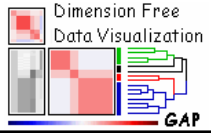
Introduction to

Generalized Association Plots (GAP)

for Dimension-Free Data Visualization

Han-Ming Wu

Institute of Statistical Science, Academia Sinica,
Taipei, Taiwan
hmwu@stat.sinica.edu.tw
http://www.sinica.edu.tw/~hmwu/



中央研究院 統計科學研究所
Institute of Statistical Science, Academia Sinica

2006/12/22

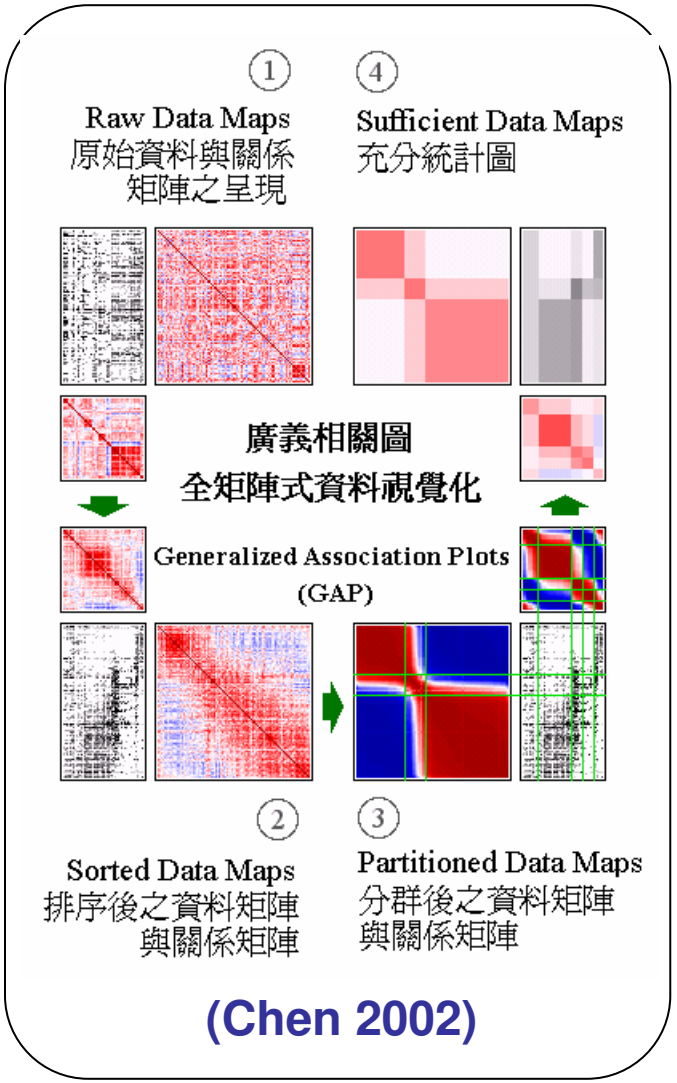
Outlines

- Two Demo Datasets
- Four Steps of Generalized Association Plots (GAP)

Raw Data Matrix and Two Proximity Matrices

Presentation 呈現 → Seriation 排序 → Partition 分割 → Sufficient 充分

- Generalization and Flexibility
- Modules/Software/Conclusion



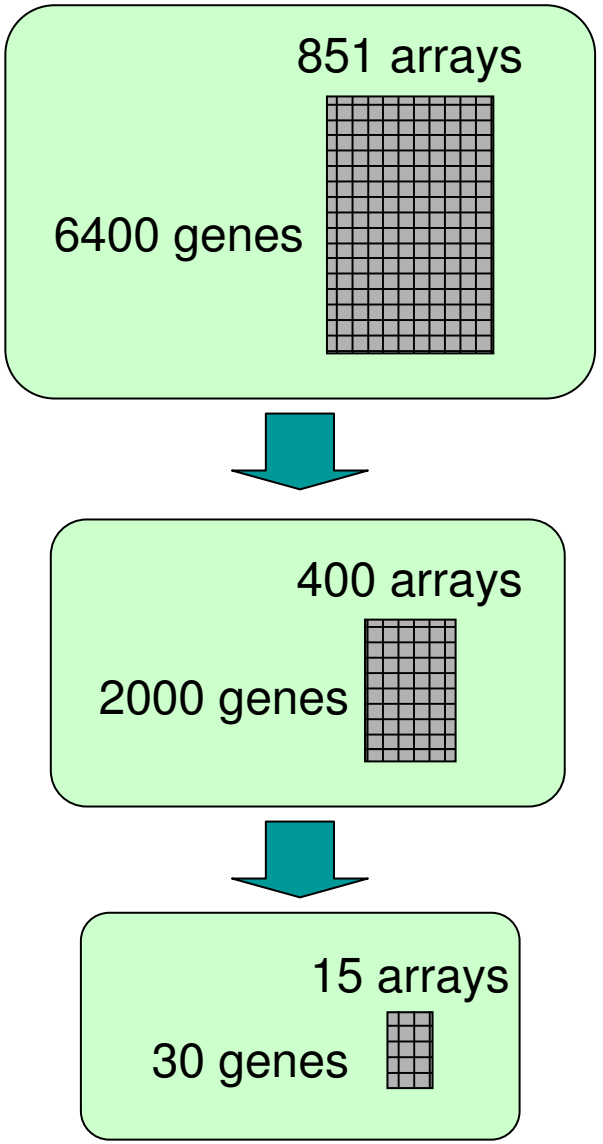
(Chen 2002)

NOTE: Matrix Visualization (MV): reorderable matrix, the heatmap, color histogram, data image and matrix visualization.

Microarray Gene Expression Data of Yeast Cell Cycle

yMGV: yeast Microarray Global Viewer

http://transcriptome.ens.fr/ymgv/



Psychosis Disorder Data

The Andreasen's Positive and Negative Symptom Table

Hallucinations (AH1-6)

Behavior (BE1-4)

Delusions (DL1-12)

Thought disorder (TH1-8)

Scale for Assessment of Positive Symptoms (**SAPS**): **30 items**, 4 subgroups.

Scale for Assessment of Negative Symptoms (**SANS**): **20 items**, 5 subgroups.

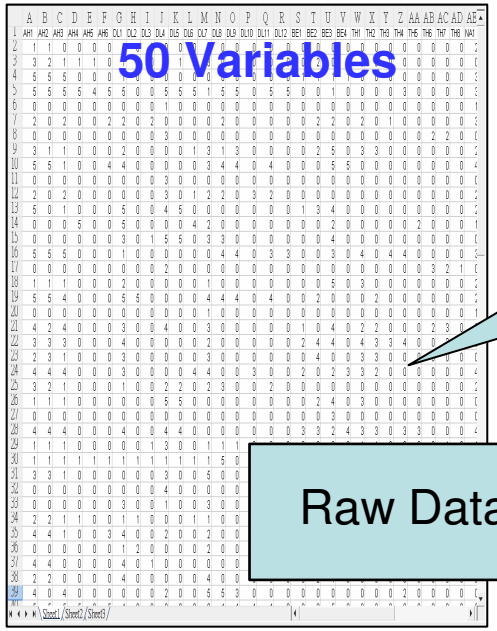
Expression (NA1-7)

Speech (NB1-4)

Hygiene (NC1-3)

Activity (ND1-4)

Inattentiveness (NE1-2)



50 Variables

All the symptoms are recorded on a six point scale (**0-5**).

95 Subjects

69 schizophrenic

26 bipolar disorders

Raw Data Matrix

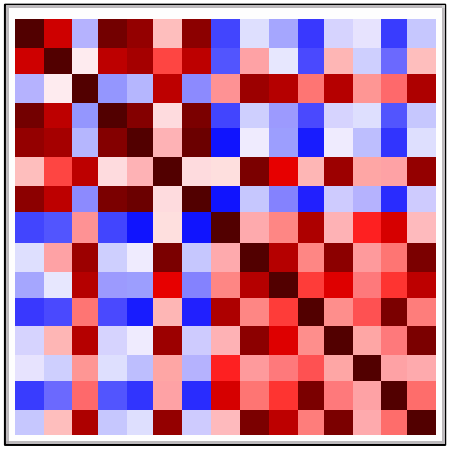
The 1st Step of GAP

Presentation of Raw Data Matrix

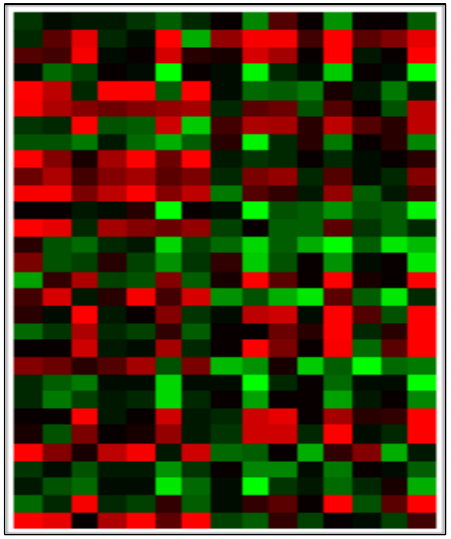
- Data Transformation
- Selection of Proximity Measures
- Color Spectrum
- Display Conditions

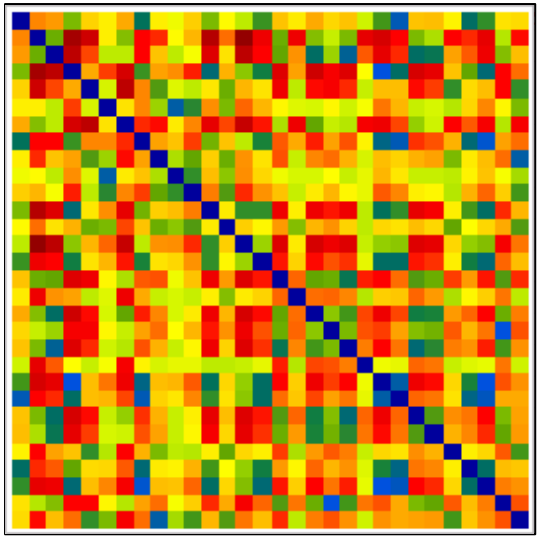
Presentation of Raw Data Matrix

Proximity Matrix for Columns



Proximity Matrix for Rows





(1) Selection of Proximity Measures

Pearson Correlation Coefficient

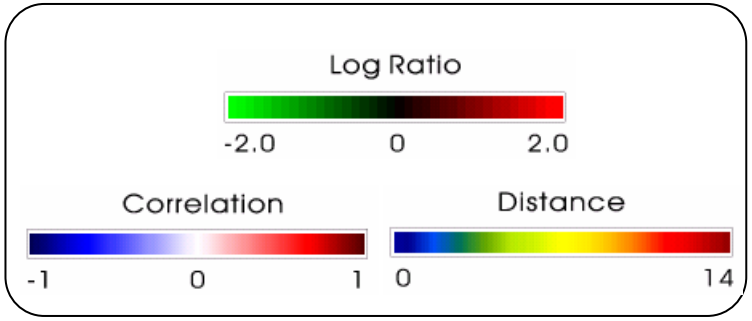
$$r_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

Euclidean Distance

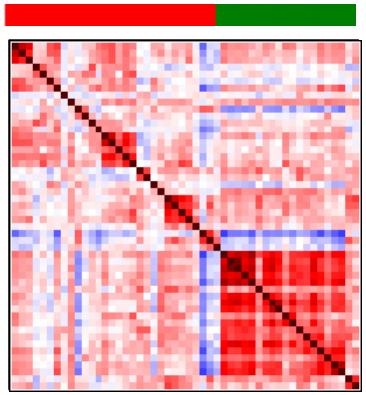
$$d_{xy} = \sqrt{\sum_{i=1}^{p}(x_i - y_i)^2}$$

