Functionally related genes behave similarly across experiments

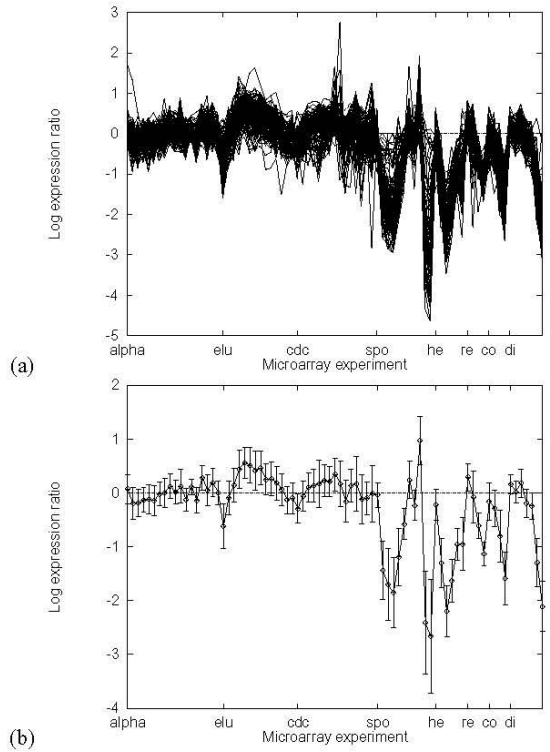


Figure 1: **Expression profiles of the cytoplasmic ribosomal proteins.** Figure (a) shows the expression profiles from the data in [Eisen et al., 1998] of 121 cytoplasmic ribosomal proteins, as classified by MYGD [MYGD, 1999]. The logarithm of the expression ratio is plotted as a function of DNA microarray experiment. Ticks along the X-axis represent the beginnings of experimental series. They are, from left to right, cell division cycle after synchronization with α factor arrest (alpha), cell division cycle after synchronization by centrifugal elutriation (elu), cell division cycle measured using a temperature sensitive *cdc15* mutant (cdc), sporulation (spo), heat shock (he), reducing shock (re), cold shock (co), and diauxic shift (di). Sporulation is the generation of a yeast spore by meiosis. Diauxic shift is the shift from anaerobic (fermentation) to aerobic (respiration) metabolism. The medium starts rich in glucose, and yeast cells ferment, producing ethanol. When the glucose is used up, they switch to ethanol as a source for carbon. Heat, cold, and reducing shock are various ways to stress the yeast cell. Figure (b) shows the average, plus or minus one standard deviation, of the data in Figure (a).

Self-Organizing Maps [Kohonen]

- Kind of neural network.
- Clusters data and find complex relationships between clusters.
- Helps reduce the dimensionality of the data.
- Map of 1 or 2 dimensions produced.
- Unsupervised Clustering
- Like K-Means, except for visualization

SOM Architectures

- 2-D Grid
- 3-D Grid
- Hexagonal Grid

SOM Algorithm

- Select SOM architecture, and initialize weight vectors and other parameters.
- **While** (stopping condition not satisfied) **do** for each input point x
  - winning node q has weight vector closest to x.
  - Update weight vector of q and its neighbors.
  - Reduce neighborhood size and learning rate.

SOM Algorithm Details

- Distance between x and weight vector: $\|x - w_i\|$
- Winning node: $q(x) = \min_i \|x - w_i\|$
- Weight update function (for neighbors):

