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2022

# Reconstructability Analysis: Discrete Multivariate Modeling

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#### Citation Details

Zwick, Martin, "Reconstructability Analysis: Discrete Multivariate Modeling" (2022). *Systems Science Faculty Publications and Presentations*. 235.

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# Reconstructability Analysis

# Martin Zwick

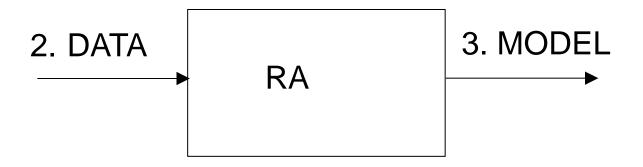
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Discrete Multivariate Modeling SySc 551-651

# 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 <u>hypergraphs</u> (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)</li>
- Standard application: frequency data f(A<sub>i</sub>, B<sub>i</sub>, C<sub>k</sub>, Z<sub>l</sub>)
- 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
- https://www.occam-ra.io/
- 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

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

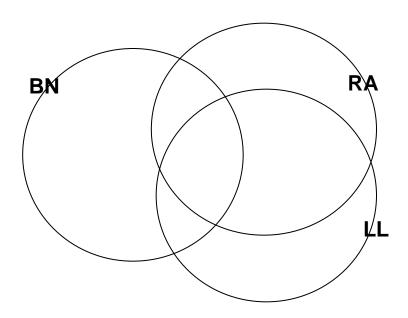
#### OTHER

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



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#### 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( $A_i, B_i, C_k, Z_l$ )

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

			frequency
$B_0$	$C_0$	$Z_0$	13
$B_0$	$C_0$	$Z_1$	2
$B_0$	$C_1$	$Z_0$	9
$B_0$	$C_1$	$Z_1$	11
			N
	B <sub>0</sub>	B <sub>0</sub> C <sub>0</sub> B <sub>0</sub> C <sub>1</sub>	$\begin{array}{c cccc} & & & & & & \\ B_0 & C_0 & Z_0 \\ B_0 & C_1 & Z_0 \\ B_0 & C_1 & Z_1 \\ & & & \\ \end{array}$

N = sample size

В  $B_0$  $A_0$ case<sub>1</sub>  $B_2$ case<sub>2</sub>  $A_1$  $A_0$  $B_0$ case<sub>N</sub>

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
                                          DEMENTIA EXAMPLE
Education
             ,3,1,Ed
                                         Z = 0 no disease; Z = 1 disease
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
```

```
#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 2 1 1 2 2 0 1 0
112 0 0 2 2 2 2 1 1 1 0 1 1 2 1 1 2 2 0 0 2 0
118 0 1 0 2 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 2 0 . 1
121 0 0 2 2 2 2 2 1 1 2 1 1 0 0 2 2 0 1 1 1 . . 1
122 0 0 1 2 1 2 1 1 1 2 0 0 2 2 0 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	Υ	Z				
t-4	-						
t-3	0	1	2				
t-2	3	4	5				
t-1	6	7	8				
t	9	10	11				
original data							

Α	В	С	X	Υ	Z
	1	1	I		-
				-	
0	1	2	3	4	5
3	4	5	6	7	8
6	7	8	တ	10	11

original data

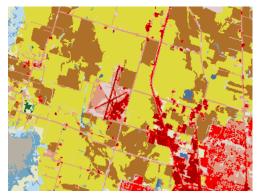
transformed data

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
1,14,1,1



	A	В	С	
	D	E	F	
	G	Н	I	

Moore neighborhood

 $\mathbf{E} = \mathsf{DV}$ A,B,C,D,F,G,H,I = IVs

IVs & DV have 14 possible states

I,14,1,I	A	A THE						
#A	В	С	D	E	F	G	Н	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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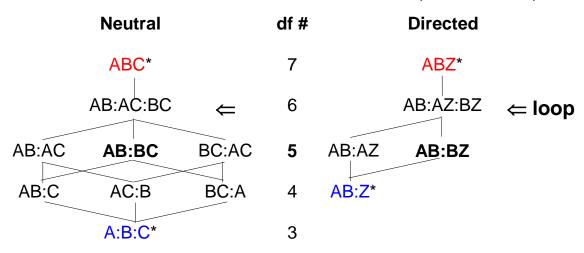
#### MODEL = STRUCTURE APPLIED TO DATA