Other Similarity/Dissimilarity Measures

(2) Color Spectrum

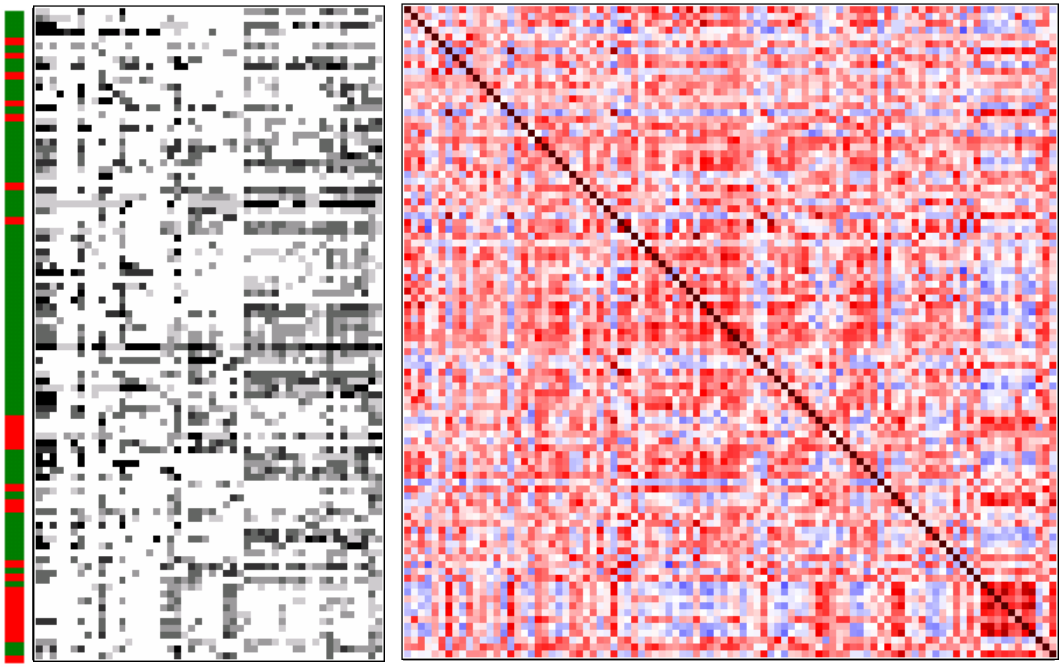


Presentation of Raw Data Matrix



Correlation Matrix for Variables

Correlation Matrix for Subjects

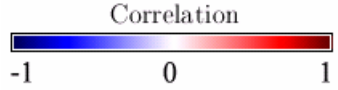


Raw Data Matrix

(1) Selection of Proximity Measures

Pearson Correlation Coefficient

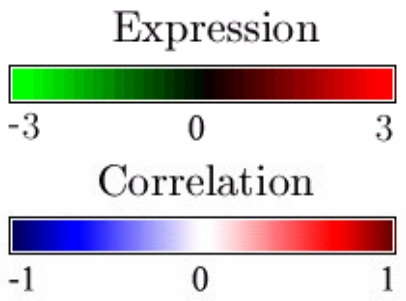
(2) Color Spectrum

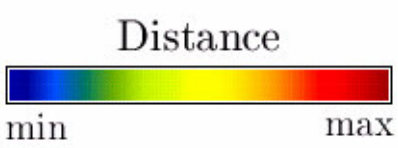


Symptoms
- SAPS
- SANS

Patients
- Schizophrenic
- Bipolar disorders

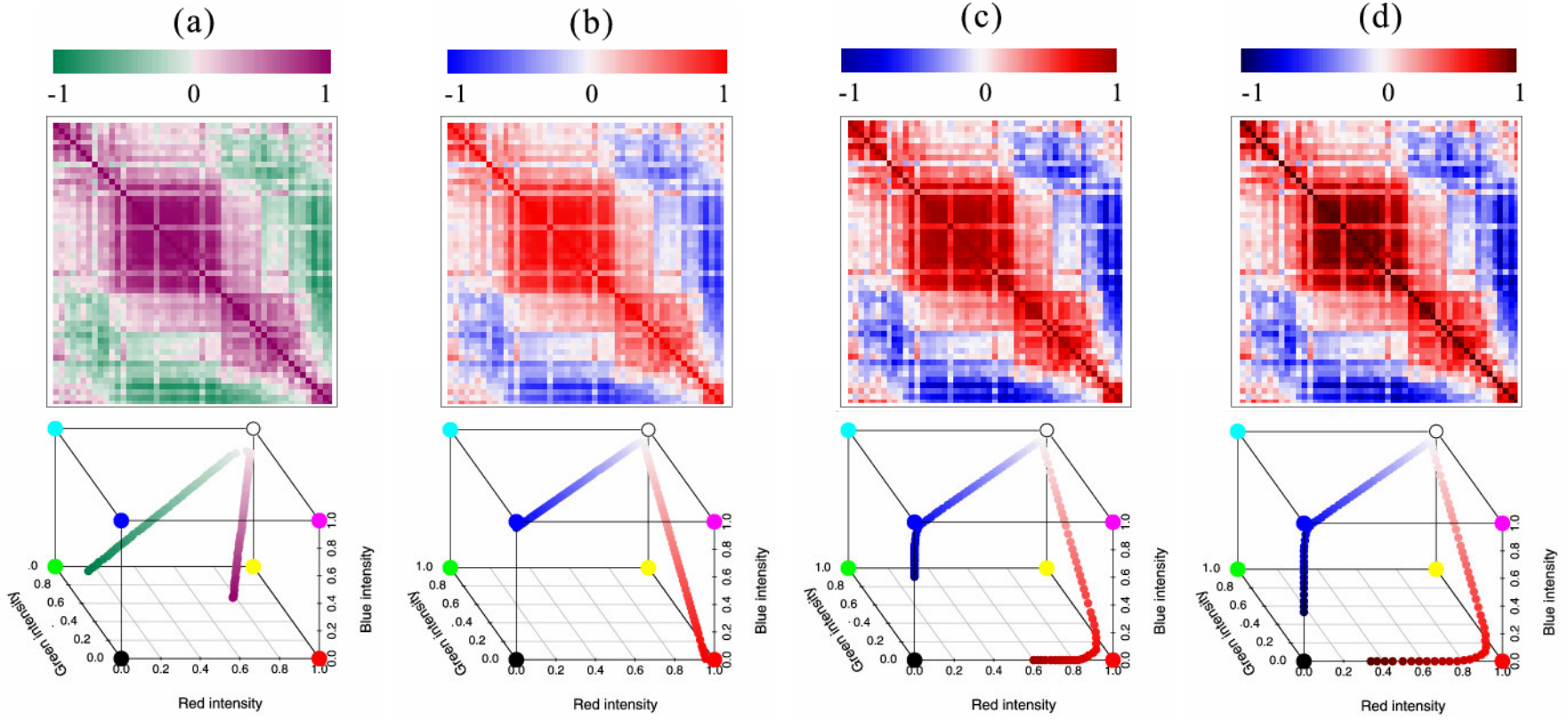
Color Spectra



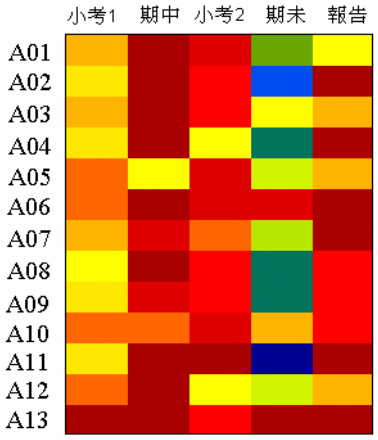


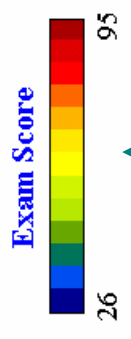
Correlation matrix map of 50 psychosis disorder variables

RGB

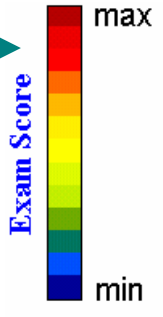


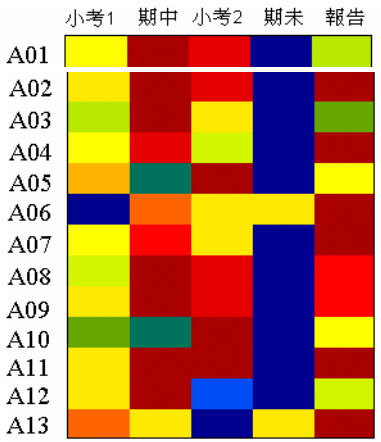
Display Conditions





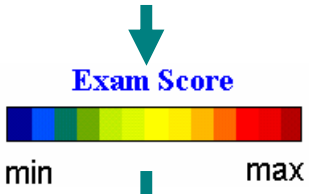
	A	B	C	D	E	F
1	學號	小考1	期中考	小考2	期末考	報告
2	A01	69	92	85	45	62
3	A02	66	90	83	36	90
4	A03	72	92	80	62	70
5	A04	68	90	60	37	95
6	A05	74	60	86	54	70
7	A06	77	90	88	88	95
8	A07	73	88	77	51	95
9	A08	61	90	84	40	82
10	A09	66	88	82	39	80
11	A10	76	75	87	72	80
12	A11	64	90	90	26	95
13	A12	75	90	60	55	70
14	A13	92	90	83	90	95

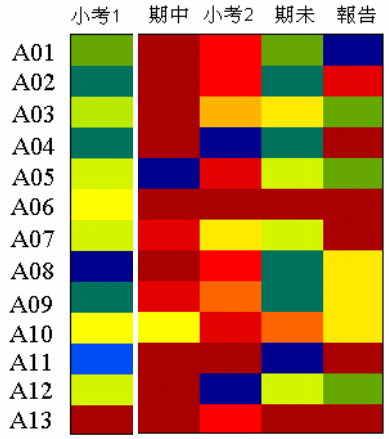




Range Matrix Condition

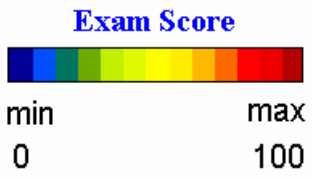
Range Row Condition





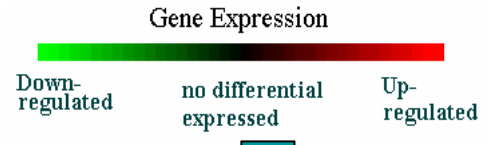
Range Column Condition

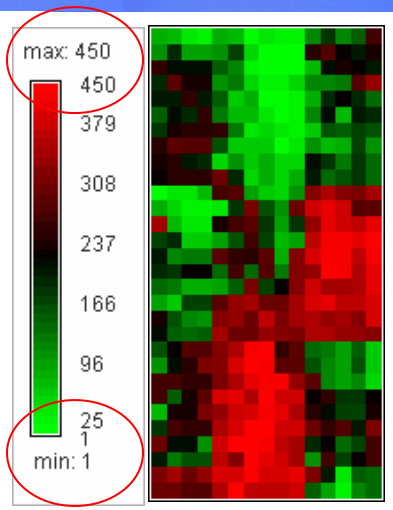
What about this one?



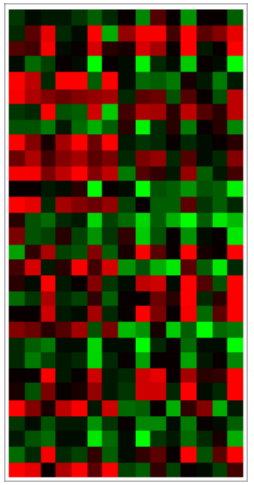
Display Conditions

	A	B	C	D	E	F	G	H	I
1	-1.37	-2.30	-1.80	-0.55	2.45	-0.13	1.49	3.03	2.48
2	-0.68	-2.11	-3.42	4.67	4.57	1.75	0.61	0.92	2.52
3	-1.19	-2.49	-3.66	3.14	1.70	3.29	3.33	2.92	2.48
4	-1.93	-2.28	-3.16	2.51	0.32	1.49	0.21	2.20	1.03
5	-2.21	-0.79	-3.29	2.55	2.44	1.45	2.68	3.03	0.19
6	-4.14	-2.91	-1.64	3.21	0.37	1.93	0.14	1.27	2.67
7	0.21	-1.36	-0.44	2.22	1.85	3.11	2.03	0.67	2.40
8	1.13	0.79	2.25	3.65	2.52	2.09	1.13	-2.59	0.67
9	0.95	2.33	-0.07	3.89	2.72	2.13	1.75	-2.17	-0.90
10	3.04	1.85	0.21	7.07	2.01	3.05	0.76	-2.58	-1.04
11	-1.02	1.65	1.53	0.95	0.60	3.12	2.52	-0.77	-1.40
12	1.21	0.24	1.04	2.50	3.69	1.81	3.98	-0.33	0.11
13	1.74	1.60	1.70	2.02	3.45	4.46	2.69	0.41	-0.09
14	1.34	1.06	0.06	1.81	2.90	3.64	3.04	0.49	-2.33
15	0.57	1.81	-0.47	1.40	2.70	0.99	0.82	-1.61	-2.56
16	0.61	4.22	-2.03	-2.61	-4.00	-4.64	-2.92	1.55	-0.71
17	-1.13	1.64	0.01	-1.77	-2.85	-1.24	-3.41	-0.59	-1.64
18	-0.86	-1.17	-0.41	-2.20	-1.30	-2.37	-1.41	0.08	0.25
19	0.75	0.66	1.04	-4.26	-1.41	-3.99	-3.53	-2.17	0.34
20	0.15	0.68	3.18	-2.86	-2.01	-3.18	-1.58	0.10	1.28

