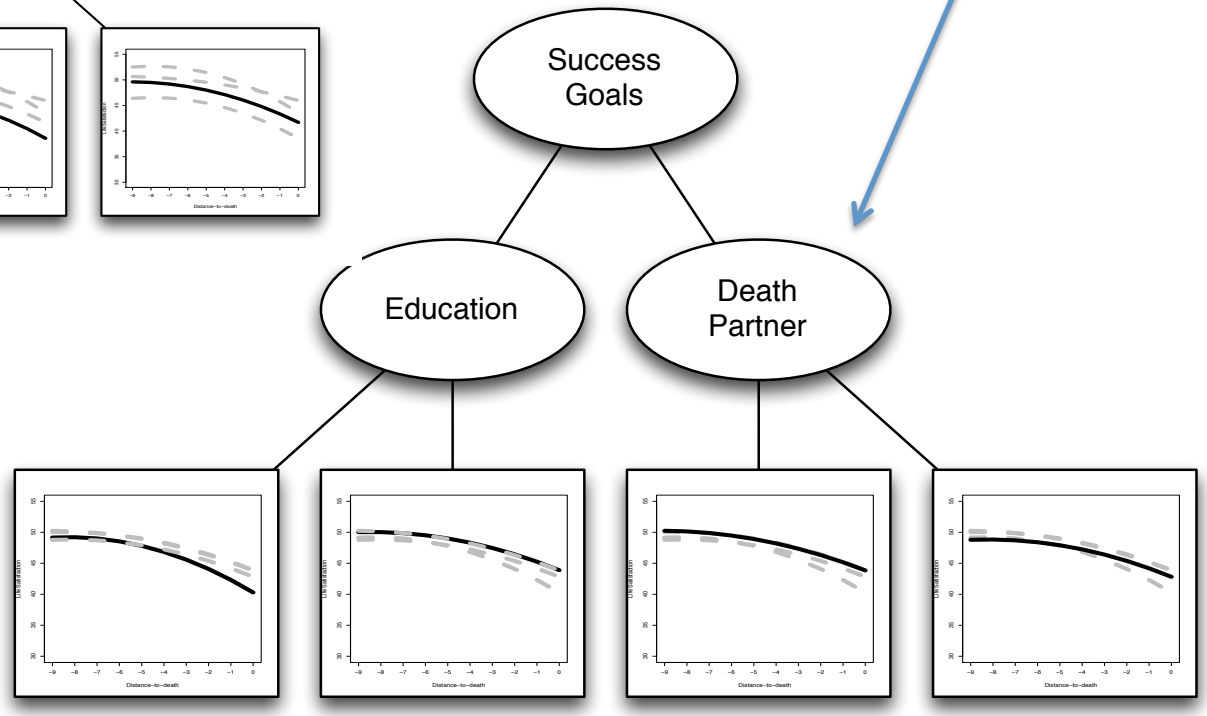
1. Compute likelihood of each tree on the OOB
2. Permute one predictor at a time
3. Compute drop in likelihood as measure of importance
4. Average over all trees

