Reconstructability Analysis: Discrete Multivariate Modeling

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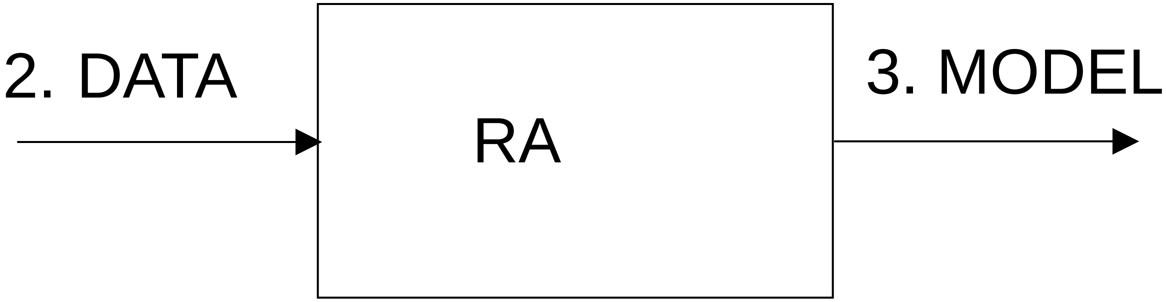
1. Introduction: what is RA

2. Input data to RA
3. Output model from RA



INTRODUCTION: WHAT IS RA?

- Reconstructability Analysis (RA) = a probabilistic graphical modeling methodology

- RA = Information theory (IT) + Graph theory (GT)

- Graphs, applied to data, are models:
- node = variable; link = relationship

- RA uses not only graphs (a link joins 2 nodes), but hypergraphs (a link can join >2 nodes)

WHY RA MIGHT BE OF INTEREST *1/2*

- Can detect many-variable or non-linear interactions not hypothesized in advance, i.e., it is explicitly designed for exploratory search
- Transparent -- not a black box like deep learning NNs
- Easily interpretable & communicable
- Designed for nominal variables
- Can also analyze continuous variables via binning
- Prediction/classification, clustering/network models
- Time series, spatial analyses
- Overlaps common statistical & machine-learning methods, but has unique features

WHY RA MIGHT BE OF INTEREST *2/2*

- Analyses at 3 levels of refinement:
  - coarse (very fast, in principle *many* variables)
  - fine (slower, 100s of variables) (~500 is max so far)
  - ultra-fine (slow, < 10 variables)
- Standard application: frequency data $f(A_i, B_j, C_k, Z_l)$
- Variety of non-standard capabilities
  - Data: set-theoretic relations & mappings
  - Predict continuous dependent variables
  - Integrate multiple inconsistent data sets (not yet in Occam)
  - Regression-like Fourier version (not yet in Occam)

OCCAM, SOFTWARE FOR RA

- OCCAM, developed by Systems Science Program, Portland State University, is now **open source**

- github.com/occam-ra/occam

- Contact me if you want to become involved:
- zwick@pdx.edu

PAST RA APPLICATIONS

- *BIOMEDICAL*

  Gene-disease association, disease risk factors, gene expression, health care policy & outcomes, dementia, diabetes, heart disease, prostate cancer, brain injury, primate health, surgery

- *FINANCE-ECONOMICS-BUSINESS*

  Stock market, bank loans, credit decisions, apparel analyses, market segmentation

- *SOCIAL-POLITICAL-ENVIRONMENTAL*

  Socio-ecological interactions, wars, urban water use, rainfall, forest attributes

- *MATH-ENGINEERING*

  Energy generation, logic circuits, automata dynamics, genetic algorithm & neural network preprocessing, chip manufacturing, pattern recognition, decision analysis