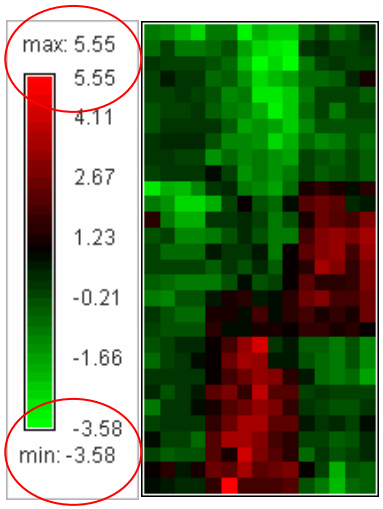




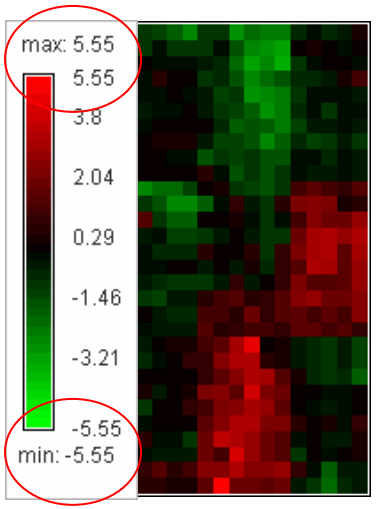
Rank Matrix Condition



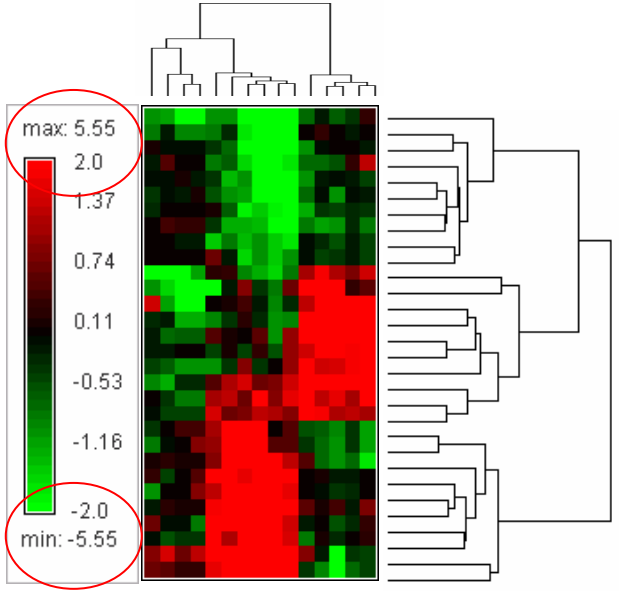
Without ordering



Range Matrix Condition



Center Matrix Condition



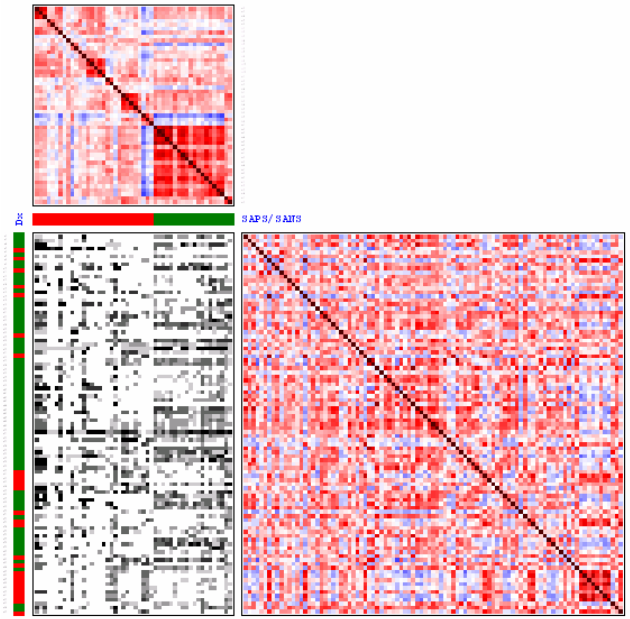
The 2nd Step of GAP

Seriation of Proximity Matrices and Raw Data Matrix

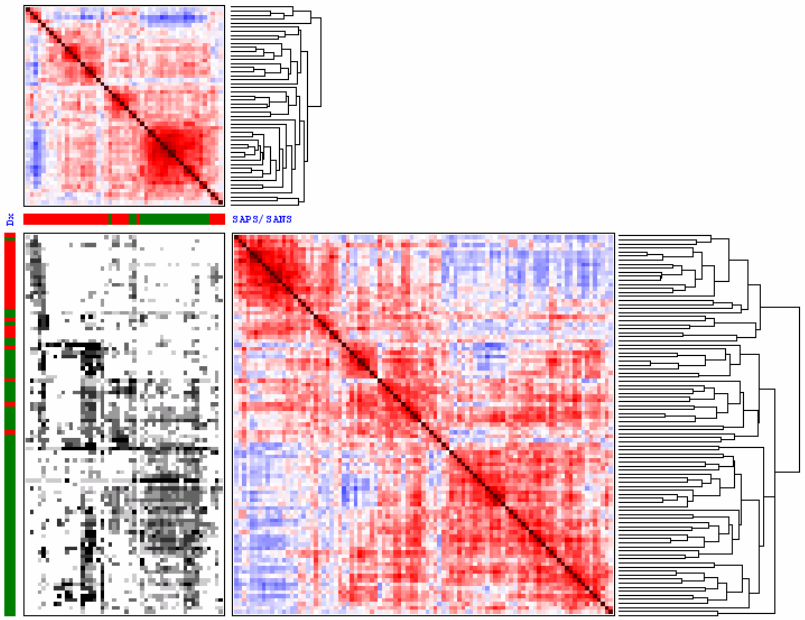
- Relativity of a Statistical Graph
- Global Criterion
  - GAP Rank-Two Elliptical Seriation
- Local Criterion
  - Tree Seriation
  - Flipping of Tree Intermediate Nodes

Relativity of a Statistical Graph

Placing similar (different) objects at closer (distant) positions.

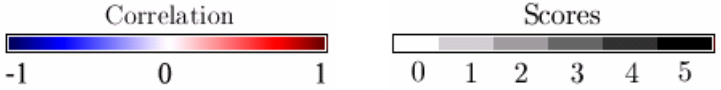


Seriation Methods



(1) Rank Two Ellipse Ordering (Chen, 2002)

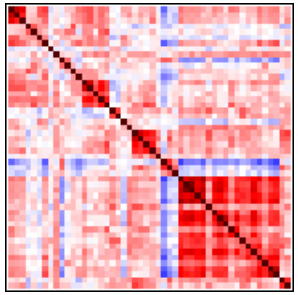
(2) Hierarchical Clusterting Tree (Average-Linkage)

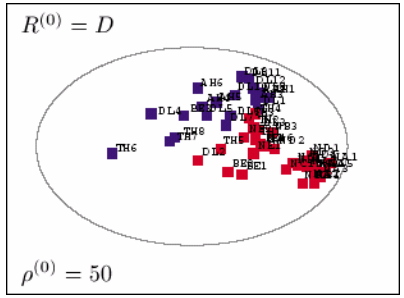


GAP Rank-Two Elliptical Seriation

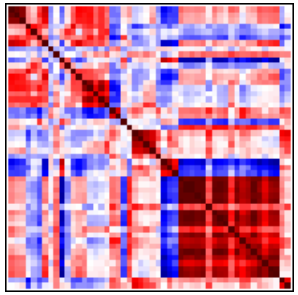
Seriation Algorithms with Converging Correlation Matrices

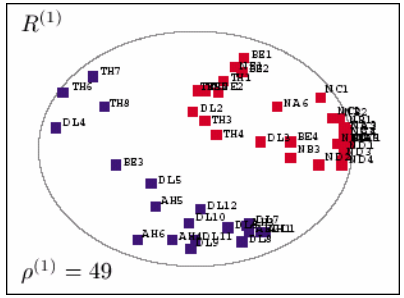
Correlation Matrix (without ordering)

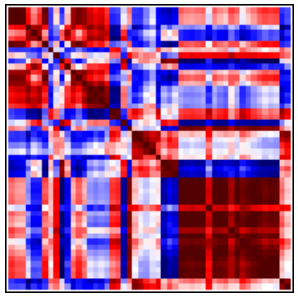


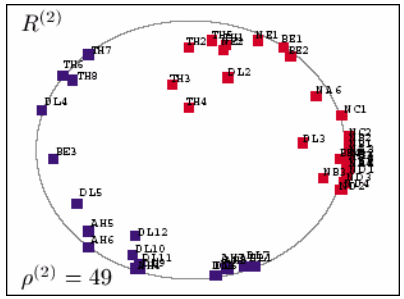


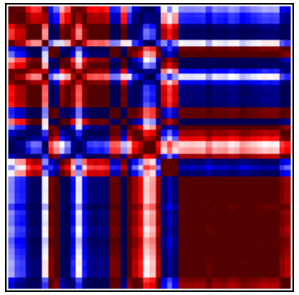
First two Eigenvectors

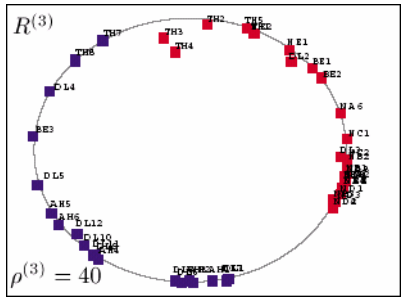


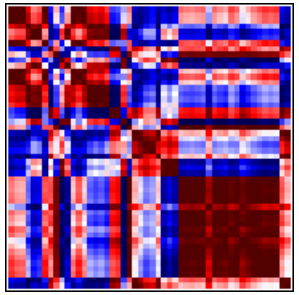


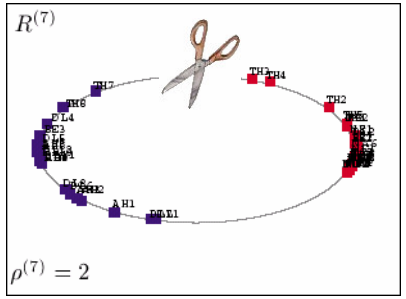




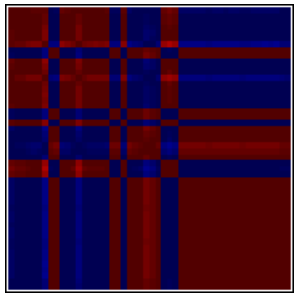


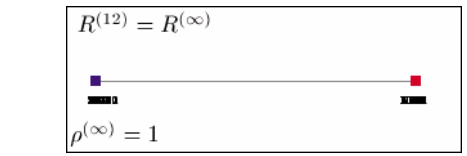


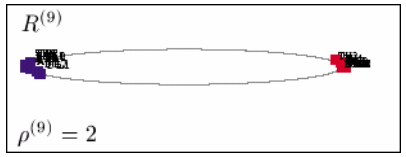


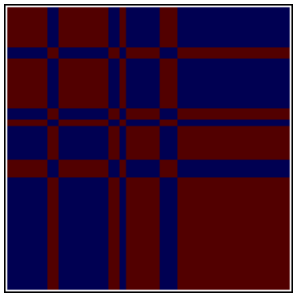


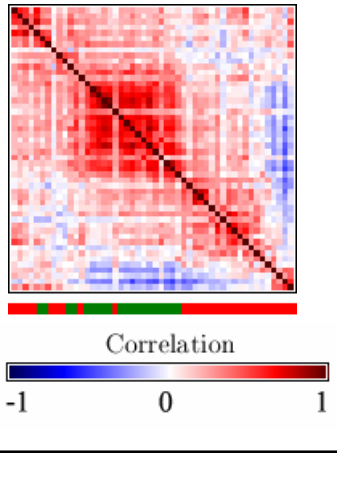
The p objects fall on an ellipse and have unique relative position on the ellipse (Chen 2002).