$$w_i(k+1) = w_i(k) + \mu(k, x, i)[x(k) - w_i(k)]$$

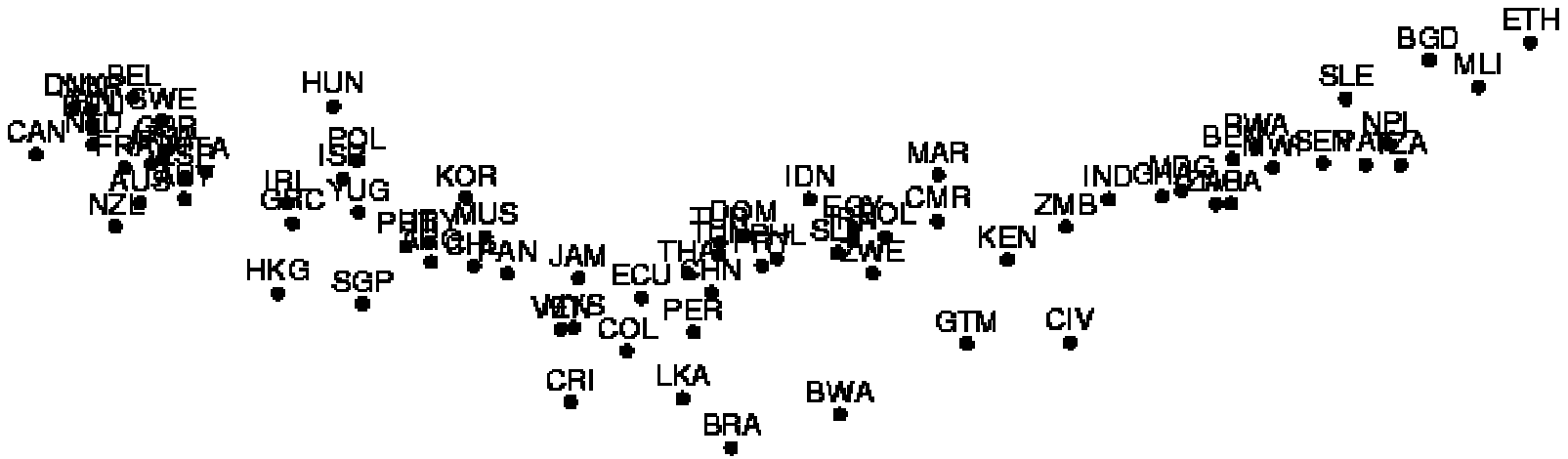
- Learning rate:

$$\mu(k, x, i) = \eta_0(k) \exp\left(\frac{-\|r_i - r_{q(x)}\|^2}{\sigma^2} \right)$$