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

Specific structure AB:BC General structure

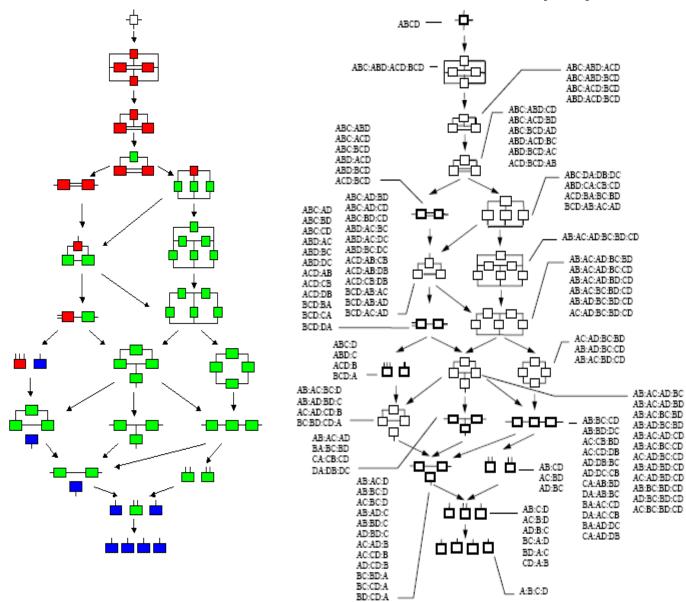


LATTICE OF SPECIFIC STRUCTURES (3 variables)



\* 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.

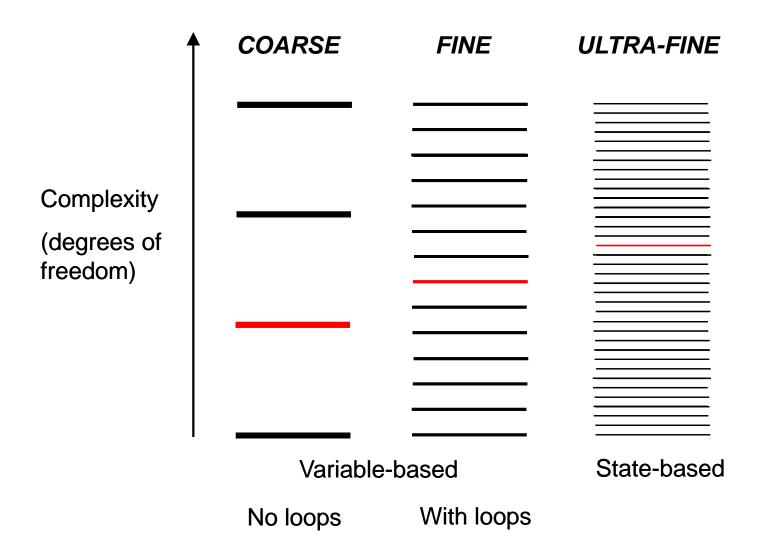
## TYPES OF STRUCTURES (GT)

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)</li>
   IV:Z: A<sub>1</sub>B<sub>1</sub>Z: B<sub>2</sub>C<sub>3</sub>Z<sub>1</sub> best prediction; detailed models