- *OTHER*

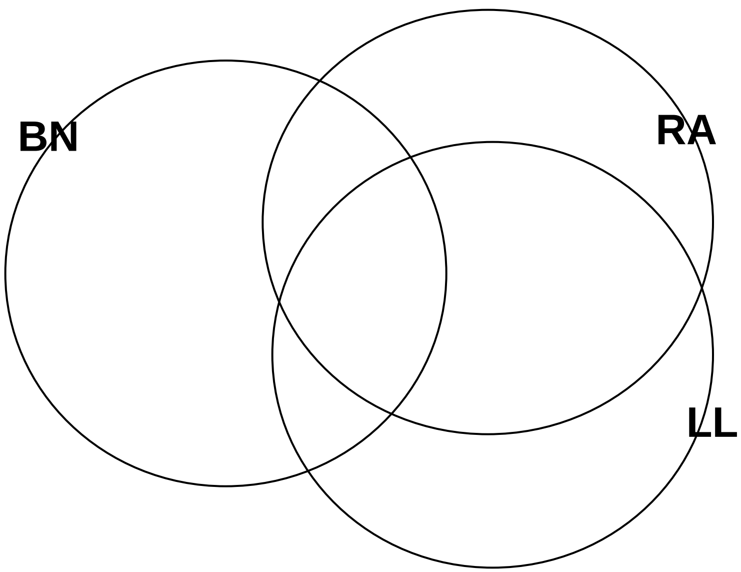
  Textual analysis, language analysis

OVERLAP WITH STATISTICAL, ML METHODS

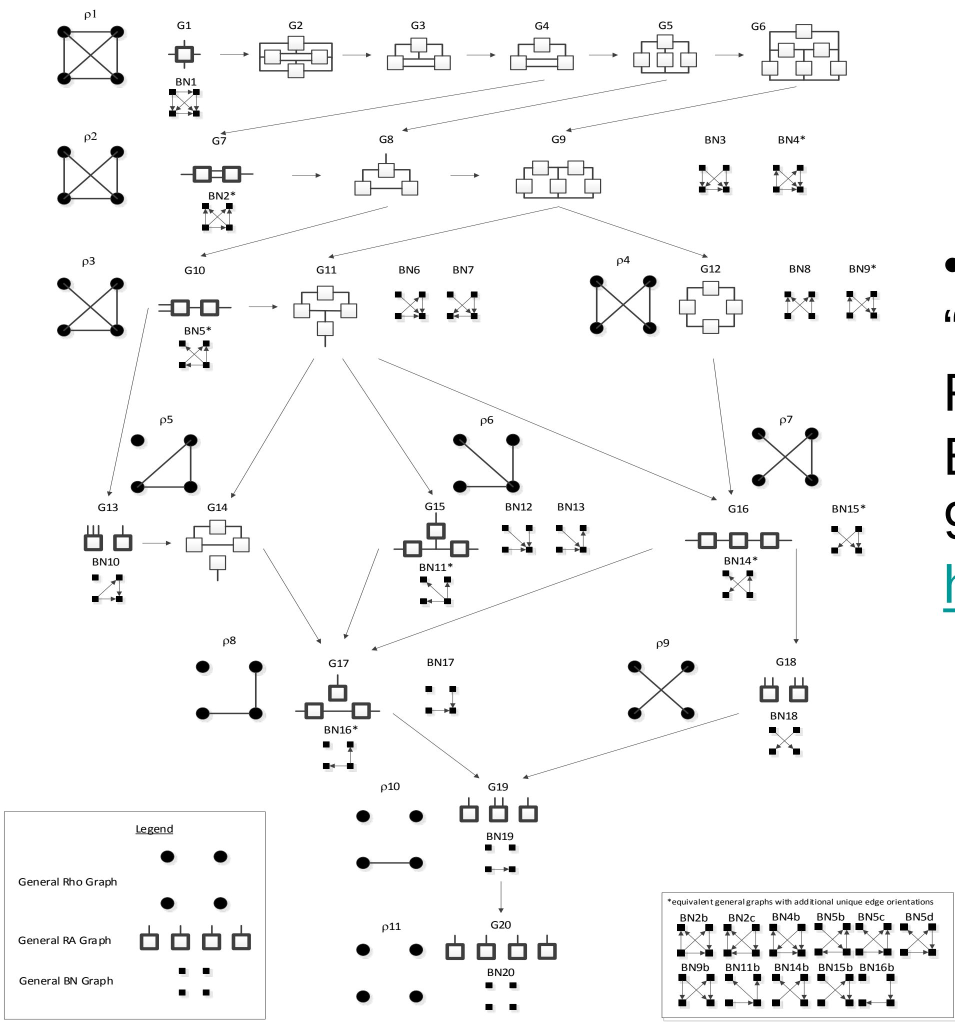
Closely related to other PGM methods, e.g., log linear (LL) (& logistic regression) models & Bayesian networks (BN)

Where methods overlap, they're equivalent

These PGM methods totally different from neural nets



4-VARIABLE GENERAL RHO, RA, BN GRAPHS



•Harris, M. and Zwick, M. (2021). “Graphical Models in Reconstructability Analysis and Bayesian Networks.” Entropy, 23: 986. https://doi.org/10.3390/e23080986

COMPARING RA TO BN, SVR, MLP (NN)

R Squared: bigger is better							
Method	ABC Train E Test	ABE Train D Test	ADE Train C Test	CDE Train B Test	BCD Train A Test	Average	Standard Deviation
Industry Model	n/a	n/a	n/a	n/a	n/a	7.5%	n/a
BN	13.3%	13.7%	14.2%	13.7%	14.4%	13.9%	0.5%
RA	**33.5%**	**33.2%**	**35.2%**	**33.2%**	**34.1%**	**33.8%**	**0.9%**
SVR-rbf	7.5%	7.5%	7.5%	7.2%	8.0%	7.5%	0.3%
SVR-Linear	6.3%	6.4%	6.5%	6.1%	6.9%	6.4%	0.3%
SVR-poly	6.6%	6.7%	6.8%	6.3%	7.1%	6.7%	0.3%
SVR-sigmoid	0.4%	0.1%	0.1%	0.4%	0.4%	0.3%	0.2%
MLP	16.8%	18.2%	17.9%	18.2%	19.3%	18.1%	0.9%

MAE: smaller is better							
Method	ABC Train E Test	ABE Train D Test	ADE Train C Test	CDE Train B Test	BCD Train A Test	Average	Standard Deviation
Industry Model	n/a	n/a	n/a	n/a	n/a	121.7	n/a
BN	103.0	102.2	102.4	103.4	102.7	102.7	0.5
RA	**86.6**	**86.7**	**85.8**	**87.6**	**86.8**	**86.7**	**0.6**
SVR-rbf	108.4	107.9	108.3	109.2	108.6	108.5	0.5
SVR-Linear	109.6	109.0	109.4	110.3	109.7	109.6	0.5
SVR-poly	109.1	108.6	109.0	109.9	109.4	109.2	0.5
SVR-sigmoid	588.3	579.6	580.7	600.5	582.8	586.4	8.5
MLP	100.5	99.2	99.8	100.4	99.7	99.9	0.5

MSE: smaller is better							
Method	ABC Train E Test	ABE Train D Test	ADE Train C Test	CDE Train B Test	BCD Train A Test	Average	Standard Deviation
Industry Model	n/a	n/a	n/a	n/a	n/a	27,339.7	n/a
BN	21,717.9	21,038.1	20,962.8	21,710.6	21,509.5	21,387.8	364.3
RA	**16,717.4**	**16,425.5**	**15,894.2**	**16,904.0**	**16,616.8**	**16,511.6**	**386.0**
SVR-rbf	23,164.5	22,576.3	22,603.6	23,361.5	23,164.7	22,974.1	359.9
SVR-Linear	23,470.0	22,822.8	22,860.1	23,631.9	23,410.9	23,239.2	372.2
SVR-poly	23,395.3	22,765.9	22,790.8	23,581.3	23,360.2	23,178.7	375.1
SVR-sigmoid	699,725.9	703,145.2	709,064.7	743,823.7	697,264.0	710,604.7	19,090.9
MLP	20,831.0	19,953.1	20,064.1	20,580.2	20,290.0	20,343.7	363.0

Harris, M., Kirby, E., Agrawal, A., Pokharel, R., Puyleart, F., and Zwick, M. (2023). “Machine Learning Predictions of Electricity Capacity.” Energies 2023, 16, 187.

https://doi.org/10.3390/en16010187

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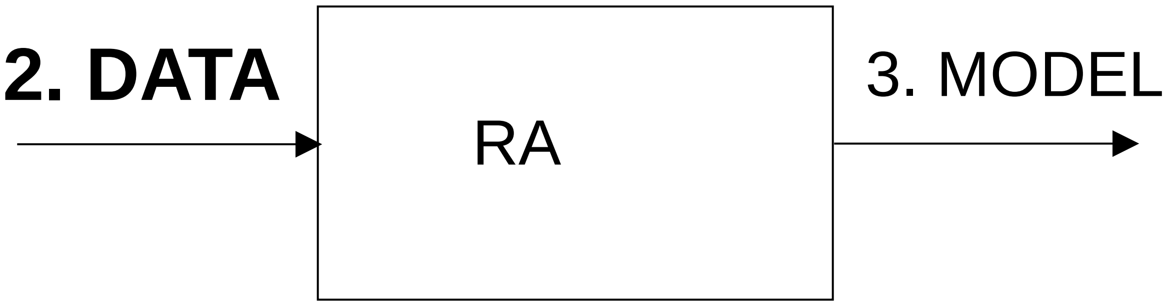
3. Output model from RA