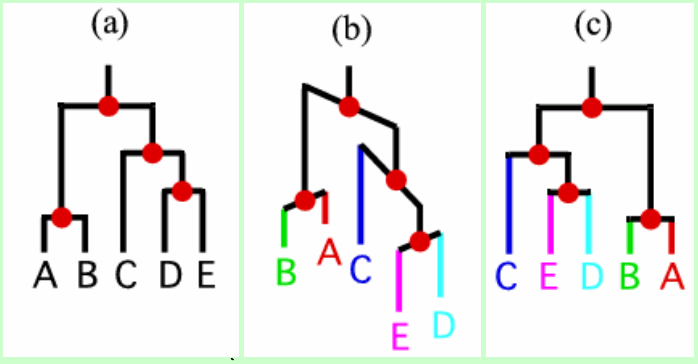




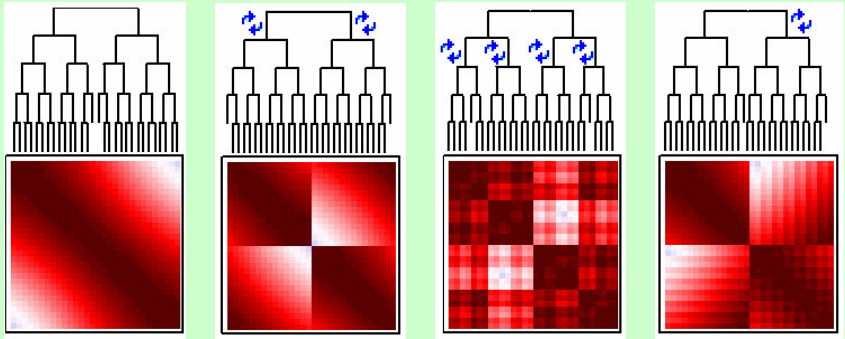


Hierarchical Clustering Tree with a Dendrogram

Tree seriation

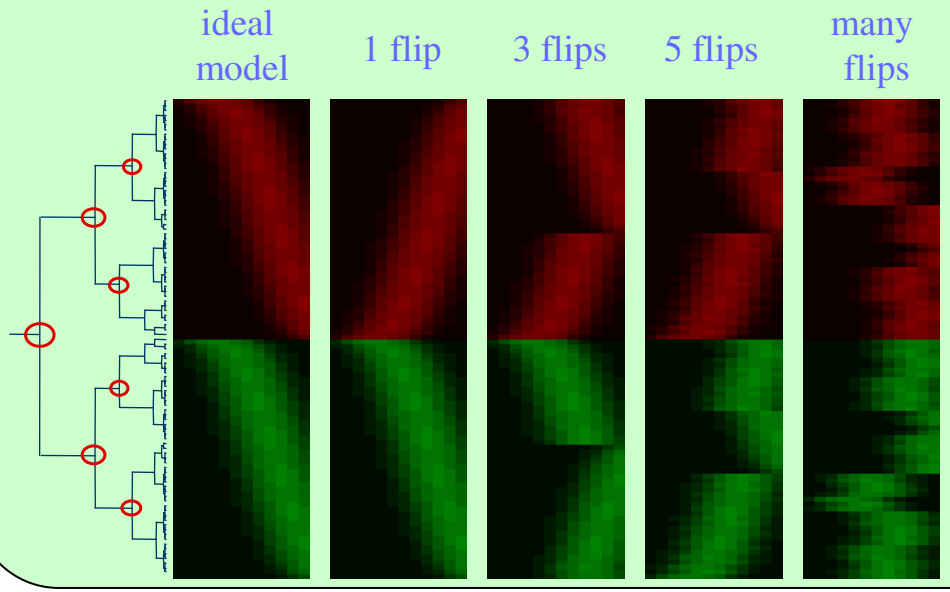


Tree seriation for proximity matrices



Different Seriations Generated from Identical Tree Structure

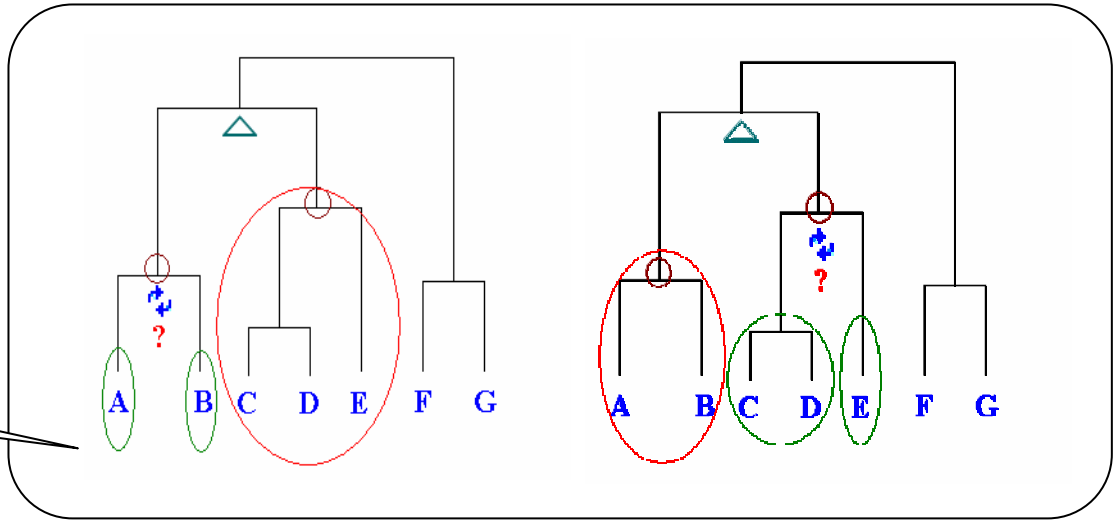
Tree seriation for raw data matrices



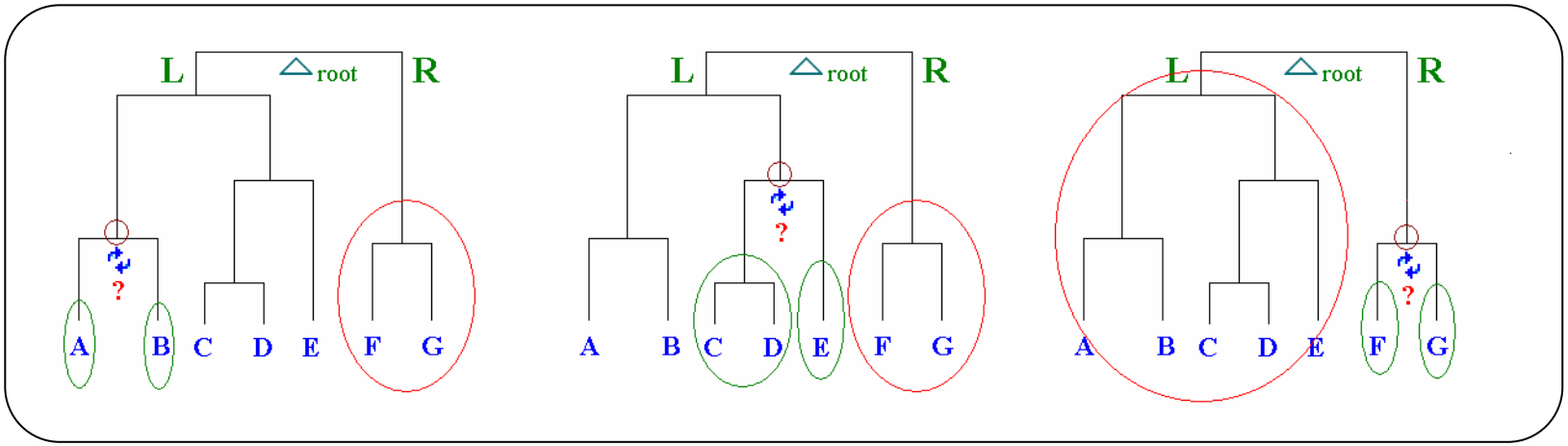
Internal Tree Flips

Uncle Approach

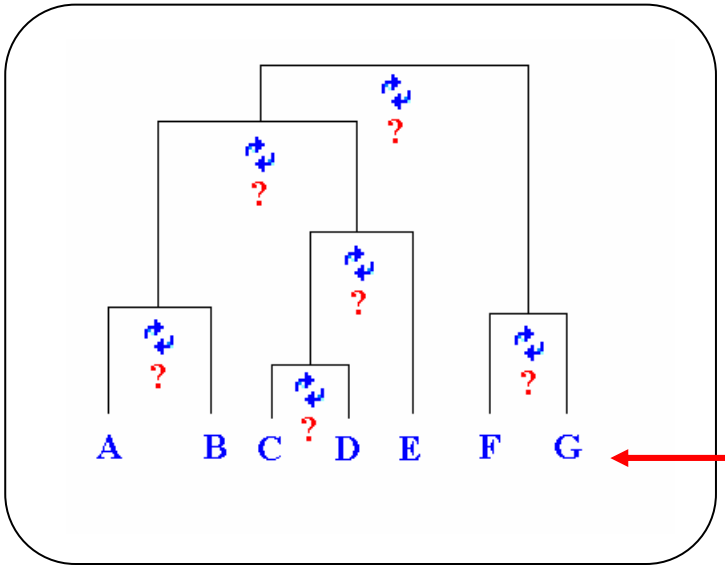
if d(A, {C,D, E}) < d(B, {C,D, E})
then flip



GrandPa Approach



External Tree Flips



As close as possible

External Ordering D E A F B C G

How to build an external ordering?

(1) Based on average expression level (Cluster Software, Eisen et al 1998)
(2) Using the results of a one-dimensional SOM
(3) …

Global vs. Local Seriation

Data: 517 genes by 13 arrays

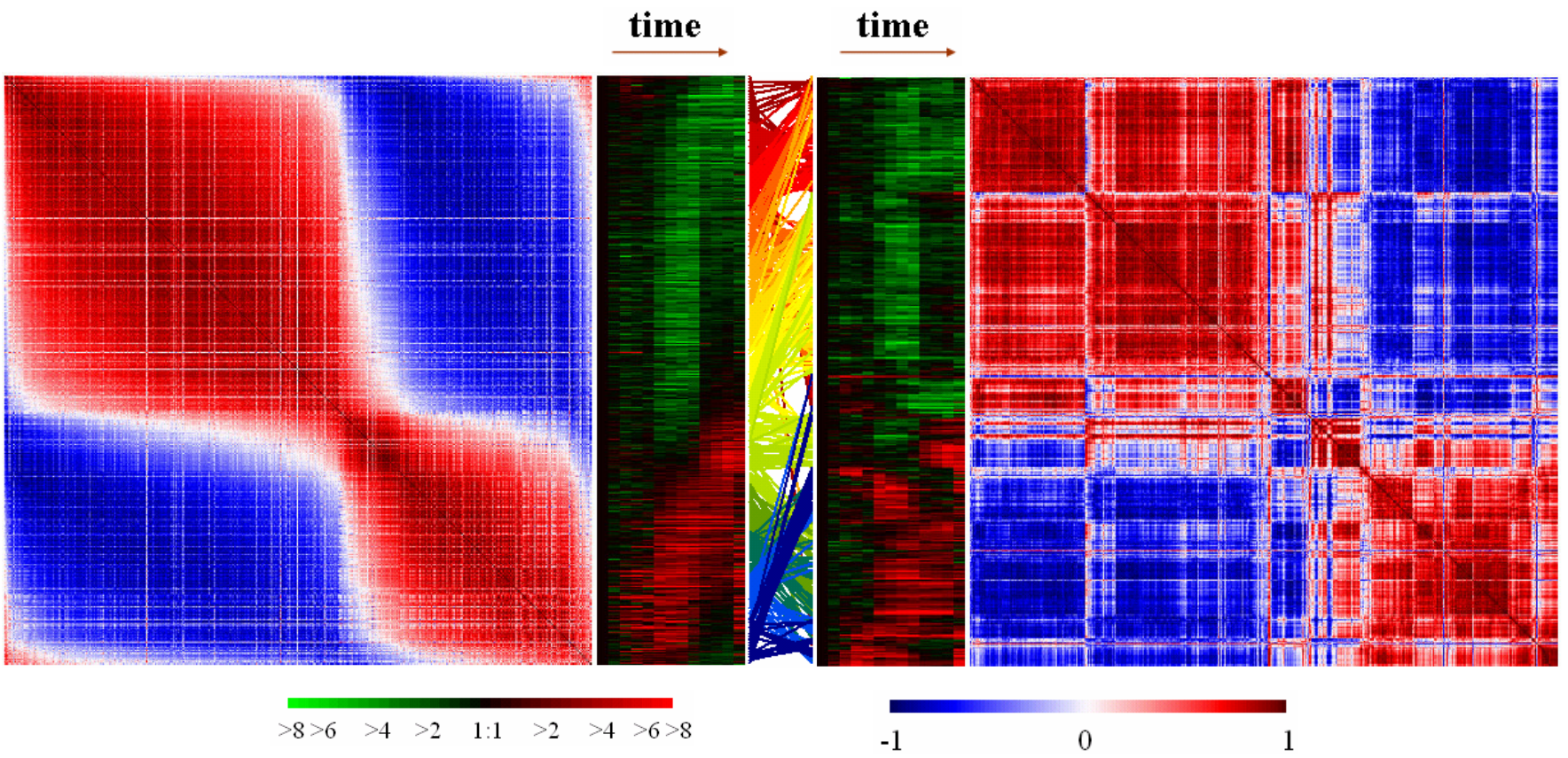
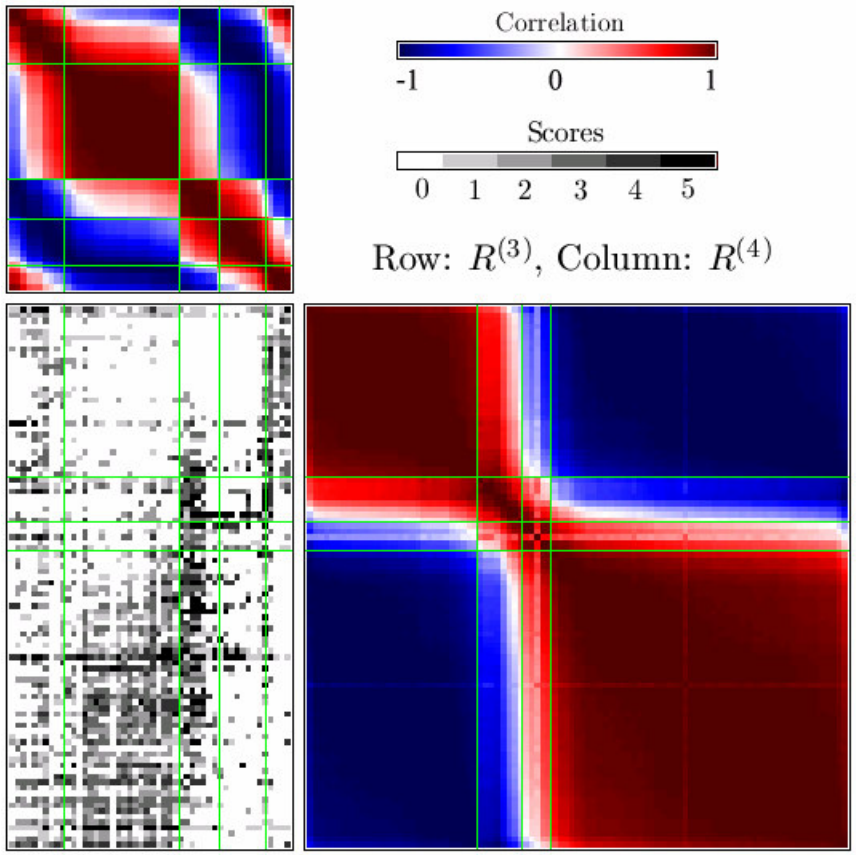
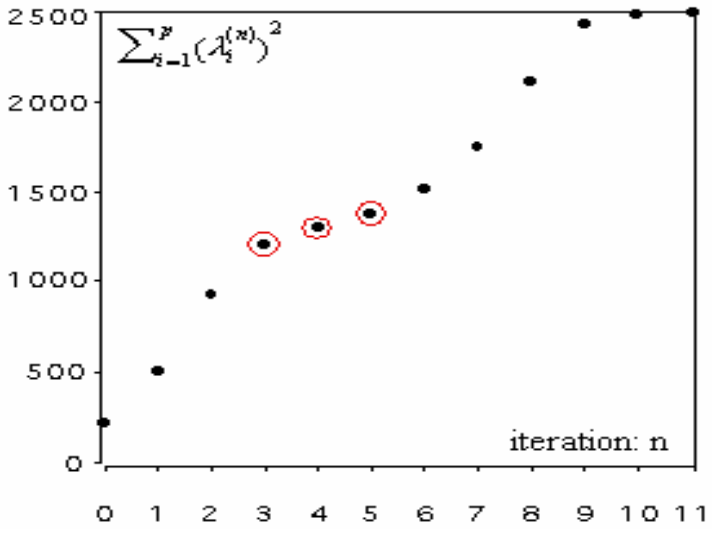