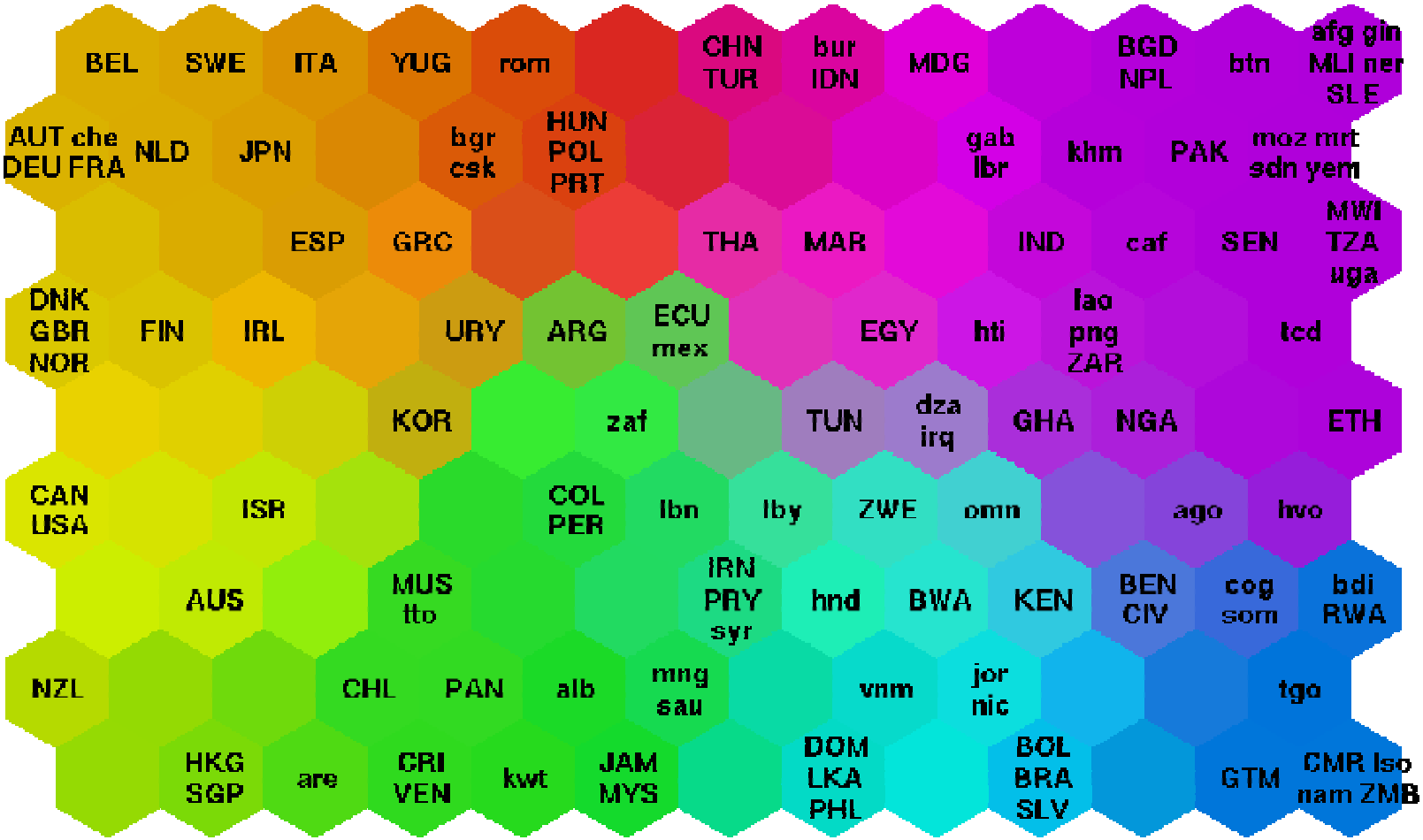
World Bank Statistics

- Data: World Bank statistics of countries in 1992.
- 39 indicators considered e.g., health, nutrition, educational services, etc.
- The complex joint effect of these factors can can be visualized by organizing the countries using the self-organizing map.