FORM OF DATA

Variables

- Type: nominal; bin if continuous (continuous DV needn't be binned)

- Number: few variables to 100s (in principle >1000s coarse analysis)

Data analysis

directed system

– IV-DV distinction: *predict/classify* a DV from IVs

neutral system

– No IV-DV distinction: model association, clustering

FORM OF DATA

- frequency(A_i,B_j,C_k,Z_l) or individual cases

				frequency
A_0	B_0	C_0	Z_0	13
A_0	B_0	C_0	Z_1	2
A_0	B_0	C_1	Z_0	9
A_0	B_0	C_1	Z_1	11
…	…	…	…	___
				N

N = sample size

	A	B	C	Z
$case_1$	A_0	B_0	C_0	Z_0
$case_2$	A_1	B_2	C_3	Z_1
…				
$case_N$	A_0	B_0	C_0	Z_0

Cases are indexed by

individual (in a population),

time, or

space

frequency(ABCZ) / N = p_{data}(ABCZ)

OCCAM input file, DATA CASES INDEXED BY INDIVIDUAL

```
ID            ,413,0,ID  #Index specifying individual
APOE          ,2,1,Ap
Gender        ,2,1,Sx
Education     ,3,1,Ed
AgeLastExam   ,3,1,Ag
rs1801133     ,3,1,A
rs3818361     ,4,1,B
rs7561528     ,3,1,C
rs744373      ,3,1,D
rs6943822     ,3,1,E
rs4298437     ,3,1,F
rs7012010     ,3,1,G
rs11136000    ,3,1,H
rs10786998    ,4,1,J
rs11193130    ,4,1,K
rs610932      ,3,1,L
rs3851179     ,3,1,M
rs3764650     ,4,1,N
rs3865444     ,4,1,P
Dementia      ,2,2,Z
```

DEMENTIA EXAMPLE

Z = 0 no disease; Z = 1 disease

#ID	Ap	Sx	Ed	Ag	A	B	C	D	E	F	G	H	J	K	L	M	N	P	Z
101	0	0	2	2	1	1	0	1	2	2	1	1	2	0	1	1	2	2	1
103	0	0	2	1	0	2	2	0	1	1	1	2	2	0	1	1	0	1	0
111	0	1	2	1	2	2	1	1	0	1	1	2	1	1	2	2	0	1	0
112	0	0	2	2	2	2	1	1	1	2	1	1	0	2	2	0	0	2	0
118	0	1	0	2	2	2	2	0	0	1	1	1	.	.	1	1	0	2	0
120	0	1	2	2	1	2	1	1	0	1	1	2	1	1	1	2	0	.	1
121	0	0	2	2	2	2	1	1	2	0	0	0	2	0	1	1	1	.	1
122	0	0	1	2	1	2	1	1	2	0	0	2	2	0	1	1	1	1	0
123	0	0	2	2	2	2	2	0	1	1	0	0	2	0	2	1	0	1	1

…

***DATA** CASES INDEXED BY TIME*

	X	Y	Z
t-4	--	--	--
t-3	0	1	2
t-2	3	4	5
t-1	6	7	8
t	9	10	11

original data

A	B	C	X	Y	Z
--	--	--	--	--	--
--	--	--	--	--	--
0	1	2	3	4	5
3	4	5	6	7	8
6	7	8	9	10	11

transformed data

Values are labels for variable states at particular times

XYZ = generating variables

Apply mask (here # lags = 1) to data

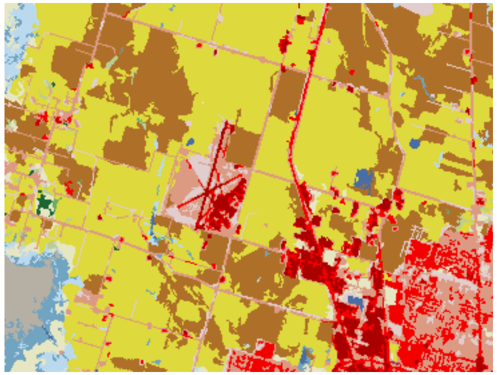
Mask adds lagged variables, ABC(t) = XYZ(t-1)

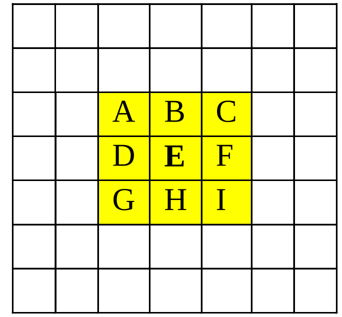
E.g., A(t) = X(t-1), labeled 6

Masking: time series data → atemporal data

DATA CASES INDEXED BY SPACE : 1 generating variable

A,14,1,A
B,14,1,B
C,14,1,C
D,14,1,D
E,14,2,E
F,14,1,F
G,14,1,G
H,14,1,H
I,14,1,I





Moore neighborhood

E = DV
A,B,C,D,F,G,H,I = IVs

IVs & DV have 14 possible states

#A	B	C	D	**E**	F	G	H	I
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	71	71	71	71	71	71
71	71	71	95	71	95	71	71	71
95	71	95	95	71	95	71	71	71
95	95	95	95	95	71	71	71	95
71	95	95	90	95	95	71	95	95
95	95	90	90	71	95	95	95	95
95	90	90	90	95	90	95	95	90

...