Image source: Dr. Chen Chun-houh's slide

Partitions of Permuted Matrix Maps

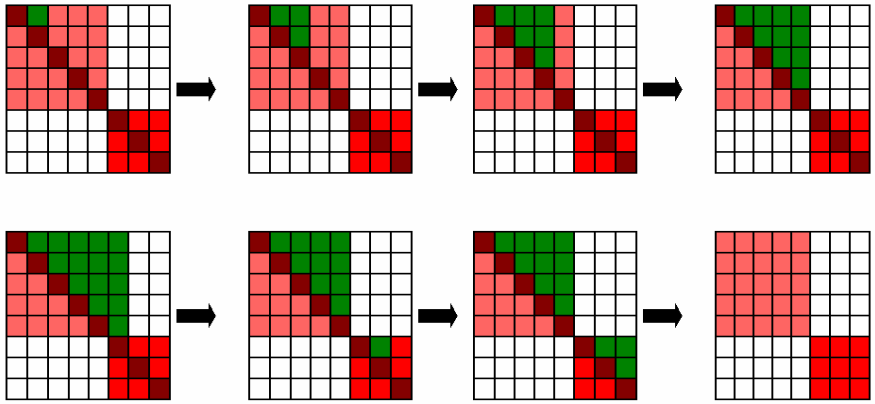


Sum squared eigenvalues (sum squared correlations)

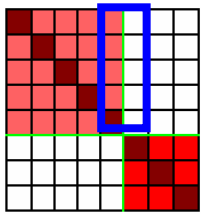


Partitions of Permuted Matrix Maps

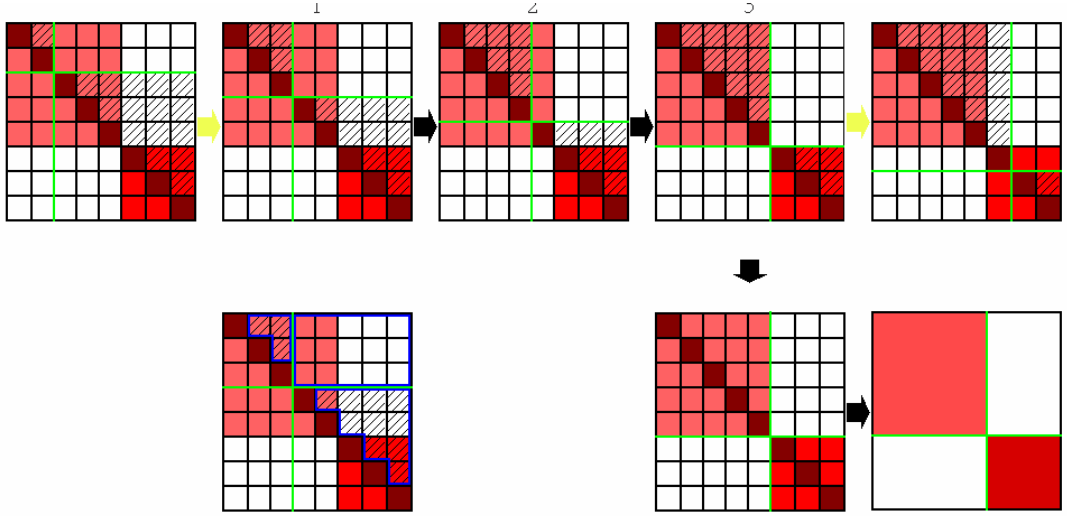
One-Way block Searching



Two-Sample Problem



Within-Sum-of-Square Approach



The 4th Step of GAP

Sufficient Graph

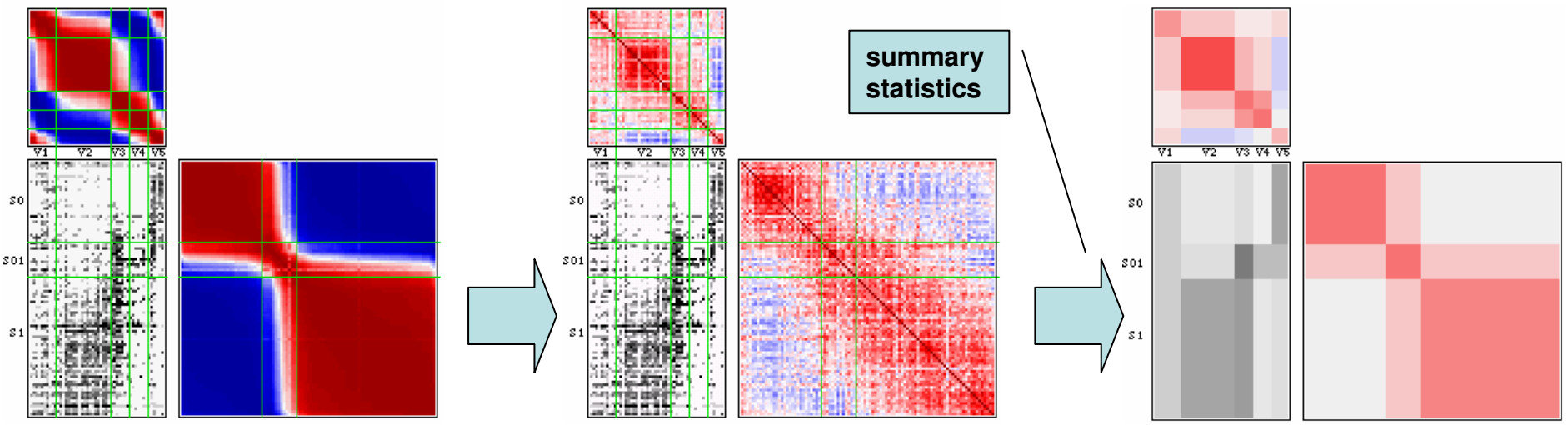
	A	B	C	D	E	F
1	學號	小考1	期中考	小考2	期末考	報告
2	A01	69	92	85	45	62
3	A02	66	90	83	36	90
4	A03	72	92	80	62	70
5	A04	68	90	60	37	95
6	A05	74	60	86	54	70
7	A06	77	90	88	88	95
8	A07	73	88	77	51	95
9	A08	61	90	84	40	82
10	A09	66	88	82	39	80
11	A10	76	75	87	72	80
12	A11	64	90	90	26	95
13	A12	75	90	60	55	70
14	A13	92	90	83	90	95