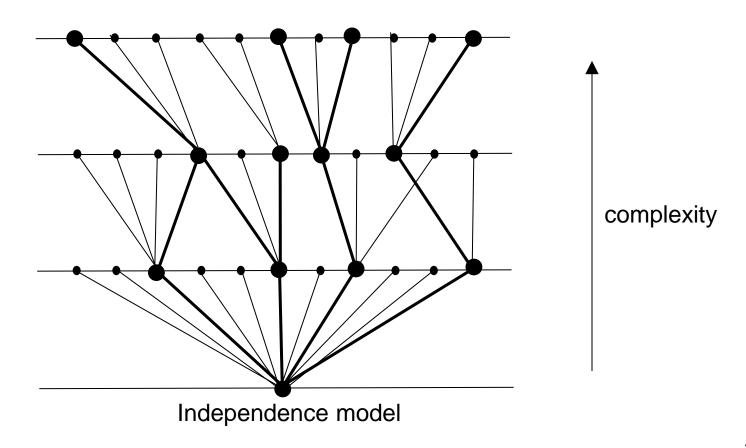
"IV" = ABC (all IVs); Z = DV All directed system models include an IV component

# 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<sub>ABC:AZ:BZ</sub>(A<sub>i</sub> B<sub>i</sub> C<sub>k</sub> Z<sub>l</sub>)

# <u>Directed system:</u>

- Model = calculated conditional distribution,
   e.g., p<sub>ABC:AZ:BZ</sub>(Z<sub>I</sub> | A<sub>i</sub> B<sub>i</sub> C<sub>k</sub>)
- Distribution gives rule to predict Z from A,B,C
   And increase/decrease risk relative to margins

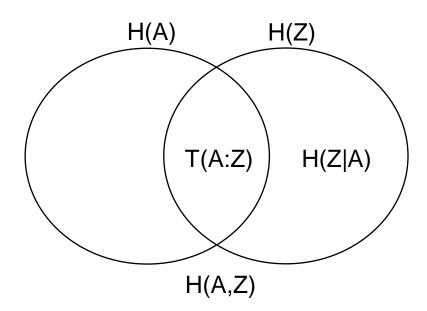
## SELECTING A MODEL (IT)

- High information (or low error) in model <u>Directed system</u>
  - Info-theory measure: high ∆H, reduction of uncertainty of DV
  - Generic measure: high %correct, accuracy of prediction
- 2. Low complexity: df, degrees of freedom
- 3. Information ↔ complexity tradeoff
  - Statistical significance (Chi-square p-values)
  - Integrated measures: AIC, BIC
     (Akaike & Bayesian Information Criteria)
  - BIC a conservative selection criterion

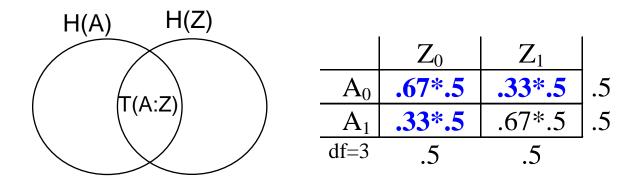
### UNCERTAINTY REDUCTION: SIMPLE EXAMPLE

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



- $p(Z_1)/p(Z_0) = 1:1$ , not knowing A  $\rightarrow$  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

<u>Criterion</u> model	<u>∆H(%)</u>	<u>∆df</u>	<u>%c</u>	<u>ΔΒΙ</u>
Variable-based with loops (fine)				
BIC IV: Ap Z: Ed Z: KZ	16	5	<b>70</b>	<b>59</b>
p-value IV: Ap Z: Ed Z: K Z: C Z: L Z	18	9	71	
AIC IV: BApZ: EdZ: KZ: CZ	20	11	72	
State-based (ultra-fine)				
BIC (model below; each interaction = 1 df)	20	6	72	81
$IV:Z:\;Ap_{1}Z:\;Ed_{0}Z:\;K_{2}Z:\;Ap_{0}Ed_{2}C_{2}Z:\;Ap_{0}Ed_{1}C_{2}K_{1}$	Z : Ap <sub>0</sub> l	$Ed_1C_0I$	$<_1Z$	