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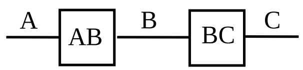
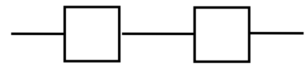
MODEL = STRUCTURE ***APPLIED TO DATA***

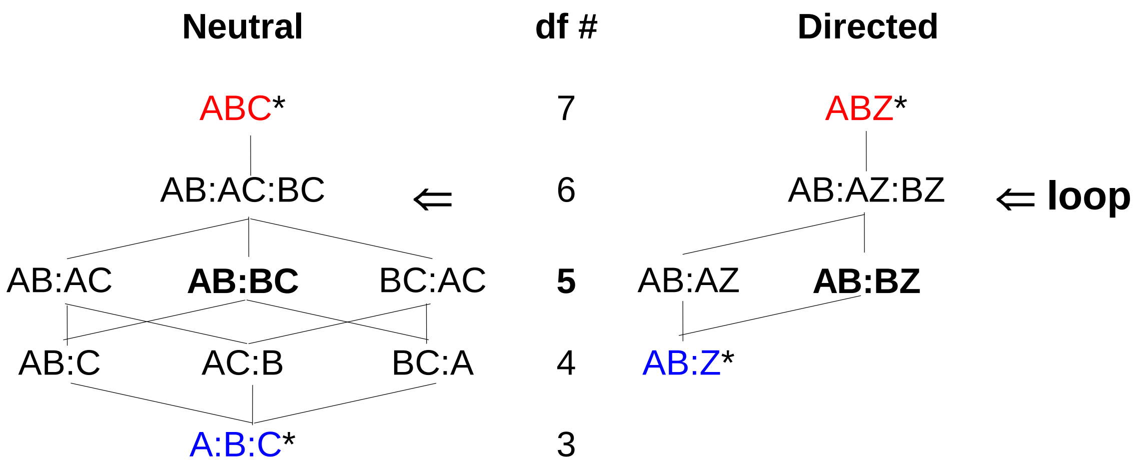
A structure (graph or hypergraph) is a set of relationships (GT)

Specific structure **AB:BC** *General* structure



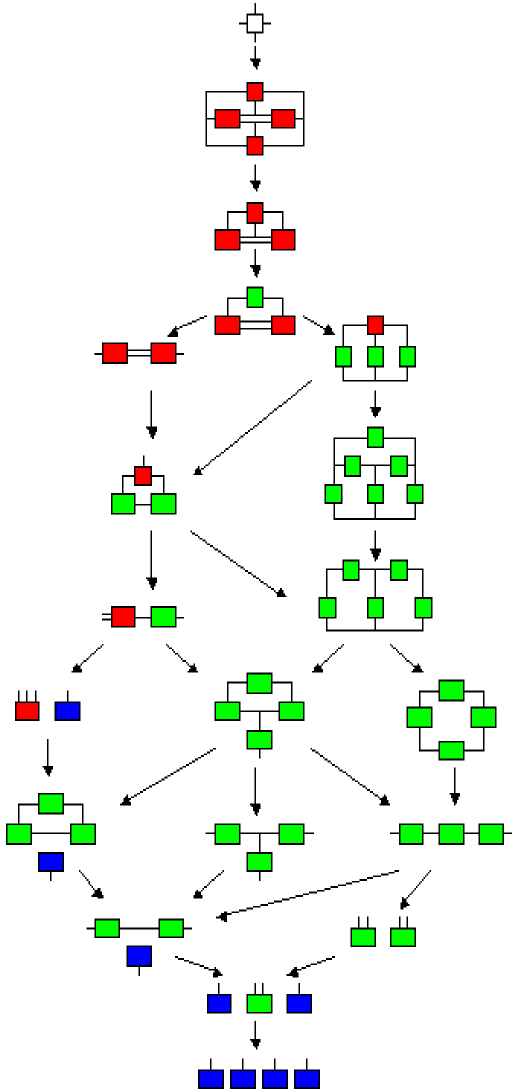


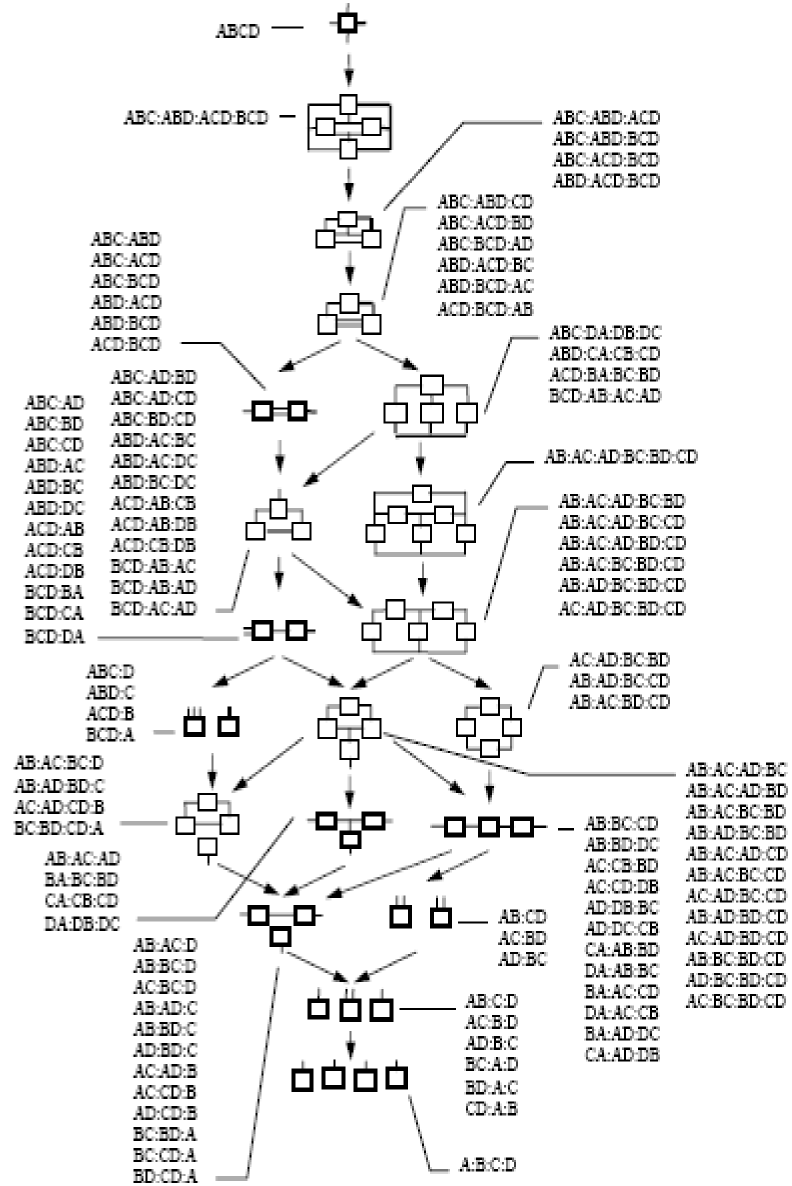
LATTICE OF *SPECIFIC* STRUCTURES (3 variables)



* **Reference model is** data or independence
# df (degrees of freedom) values are for binary variables

STRUCTURES 4 variables (GT)





STRUCTURES ***(GT)***

Combinatorial explosion

# variables	3	4	5	6
# general structures neutral	5	20	180	16,143
# specific structures neutral	9	114	6,894	7,785,062
one DV directed	5	19	167	7,580
one DV, no loops directed	4	8	16	32

NEED INTELLIGENT HEURISTICS TO **SEARCH LATTICE**

Can analyze 100s of variables, & for simple models, many more.