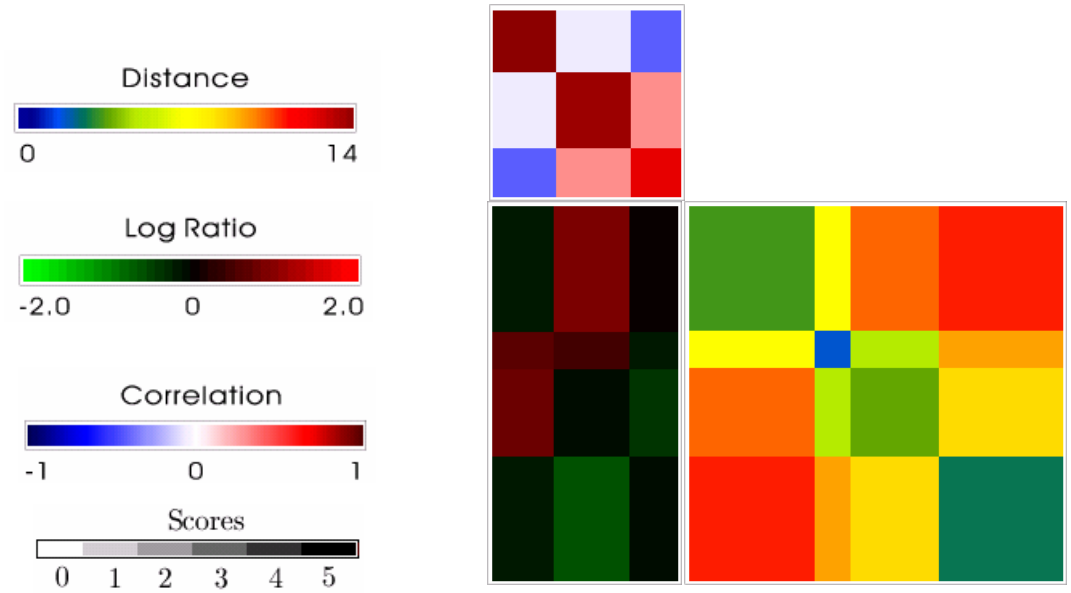
Sufficient Statistics

	小考1	期中考	小考2	期末考	報告
平均	71.77	86.54	80.38	53.46	83

70	低平均	65.67	81.83	73.67	53.67	72
	高平均	77.83	90.67	86.67	53.67	94.17

Sufficient Graph





Summarizing Display

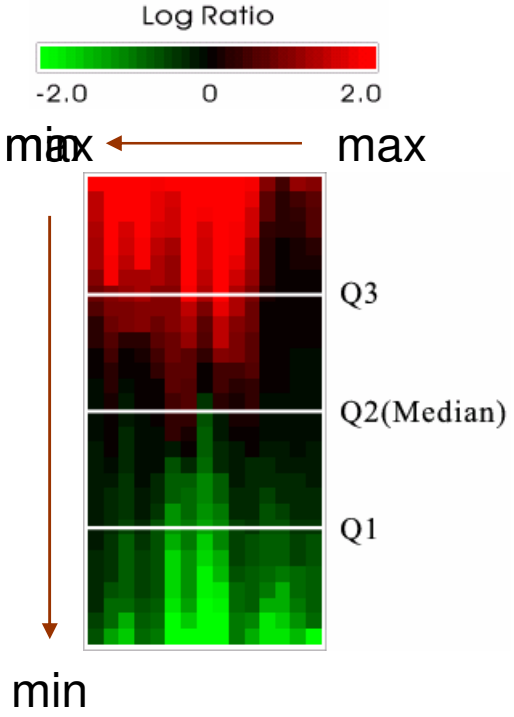
(1) subject-subject

(2) variable-variable

(3) subject-variable

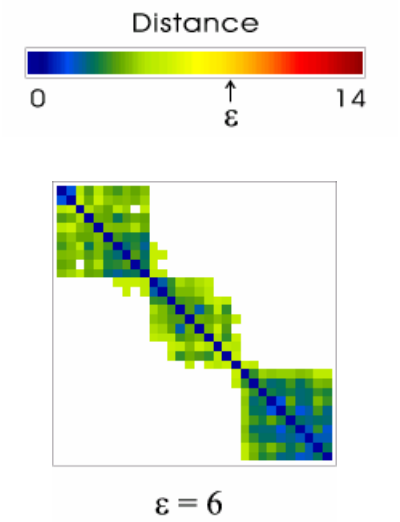
Generalization and Flexibility

Sediment Display



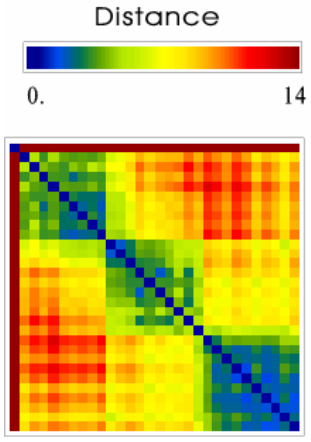
Similar information to that given by a boxplot when the color strips at the quartile positions are extracted.

Sectional Display

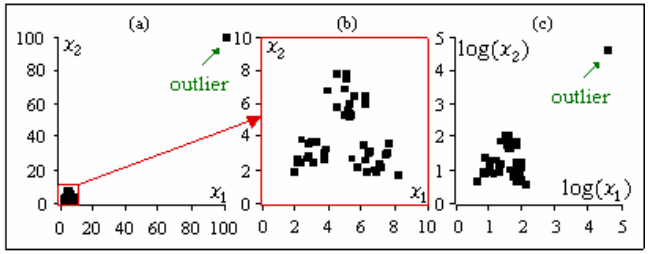


Display only those numerical values that satisfy certain conditions.

Restricted Display

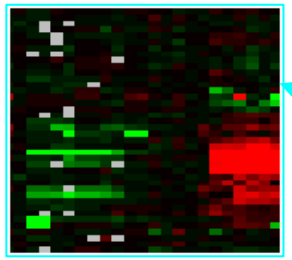


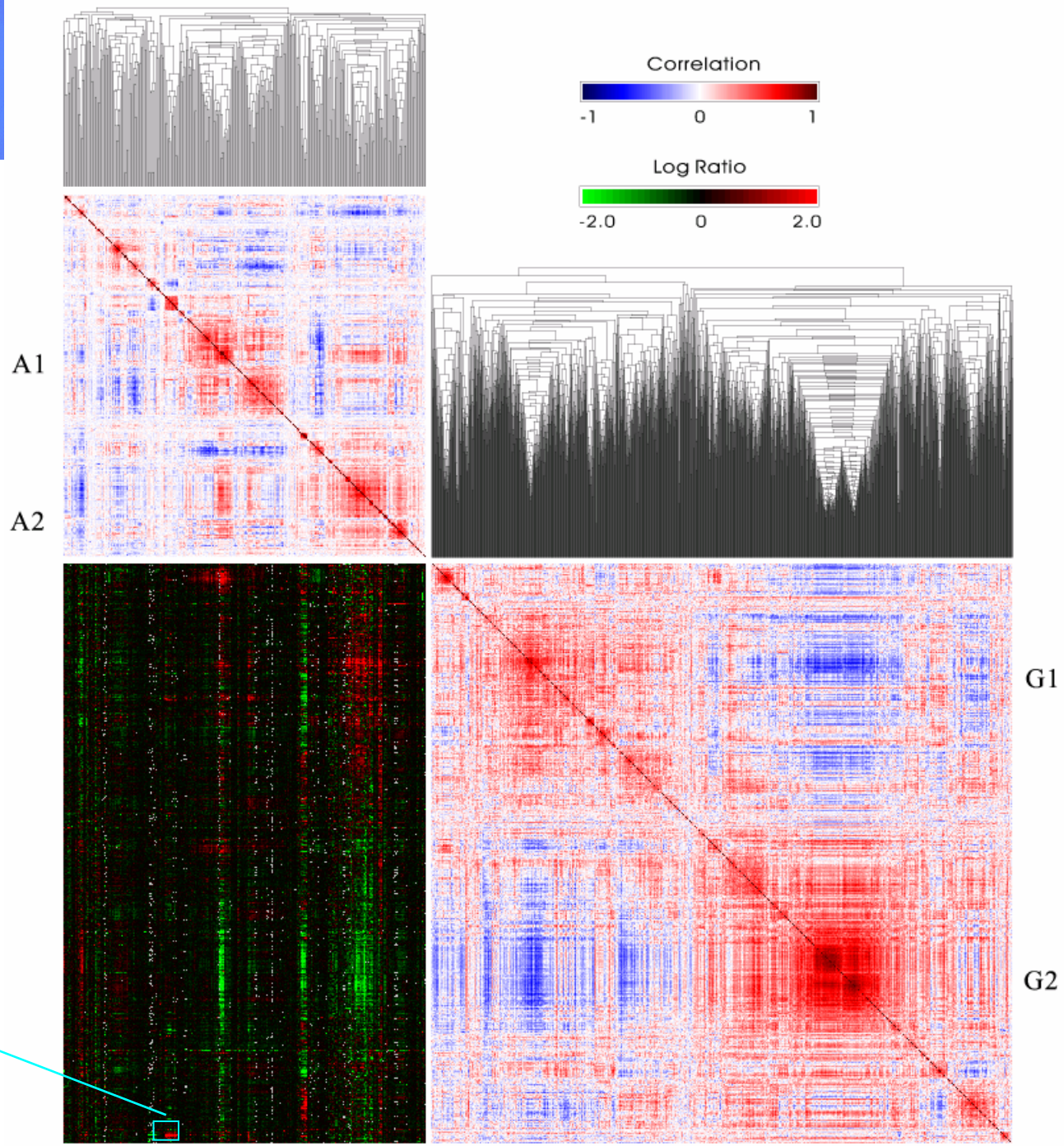
Resolution of a Statistical Graph



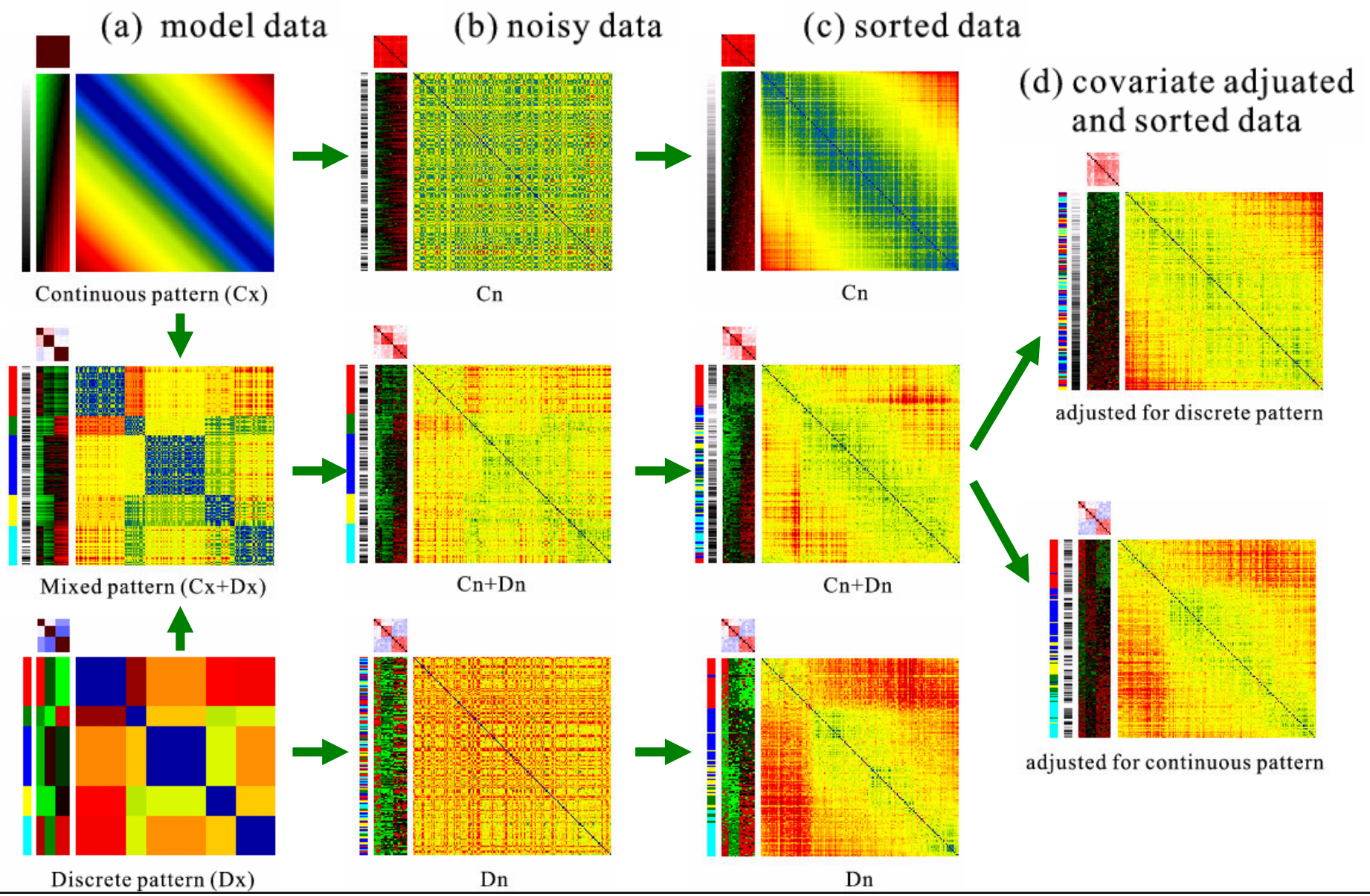
An Example

- 2000 genes by 400 arrays with relatively fewer missing values.
- Pearson's correlation coefficient.
- Average linkage clustering trees.
- The basic gene clustering structure and array (experiments) grouping patterns can be identified using these tree sorted matrix maps.