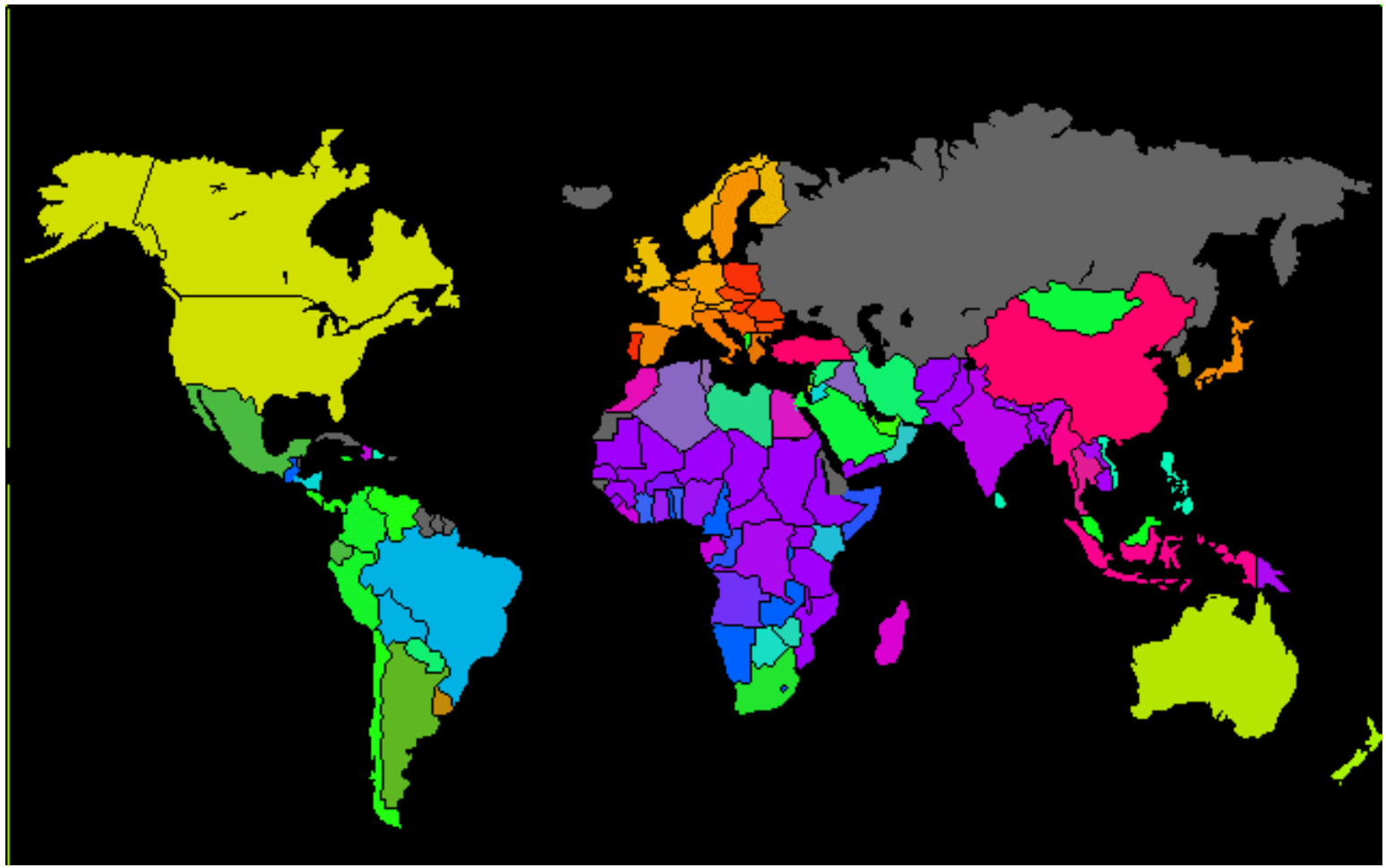
World Poverty PCA

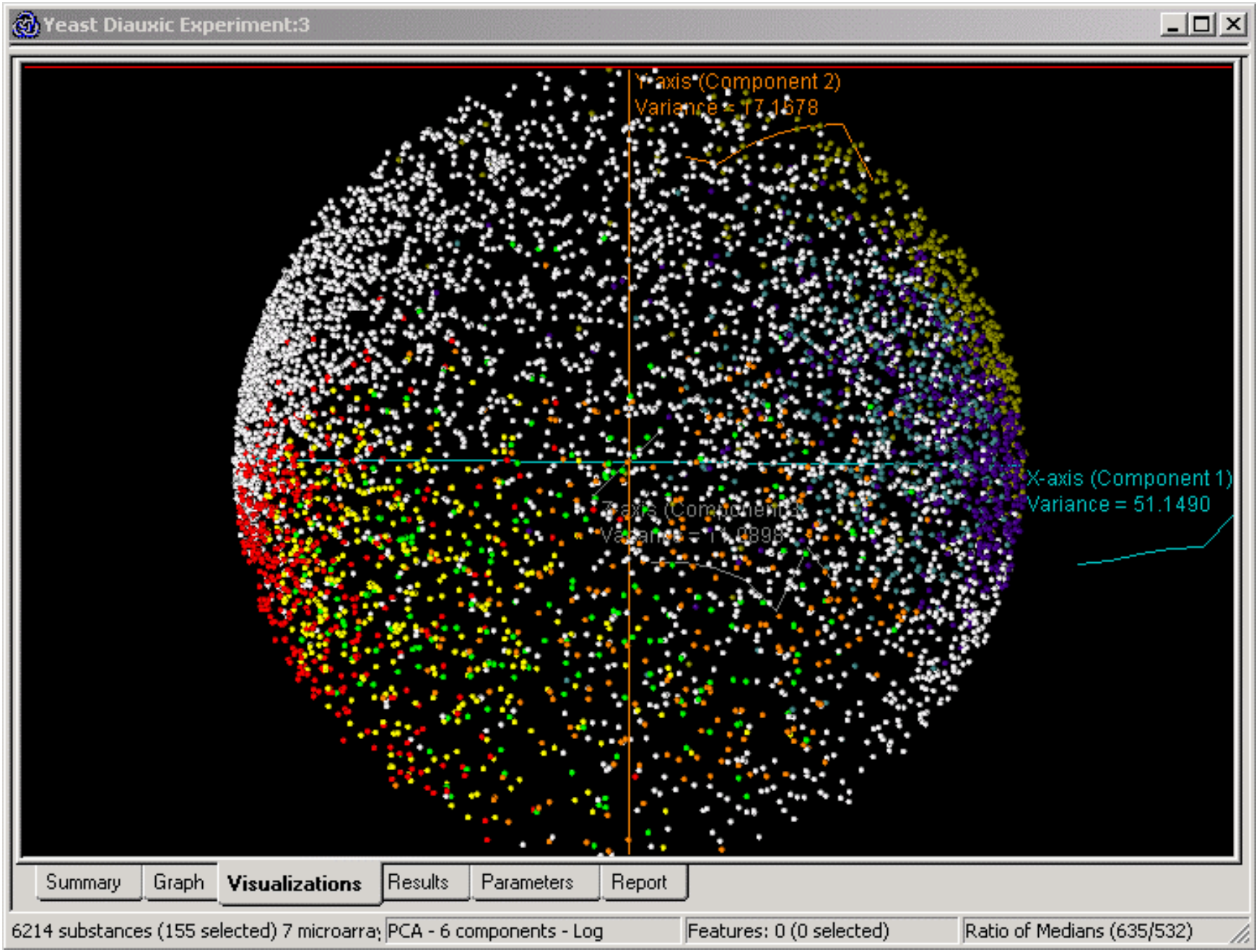


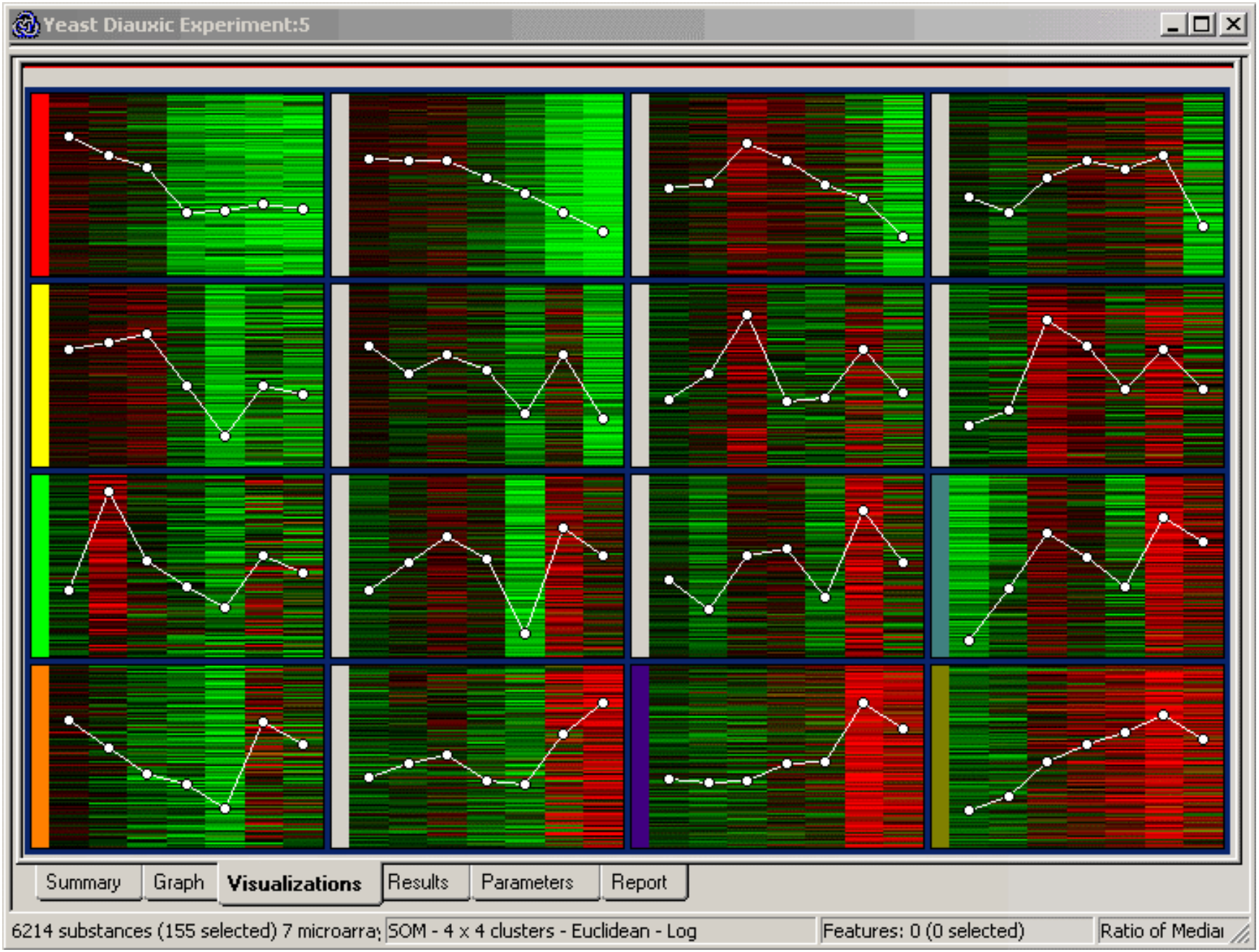
World Poverty SOM



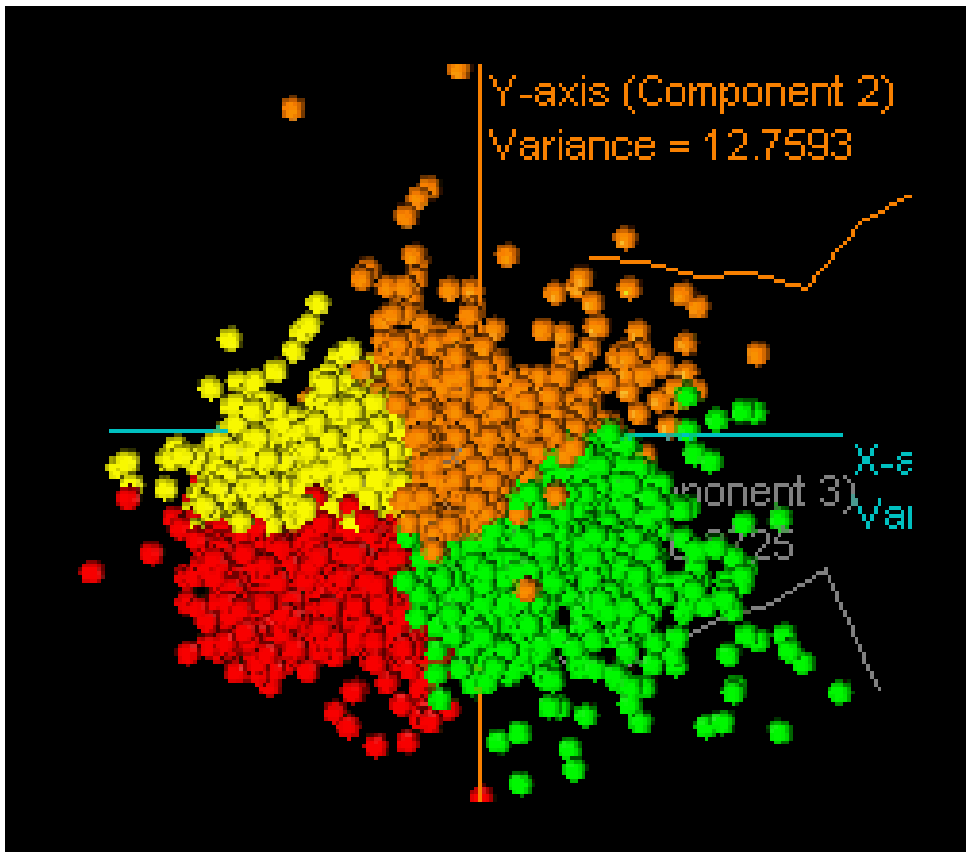