TYPES OF STRUCTURES *(GT)*

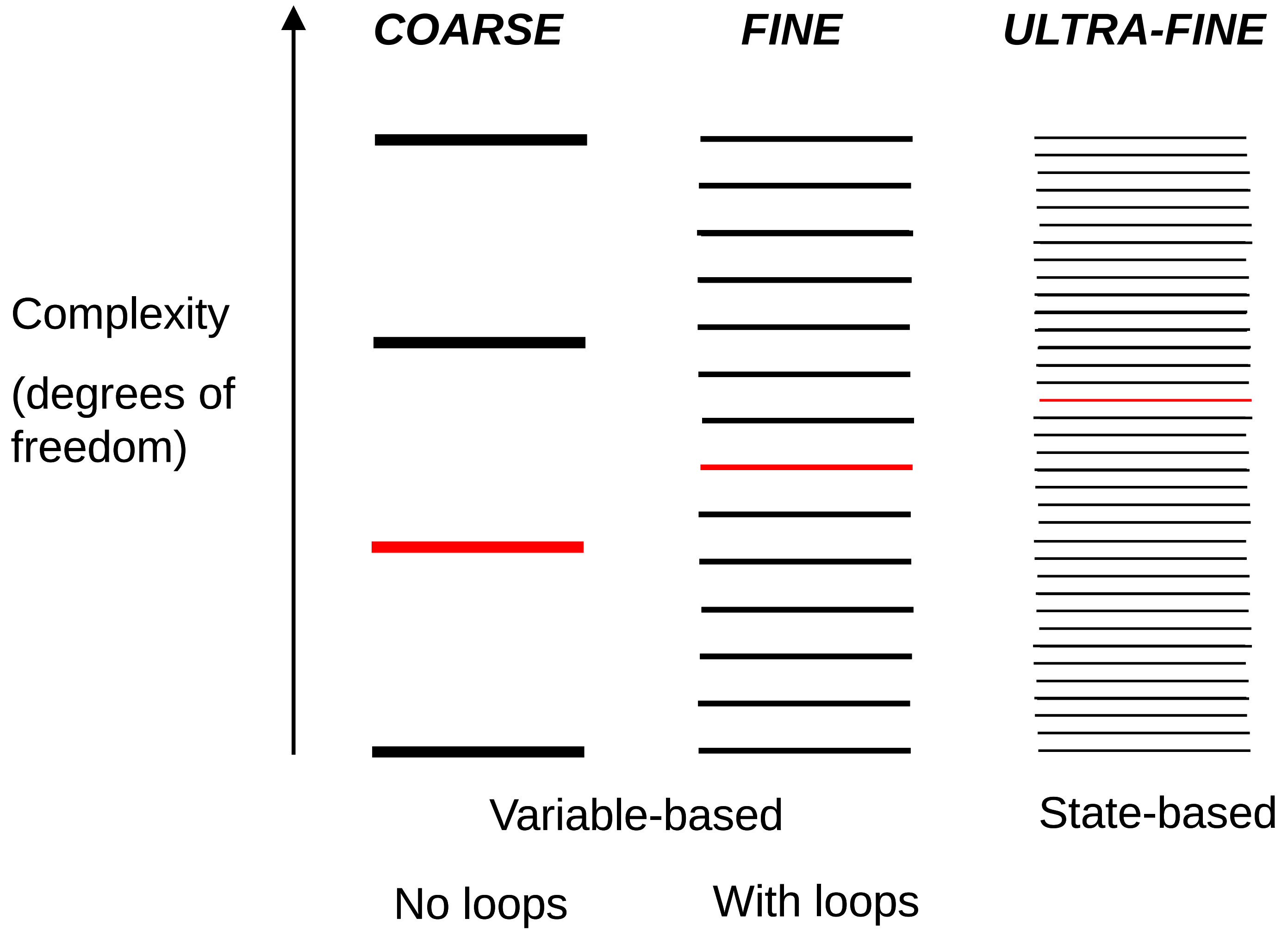
FOR PREDICTION / CLASSIFICATION (directed system)

- Variable-based
  - no loops [coarse] *many* variables (fast)
    IV:ACZ simple prediction, feature selection
  - with loops [fine] up to 100s of variables (slow)
    IV:ABZ:BCZ better prediction
- State-based [ultra-fine] < 10 variables (very slow)
  IV:Z: A_1B_1Z : $B_2C_3Z_1$ best prediction; detailed models

"IV" = ABC (all IVs); Z = DV

All directed system models include an IV component

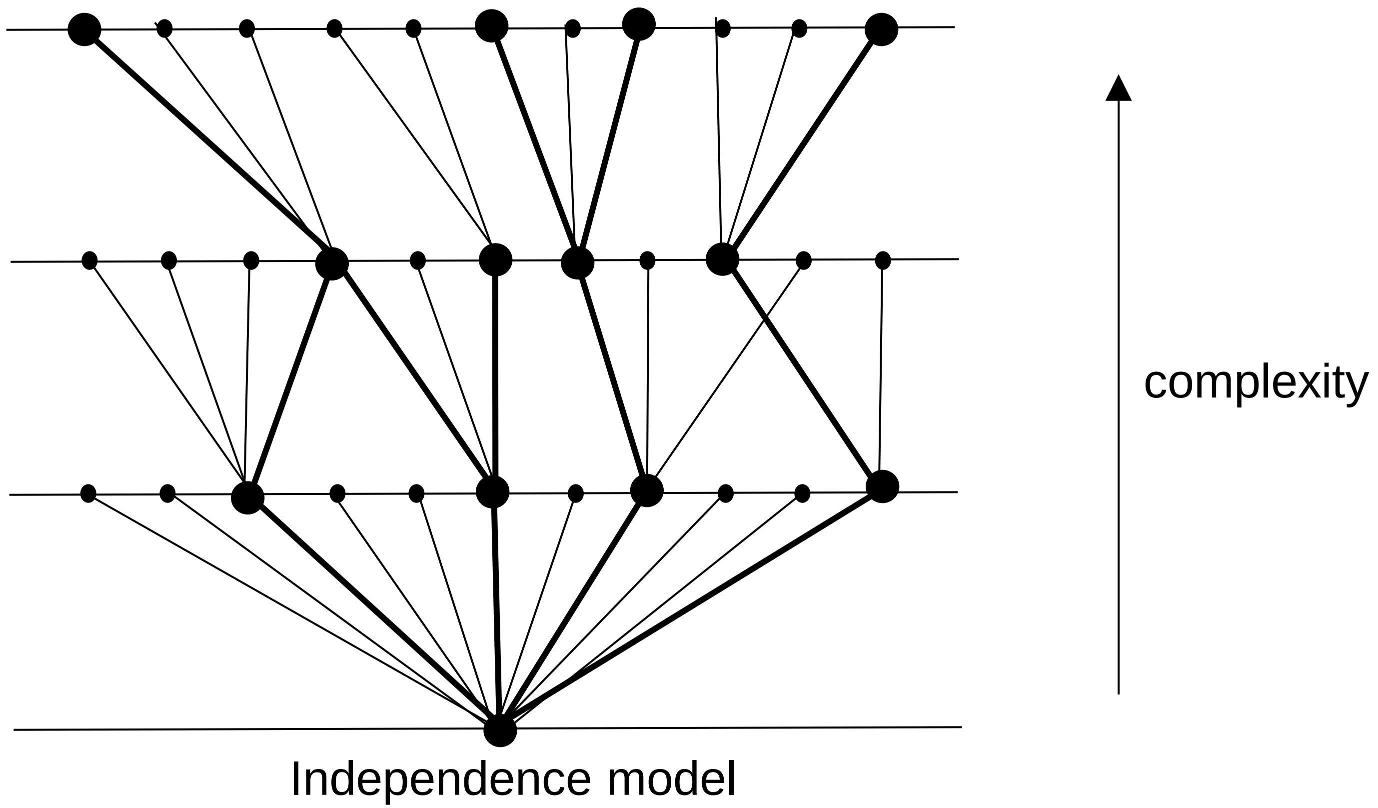
TYPES OF STRUCTURES (GT)