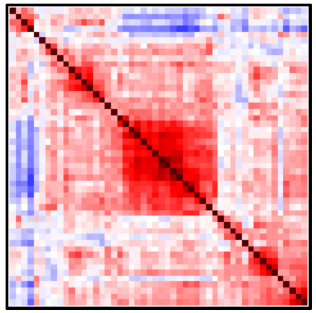


Module: MV for Covariate Adjustment



Module: Interactive Diagnostic System for Hierarchical Clustering Tree with Matrix Visualization

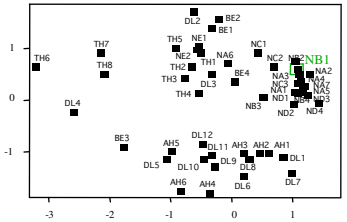
(1) Input Proximity Matrix



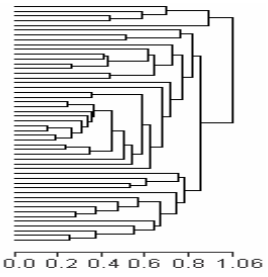
(e.g., Pearson's Correlation)

Statistical Modeling

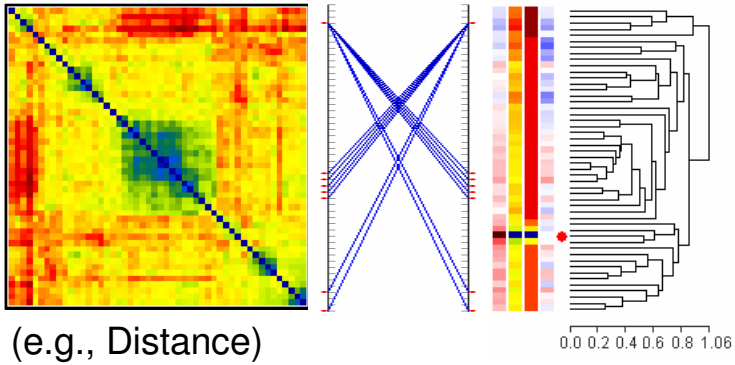
Multidimensional Scaling (MDS)



Hierarchical Clustering Tree (HCT)

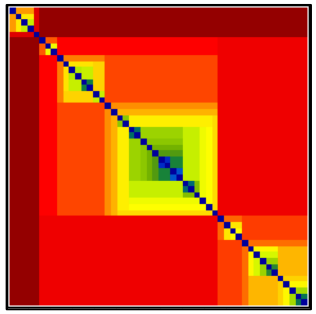


(2) Transformed Disparity Matrix

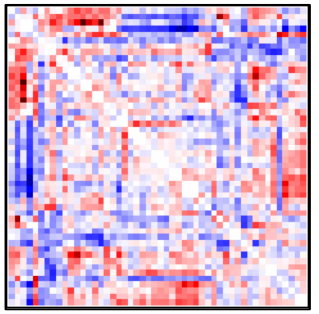


(e.g., Distance)

(e.g., Cophenetic Matrix)

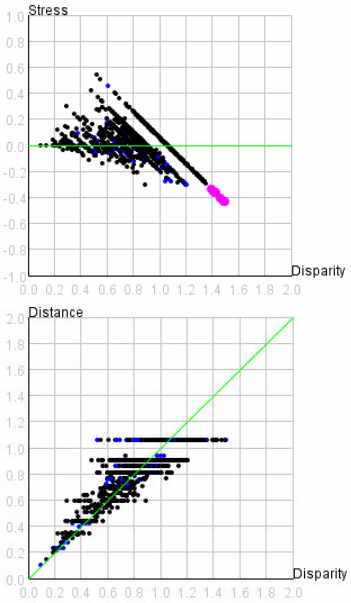


(e.g., Residual Matrix)



(3) Output Distance Matrix

(4) Stress Matrix



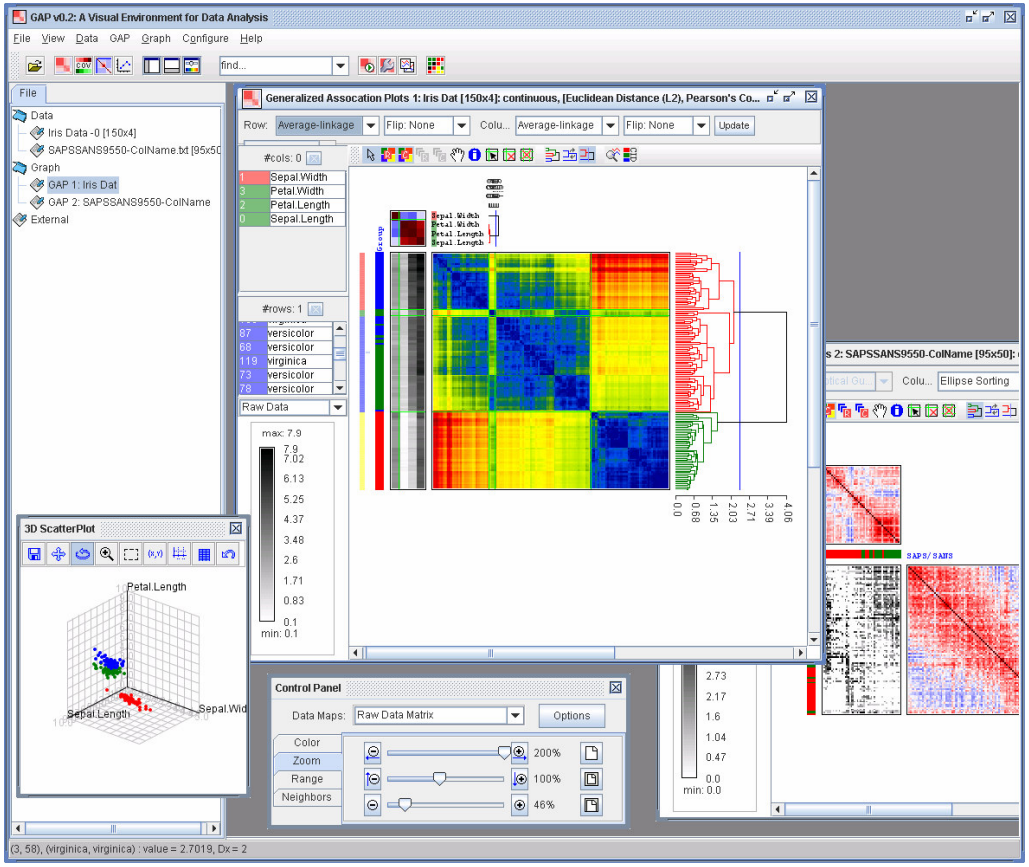
GAP Software verison 0.2

Generalized Association Plots

- Input Data Type: continuous or binary.
- Various seriation algorithms and **clustering analysis**.
- Various display conditions.
- Modules:
  GAP with Covaraite Adjusted,
  Nonlinear Association Analysis,
  Missing Value Imputation.

Statistical Plots

- 2D Scatterplot, 3D Scatterplot (Rotatable)



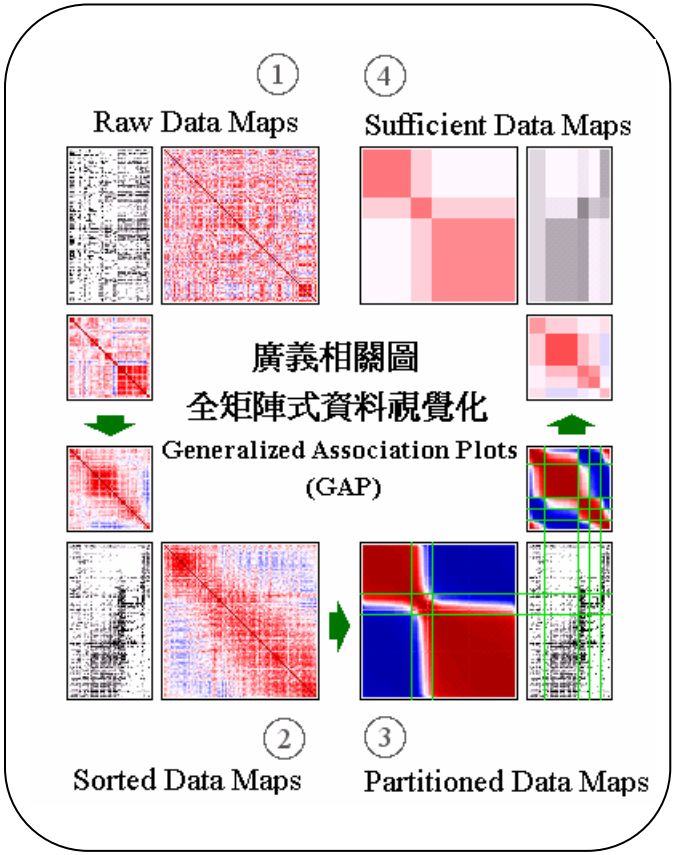
http://gap.stat.sinica.edu.tw/Software/GAP

Conclusion

MV is the **color order-based** representation of data matrices.

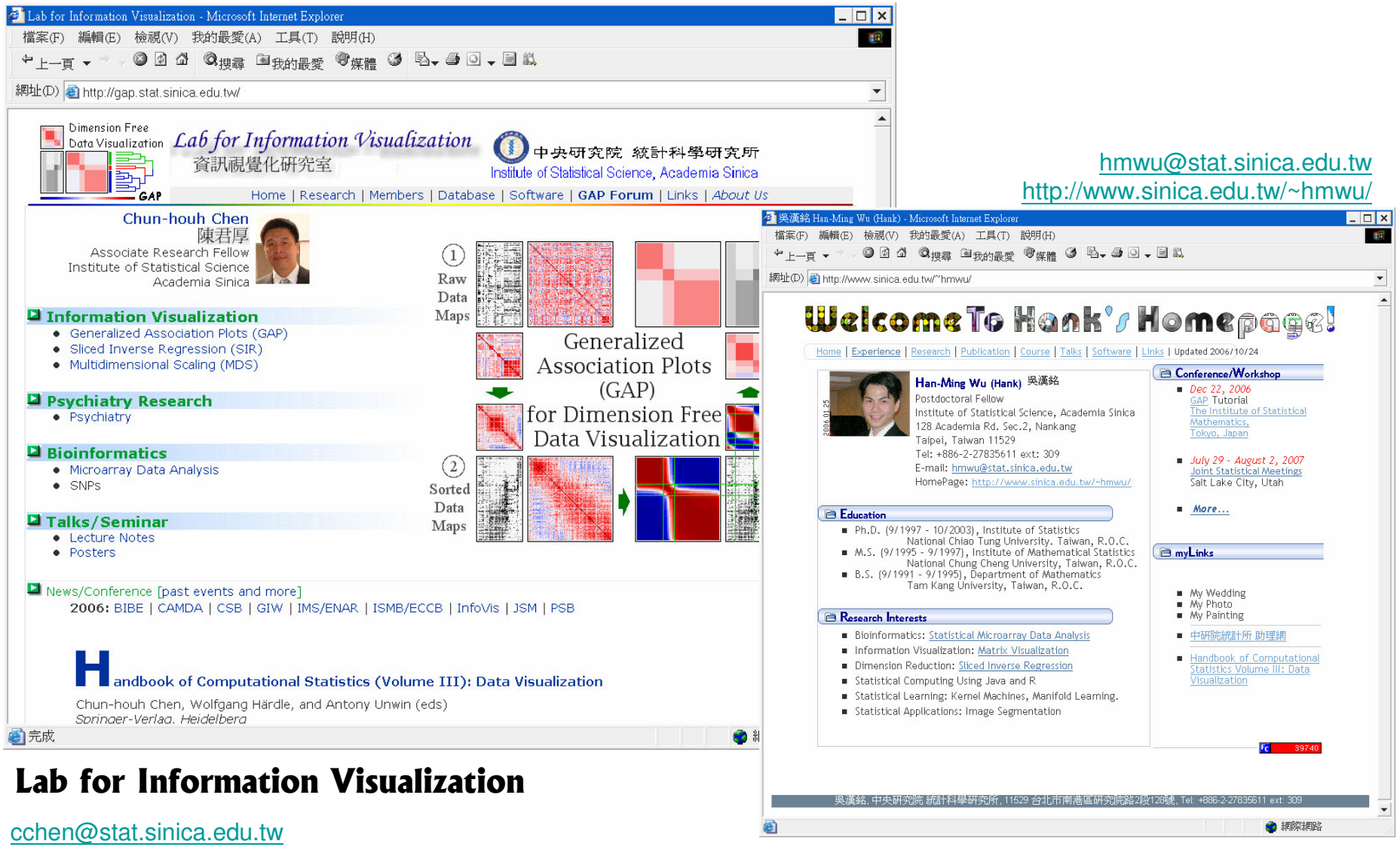
A MV displays provide five levels of information:

1. raw scores for every sample/variable combination;
2. an individual sample score vector across all variables, and an individual variable vector across all samples;
3. an association score for every sample-sample and variable-variable relationship;
4. a grouping structure for variables and a clustering effect for sample;
5. an interaction pattern of sample-clusters on variable-groups.



- **A preliminary step in modern exploratory data analysis.**
- **A continuing and active topic of research and application.**
- **New generation of exploratory data analysis (EDA) tool.**

Web Site



Lab for Information Visualization

cchen@stat.sinica.edu.tw
http://gap.stat.sinica.edu.tw

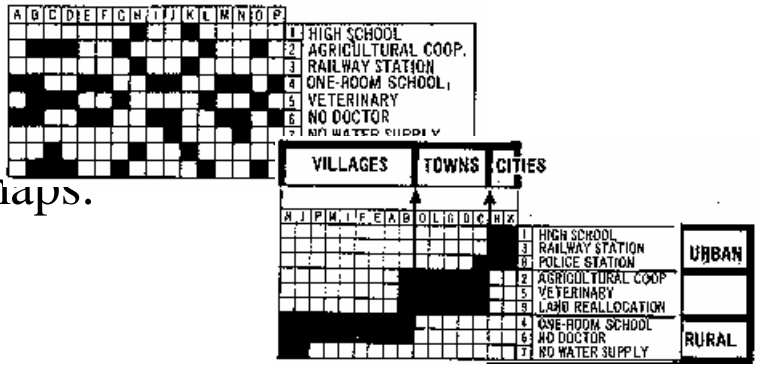
hmwu@stat.sinica.edu.tw
http://www.sinica.edu.tw/~hmwu/

Appendix

Related Works of MV

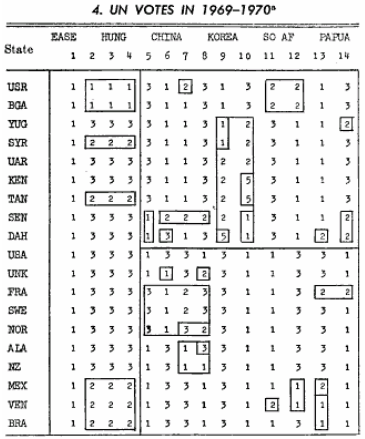
Concept:

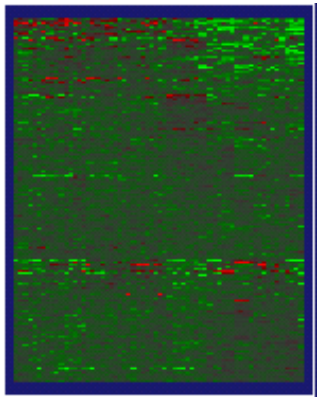
- Bertin (1967): reorderable matrix.
- Carmichael and Sneath (1969): taxometric maps.