Models integrate <u>multiple</u> predicting interactions

IV = ApEdCKL... (all the independent variables); %c(!V:Z) = 52

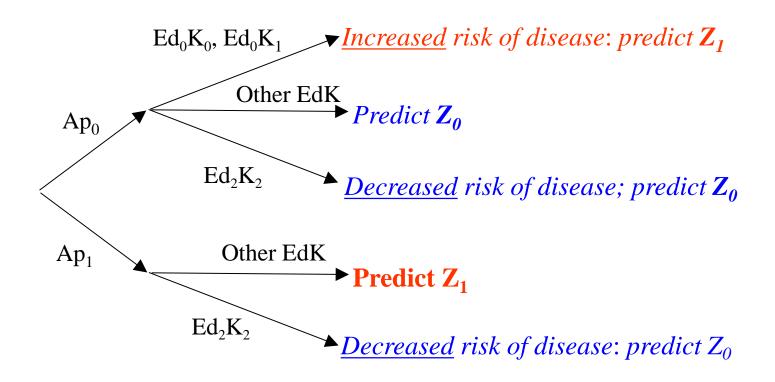
## PROBABILITY DISTRIBUTION DEMENTIA EXAMPLE

				]	DATA	MODE	dZ:KZ			
	IV			obs p(	Z   IV)	calc p(Z	Z   IV)		p-val	lue
Ap	Ed	K	freq	$Z_0$	$Z_1$	$Z_0$	$Z_1$	rule	p <sub>rule</sub>	$p_{Ap}$
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

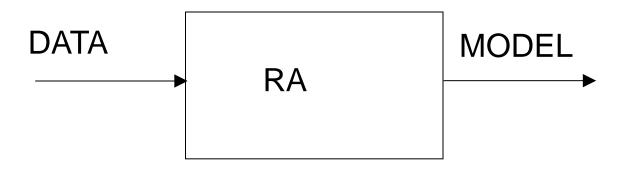


## NEUTRAL ANALYSIS EXAMPLE



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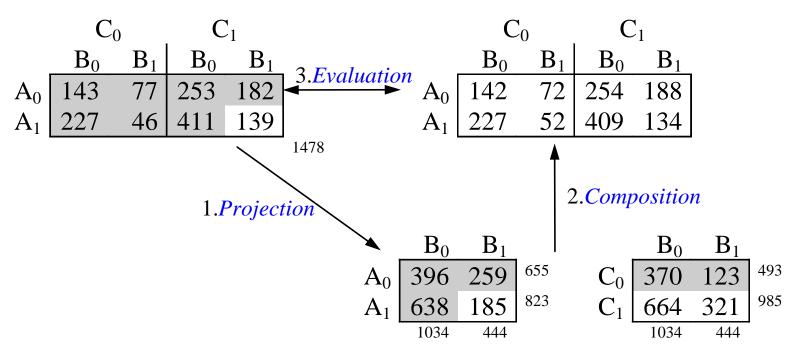
# 4. RA methodology



#### **GENERATE MODEL**

frequencies shown, not probabilities

**data**: observed ABC (df=7) **model**: calculated ABC<sub>AB:BC</sub>



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}) = -\sum 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, 
$$T_{model}$$
 =  $H_{model} - H_{data}$   
=  $\Sigma p_{data} \log_2(p_{data}/p_{model})$  data  
[reference=independence]  
information,  $I_{model}$  =  $H_{ind} - H_{model}$   
=  $\Sigma p_{data} \log_2(p_{model}/p_{ind})$  model  
uncertainty reduction =  $H(DV) - H_{model}(DV \mid IV)$   
2. [reference=independence]

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

- $\triangle AIC = \triangle LR + 2 \triangle df$
- $\triangle BIC = \triangle LR + In(N) \triangle df$

### **BASIC OCCAM ACTIONS**

 Search = exploratory modeling, examine many 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 DMM 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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