OCCAM SEARCH of LATTICE of STRUCTURES

beam search, levels = 3, width = 4 (node = model)

(there are many other search algorithms)



MODEL = PROBABILITY DISTRIBUTION (IT)

Neutral system:

- Model = calculated *joint* distribution,

  e.g., $p_{ABC:AZ:BZ}(A_i \; B_j \; C_k \; Z_l)$

Directed system:

- Model = calculated *conditional* distribution,

  e.g., $p_{ABC:AZ:BZ}(Z_l \mid A_i \; B_j \; C_k)$

- Distribution gives rule to predict Z from A,B,C

  And increase/decrease risk relative to margins

SELECTING A MODEL ***(IT)***

1. High information (or low error) in model

   <u>*Directed system*</u>

   – *Info-theory measure: high ΔH, <u>reduction of uncertainty of DV</u>*
   – *Generic measure: high %correct, accuracy of prediction*

2. Low complexity: df, degrees of freedom

3. Information $\leftrightarrow$ complexity tradeoff

   – Statistical significance (Chi-square p-values)
   – Integrated measures: AIC, BIC
     (Akaike & Bayesian Information Criteria)
   – BIC a conservative selection criterion

UNCERTAINTY REDUCTION: ***SIMPLE EXAMPLE***

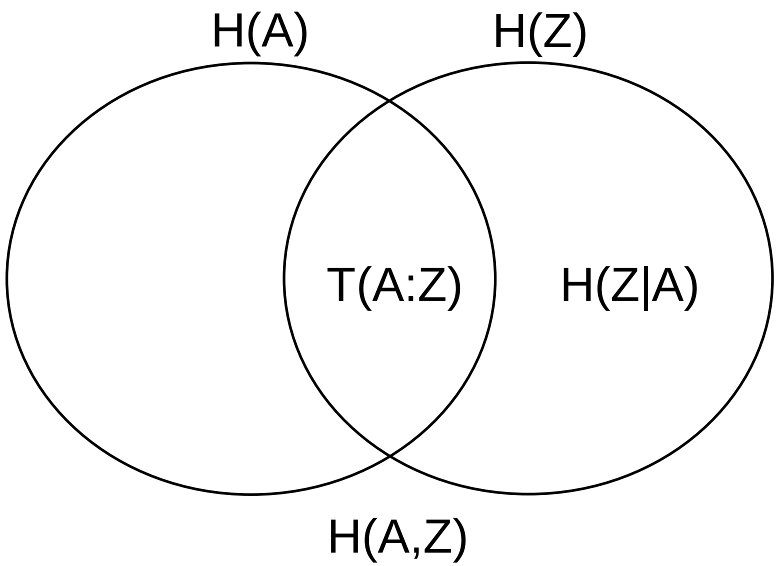
2 variables: IV=A; DV = Z; T(A:Z)=mutual information (association)

- *Uncertainty reduction* is *like* variance explained

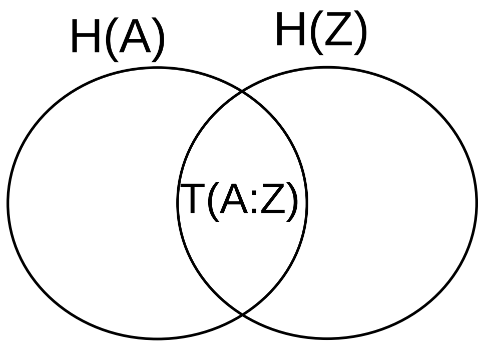
  Model AZ = predict Z, i.e., reduce H(Z), by knowing A

- Uncertainty *reduced* = T(A:Z); uncertainty *remaining* = H(Z|A)

  ΔH = T(A:Z) / H(Z) *fractional uncertainty reduction* (express in %)



UNCERTAINTY REDUCTION: ***SIMPLE EXAMPLE***



	Z_0	Z_1	
A_0	**.67*.5**	**.33*.5**	.5
A_1	**.33*.5**	.67*.5	.5
df=3	.5	.5	

- $p(Z_1)/p(Z_0)$= 1:1, not knowing A → 2:1 or 1:2, knowing A
- $\Delta H(Z) = T(A:Z) / H(Z) = 8\%$
- 8% reduction in uncertainty is *large* (unlike variance!)