Clustering of data arrays:

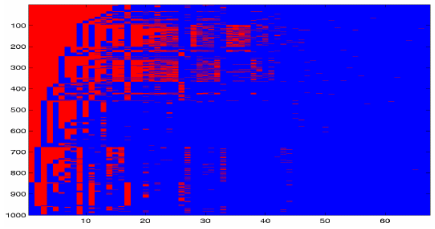
- Hartigan (1972): direct clustering of a data matrix.
- Tibshirani (1999): block clustering.
- Lenstra (1974): traveling-salesman problem.
- Slagle *et al.* (1975): shortest spanning path.

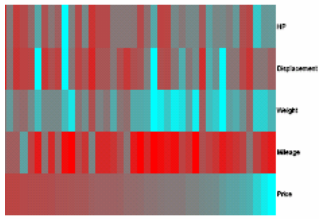




Colour Representation:

- Wegman (1990): colour histogram.
- Minnotte and West (1998): data image.
- Marchette and Solka (2003): outlier detection.

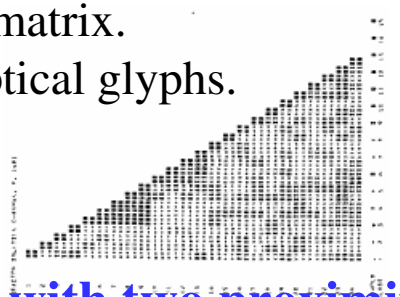


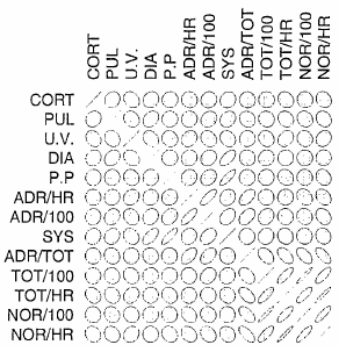


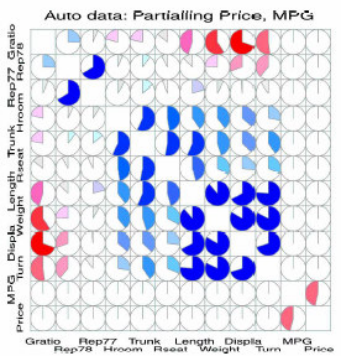
Related Works (conti.)

Exploring proximity matrices only:

- Ling (1973): shaded correlation matrix.
- Murdoch and Chow (1996): elliptical glyphs.
- Friendly (2002): corrgrams.

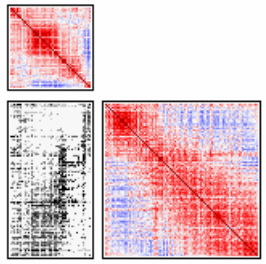






Integration of raw data matrix with two proximity matrices

- Chen (1996, 1999, and 2002): generalized association plots (GAP).

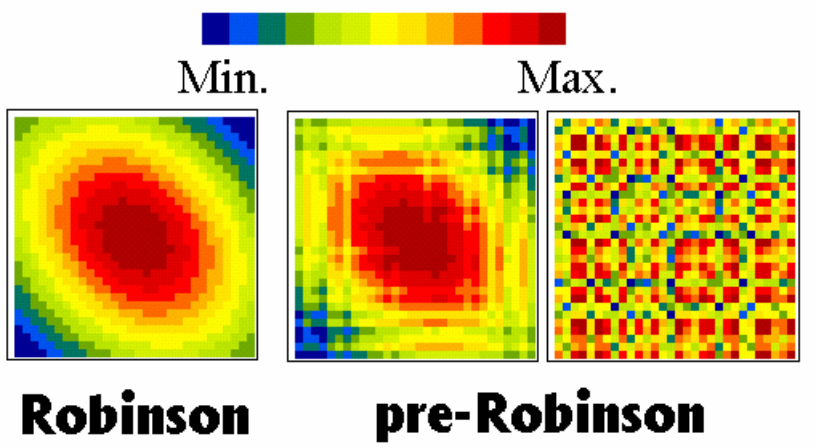


Reordering of variables and samples

- Chen (2002): concept of relativity of a statistical graph.
- Friendly and Kwan (2003): effect ordering of data displays.
- Hurley (2004): placing interesting displays in prominent positions.

Matrix Visualization (MV): reorderable matrix, the heatmap, color histogram, data image and matrix visualization.

Criteria for a *good* Permutation



Global criterion:

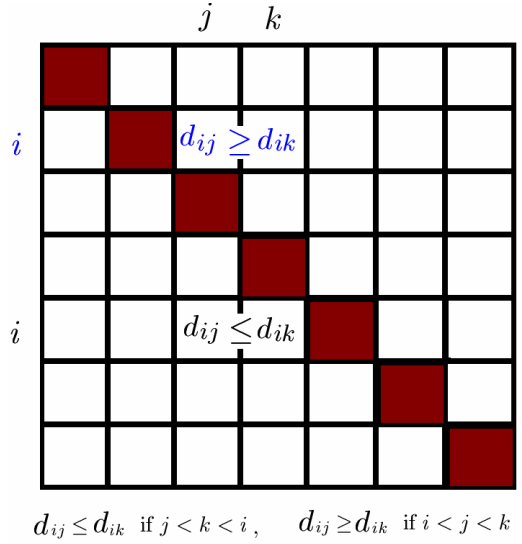
Anti-Robinson Measurements

$$AR(i) = \sum_{i=1}^{p} \Big[\sum_{j<k<i} I(d_{ij} < d_{ik}) + \sum_{i<j<k} I(d_{ij} > d_{ik}) \Big],$$

$$AR(s) = \sum_{i=1}^{p} \Big[\sum_{j<k<i} I(d_{ij} < d_{ik}) \cdot |d_{ij} - d_{ik}| + \sum_{i<j<k} I(d_{ij} > d_{ik}) \cdot |d_{ij} - d_{ik}| \Big],$$

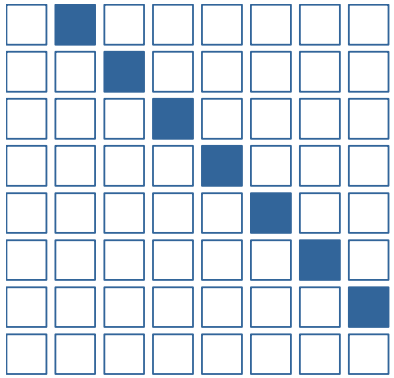
$$AR(w) = \sum_{i=1}^{p} \Big[\sum_{j<k<i} I(d_{ij} < d_{ik}) |j-k| |d_{ij} - d_{ik}| + \sum_{i<j<k} I(d_{ij} > d_{ik}) |j-k| |d_{ij} - d_{ik}| \Big].$$

When T is symmetric, we usually want T' to approximate a Robinson form (Robinson (1951)).



Local criterion:

Minimal Span Loss Function



$$MS = \sum_{i=1}^{n-1} d_{i,i+1}$$

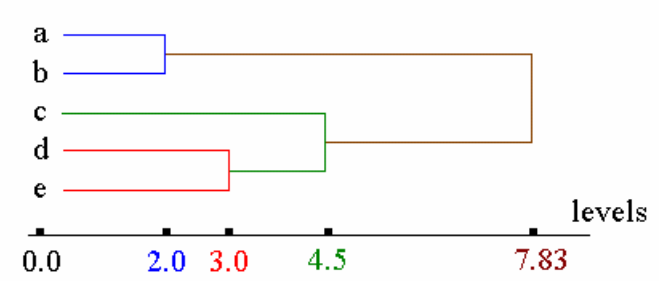
Hierarchical Clustering Tree

(Kaufman and Rousseeuw, 1990)

Example: Average-Linkage

distance matrix

	a	b	c	d	e
a	0	2	6	10	9
b		0	5	9	8
c			0	4	5
d				0	3
e					0



	{a, b}	c	d	e
{a, b}	0	5.5	9.5	8.5
c		0	4	5
d			0	3
e				0

$$D(\{a,b\},\{c\}) = \frac{1}{2}[D(a,c) + D(b,c)]$$

$$= \frac{1}{2}(6+5) = 5.5$$

	{a, b}	c	{d, e}
{a, b}	0	5.5	9.0
c		0	4.5
{d, e}			0

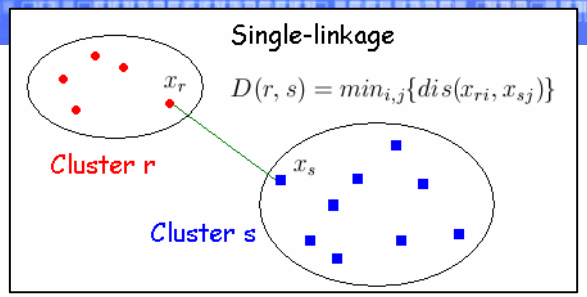
$$D(\{a,b\},\{d,e\})$$

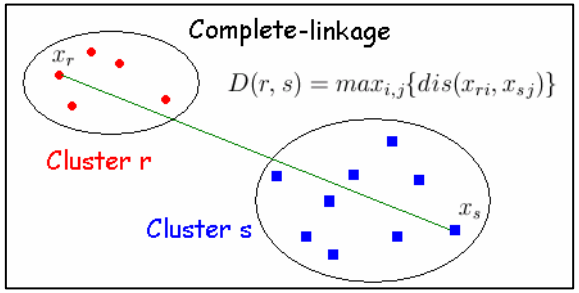
$$= \frac{1}{4}[D(a,d)+D(a,e)+D(b,d)+D(b,e)]$$

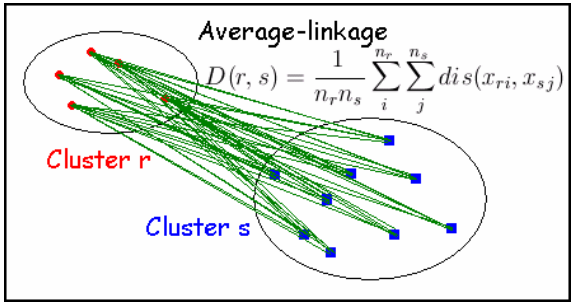
$$= \frac{1}{4}(10+9+9+8) = 9$$

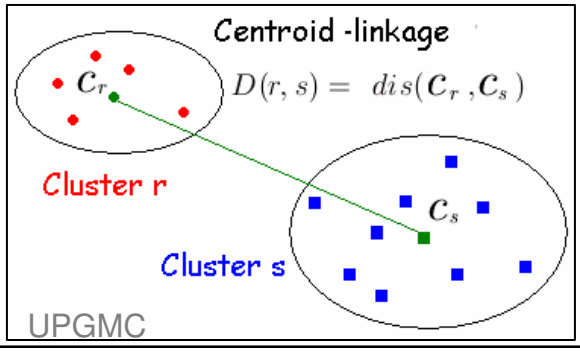
	{a, b}	{c, d, e}
{a, b}	0	7.83
{c, d, e}		0

UPGMA (Unweighted Pair-Groups Method Average)









Reference

- J. A. Hartigan. Direct clustering of a data matrix. Journal of the American Statistical Association, 67(337):123-129, March 1972.
- Duffy, D. & Quiroz, A. (1991), A permutation-based algorithm for block clustering, J. of Classification 8, 65--91.
- Chen, C. H. (2002). Generalized Association Plots: Information Visualization via Iteratively Generated Correlation Matrices. Statistica Sinica 12, 7-29.
- Wu, H. M., Tien, Y. J. and Chen, C. H. (2006). GAP: a Graphical Environment for Matrix Visualization and Information Mining.
- Ziv Bar-Joseph, David K. Gifford, and Tommi S. Jaakkola, (2001), Fast Optimal Leaf Ordering for Hierarchical Clustering. Bioinformatics 17(Suppl. 1):S22–S29.