Bootstrapped Tree #3 and #294

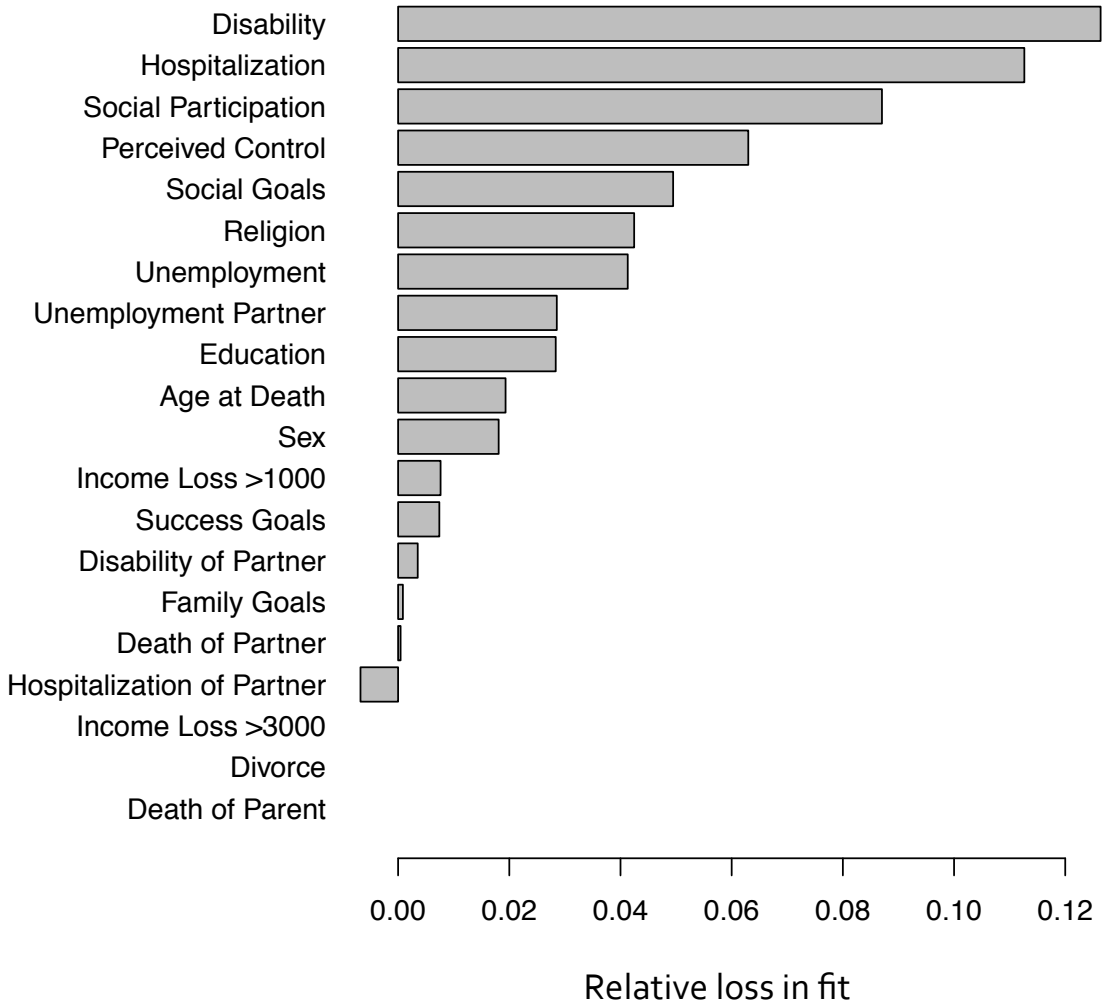


Rather important

Rather not important



Variable Importance in Well-Being



Summary: Variable Importance

- Generic, non-parametric approach (independent of method used) to assess **importance**
- VI summarizes **main effects and interactions**
- Does not require expensive re-training the forest

BUT

- Standard error depends on number of forests, so **don't use NHST**
- May have a bias for correlated predictors (but **see conditional variable importance**; Strobl et al., 2008)

Summary

SEM Trees and Forests

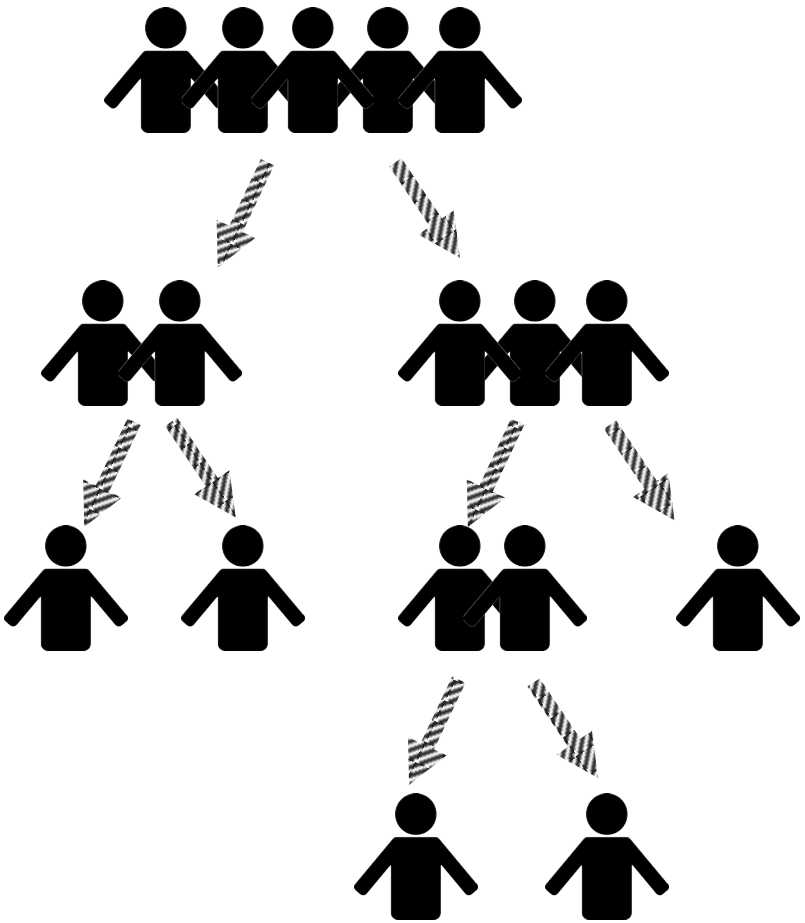
- combine **model-based and data-driven** modelling
- are tools to **recursively** identify **sub groups** and their predictors in the data
- explain **heterogeneity** in a sample
- by **reducing surprise** (increasing information)
- discover differences both on the **construct level** and on the **measurement level**

Summary

SEM Trees and Forests as a hybrid of two modeling cultures allows us:

- **Challenge established models** when comparing predictive accuracy (**hold out set!**).
- Tree/forest may lead to a **revision of the substantial theory** and the formulation of a new parametric model and/or experiment
- Conclusion that **postulated model applies only to a limited range of subjects**

Idiographic versus Nomothetic



- May be useful as an approach to "*develop the neglected territory between idiographic and nomothetic analytic approaches.*"