SELECTING A MODEL ***DEMENTIA EXAMPLE***

Criterion	model	ΔH(%)	Δdf	%c	ΔBIC
Variable-based with loops (fine)					
BIC	IV: Ap Z : Ed Z : K Z	16	5	70	59
p-value	IV: Ap Z : Ed Z : K Z : C Z : L Z	18	9	71	
AIC	IV: B Ap Z : Ed Z : K Z : C Z	20	11	72	
State-based (ultra-fine)					
BIC	(model below; each interaction = 1 df)	20	6	72	81

IV:Z: Ap_1Z : Ed_0Z : K_2Z : $Ap_0Ed_2C_2Z$: $Ap_0Ed_1C_2K_1Z$: $Ap_0Ed_1C_0K_1Z$

Models integrate ***multiple predicting interactions***

IV = ApEdCKL… (all the independent variables); %c(IV:Z) = 52

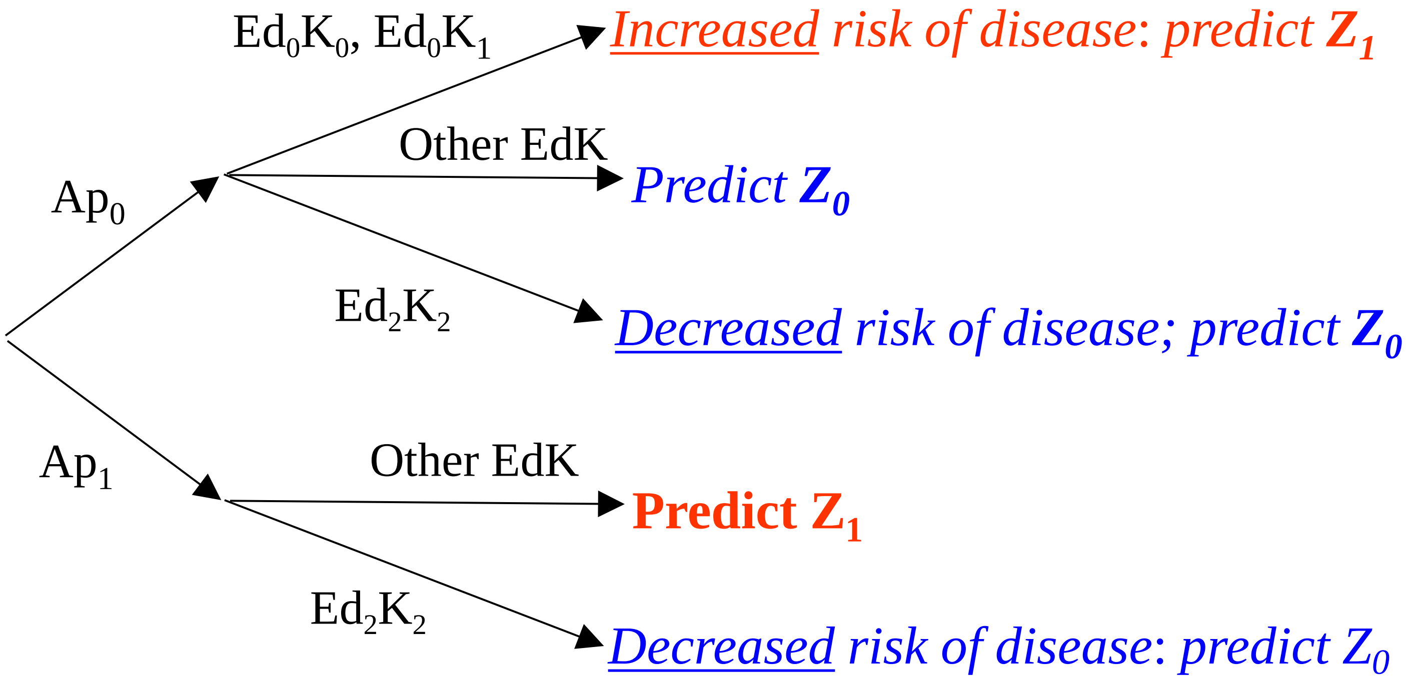
PROBABILITY DISTRIBUTION DEMENTIA EXAMPLE

				DATA		MODEL IV:ApZ:EdZ:KZ				
IV				obs p(Z | IV)		calc p(Z | IV)			p-value	
Ap	Ed	K	freq	Z_0	Z_1	Z_0	Z_1	rule	p_{rule}	p_{Ap}
0	**0**	**0**	4	0.0	1.000	.122	.878	1	0.131	**0.028**
0	**0**	**1**	8	.125	.875	**.124**	**.876**	**1**	**0.033**	**0.002**
0	0	2	4	.250	.750	.294	.706	1	0.409	0.138
0	1	0	31	.645	.355	.616	.384	0	0.198	0.707
0	1	1	37	.622	.378	.619	.381	0	0.147	0.714
0	**1**	**2**	23	.783	.217	**.827**	**.173**	**0**	**0.002**	0.072
0	**2**	**0**	66	.636	.364	**.640**	**.360**	**0**	**0.023**	0.894
0	**2**	**1**	61	.656	.344	**.644**	**.357**	**0**	**0.025**	0.942
0	**2**	**2**	33	.848	.152	**.842**	**.158**	**0**	**0.000**	**0.020**
0	--	--	267	.648	.352	**.648**	**.352**	**0**		
1	0	0	1	.000	1.000	.026	.974	1	0.343	0.571
1	**0**	**1**	7	.143	.857	**.026**	**.974**	1	**0.012**	0.134
1	0	2	2	.000	1.000	.074	.926	1	0.228	0.514
1	1	0	13	.308	.692	.234	.766	1	0.055	0.709
1	**1**	**1**	24	.167	.833	**.237**	**.763**	1	**0.010**	0.633
1	1	2	11	.545	.455	.478	.522	1	0.884	0.146
1	**2**	**0**	32	.219	.781	**.254**	**.746**	1	**0.005**	0.732
1	**2**	**1**	39	.256	.744	**.256**	**.744**	1	**0.002**	0.735
1	2	2	17	.529	.471	.504	.496	**0**	0.973	**0.040**
1	--	--	146	.281	.719	**.281**	**.719**	**1**		
			413	.518	.482	**.518**	**.482**	0		

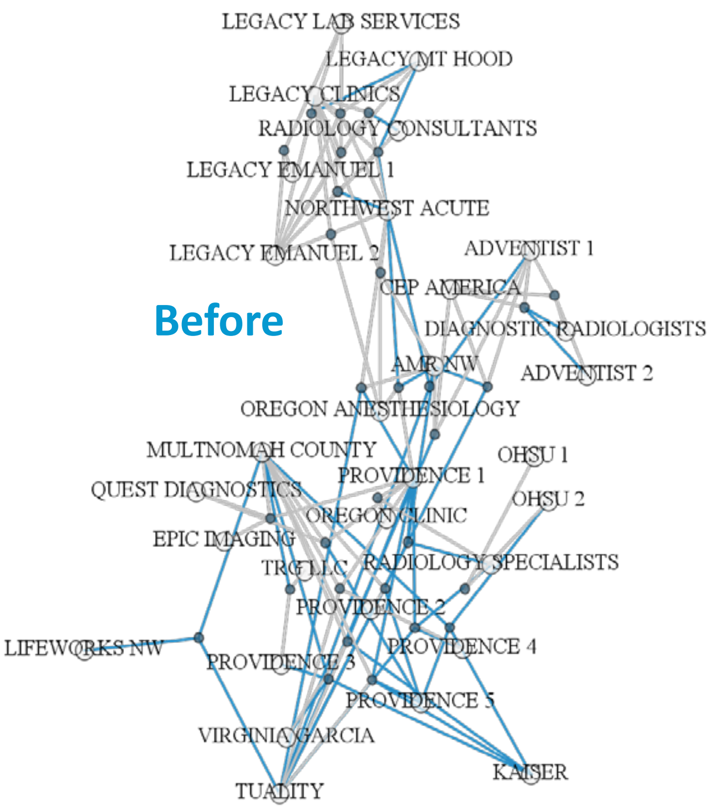
DECISION TREE ***DEMENTIA EXAMPLE***

Obtained from conditional probability distribution

Increase/decrease of risk compared to prediction based only on Ap



NEUTRAL ANALYSIS EXAMPLE



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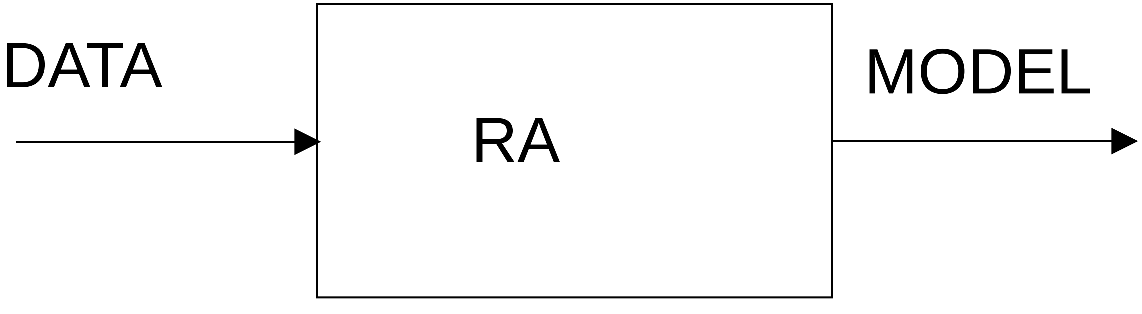
4. RA methodology



GENERATE MODEL

frequencies shown, not probabilities

data: observed ABC (df=7)

	C_0		C_1	
	B_0	B_1	B_0	B_1
A_0	143	77	253	182
A_1	227	46	411	139

1478

model: calculated $ABC_{AB:BC}$

	C_0		C_1	
	B_0	B_1	B_0	B_1
A_0	142	72	254	188
A_1	227	52	409	134

3.*Evaluation*

1.*Projection*

2.*Composition*

	B_0	B_1	
A_0	396	259	655
A_1	638	185	823
	1034	444	

	B_0	B_1	
C_0	370	123	493
C_1	664	321	985
	1034	444	

model: AB:BC (df=5)

GENERATE MODEL ***(Projection, Composition)***

- *Projection* = sum frequencies or probabilities

- *Composition*

Maximize model entropy *subject to* model constraints

Model entropy: $H(p_{model}) = - \Sigma\, p_{model} \log_2 p_{model}$

E.g., for model AB:BC, *maximize* $H(p_{AB:BC})$ *subject to*

$$p_{AB:BC}(AB)= p_{data}(AB)$$

$$p_{AB:BC}(BC)= p_{data}(BC)$$

Composition is critical computational step; done

(a) Algebraically (very fast) — loopless models

(b) Iteratively (Iterative Proportional Fitting) — models with loops

EVALUATE MODEL (1/2)

- *Evaluation* (1 = data dependent; 2 = data independent)

1. *[reference=data]*

error, T_{model} $= H_{model} – H_{data}$

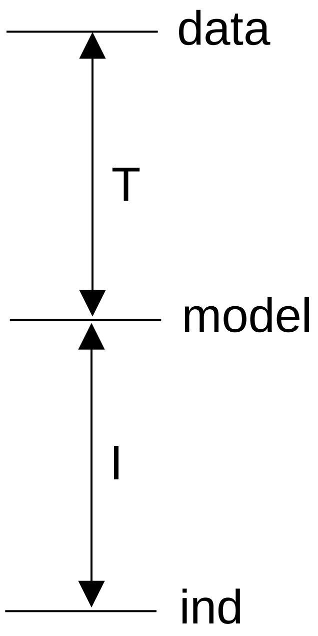
$= \Sigma\, p_{data} \log_2(p_{data}/p_{model})$

[reference=<u>ind</u>ependence]

information, I_{model} $= H_{ind} – H_{model}$

$= \Sigma\, p_{data} \log_2(p_{model}/p_{ind})$

uncertainty reduction $= H(DV) - H_{model}(DV \mid IV)$



2. *[reference=<u>ind</u>ependence]*

complexity $= \Delta df = df_{model} – df_{ind}$

EVALUATE MODEL (2/2)

Trade off information (or error) & complexity, define best model criterion, via:

Use likelihood ratio Chi-square, LR = k N T

- p-values from ΔLR, Δdf, Chi-square table

Or linear combinations of information & complexity

- ΔAIC = ΔLR + 2 Δdf
- ΔBIC = ΔLR + ln(N) Δdf

BASIC OCCAM ACTIONS

- Search = exploratory modeling, examine <u>many</u> models, find best or good ones

  (OCCAM actions: Search, SB-Search)

- Fit = confirmatory modeling, look at <u>one</u> model in detail (see probability distribution) & use for prediction

  (OCCAM actions: Fit, SB-Fit)

(OCCAM actions: Show Log, Manage Jobs = managerial functions)

OCCAM Initial Screen

INFORMATION ON RA

- Review articles on Zwick's SW page
  - "Wholes & Parts in General Systems Methodology" (accessible)
  - "An Overview of Reconstructability Analysis" (encompassing)
- Krippendorff, Klaus (1986). Information Theory. *Structural Models for Qualitative Data* (Quantitative Applications in the Social Sciences Monograph #62). New York: Sage Publications.
- *International Journal of General Systems*
- *Kybernetes*, Vol. 33, No. 5/6 2004: special RA issue

- THANK YOU.

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