(see Singer, Ryff, Carr, and Magee, 1998)

Caveats

Prediction ≠ Explanation

- No short-cut from data to theory or knowledge
- The model with **best predictions** may **not** be the **true** model
- Shmueli et al. (2010): **parsimonious** but less „true" model can **have a higher predictive validi**ty than a „truer" but more complex model, particularly when
  - Data are noisy
  - When the true effects of the left-out variables are small
  - Sample size is small

Caveats

Prediction ≠ Causation

- With correlational data: association learning and curve-fitting
- No causal claims
- No claims about (temporal) precedence of one predictor over the other

A Dark Prophecy

Reviewer #2's (2012) damning verdict :

- *„Psychologists, with their obsession with their theories, are going to find data mining hard to grasp."*
- *„Data mining and SEM make strange bedfellows. Admittedly, bad data mining practices could take over-fitting to a new, horrific level."*

Overfitting / Generalization

The term "exploratory" is considered by many as less than an approach to data analysis and more a confession of guilt

— McArdle (2013)

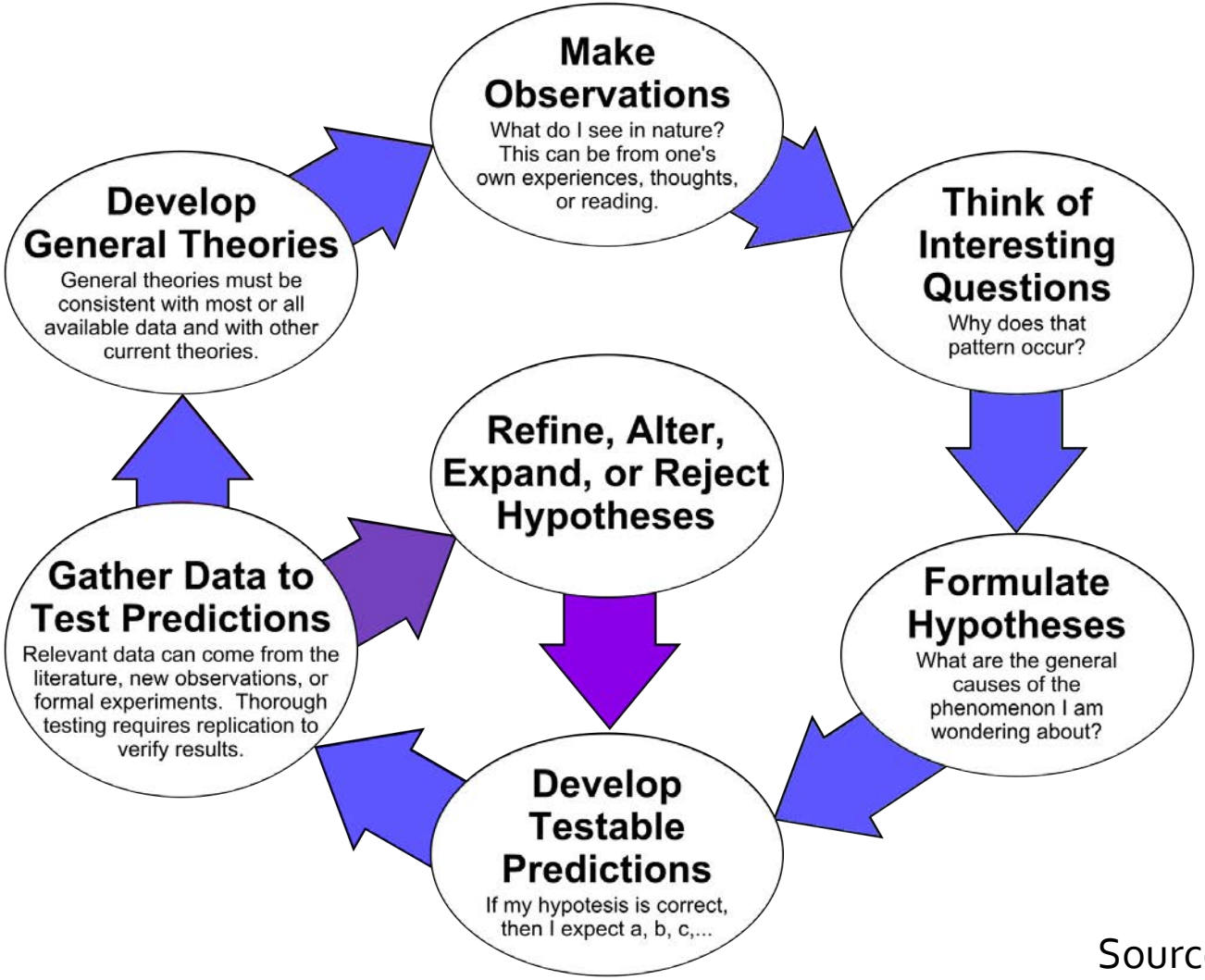
"inductive-deductive spiral" is an essential process in a good science

— Cattell, 1966

"Confirm first, then explore!"

— McArdle (2013)

Overfitting / Generalization



Source: Wikipedia

Twitter @brandmaier

Website: http://www.brandmaier.de