World Poverty Map



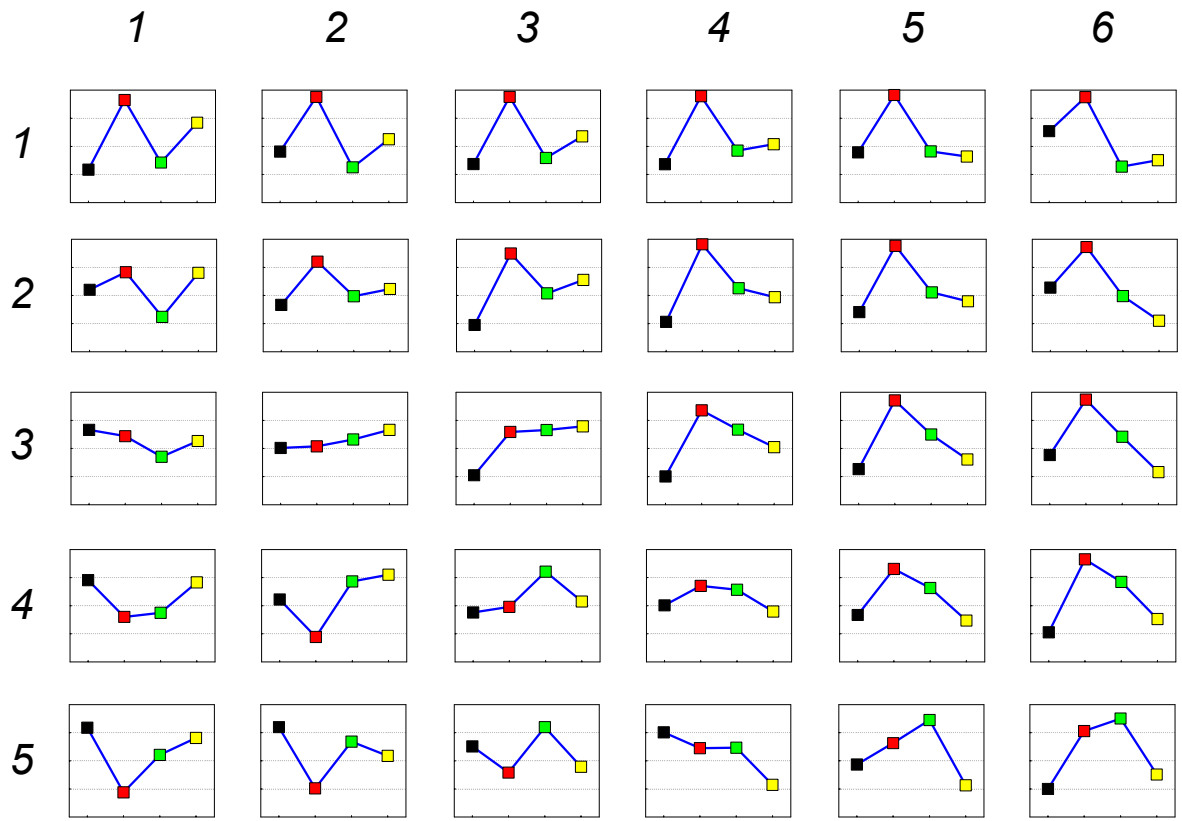

Yeast Diauxic Experiment:3
Y-axis (Component 2)
Variance = 17.1678
X-axis (Component 1)
Variance = 51.1490
Summary
Graph
Visualizations
Results
Parameters
Report
6214 substances (155 selected) 7 microarra
PCA - 6 components - Log
Features: 0 (0 selected)
Ratio of Medians (635/532)


Yeast Diauxic Experiment:5
Summary
Graph
Visualizations
Results
Parameters
Report
6214 substances (155 selected) 7 microarra
SOM - 4 x 4 clusters - Euclidean - Log
Features: 0 (0 selected)
Ratio of Media

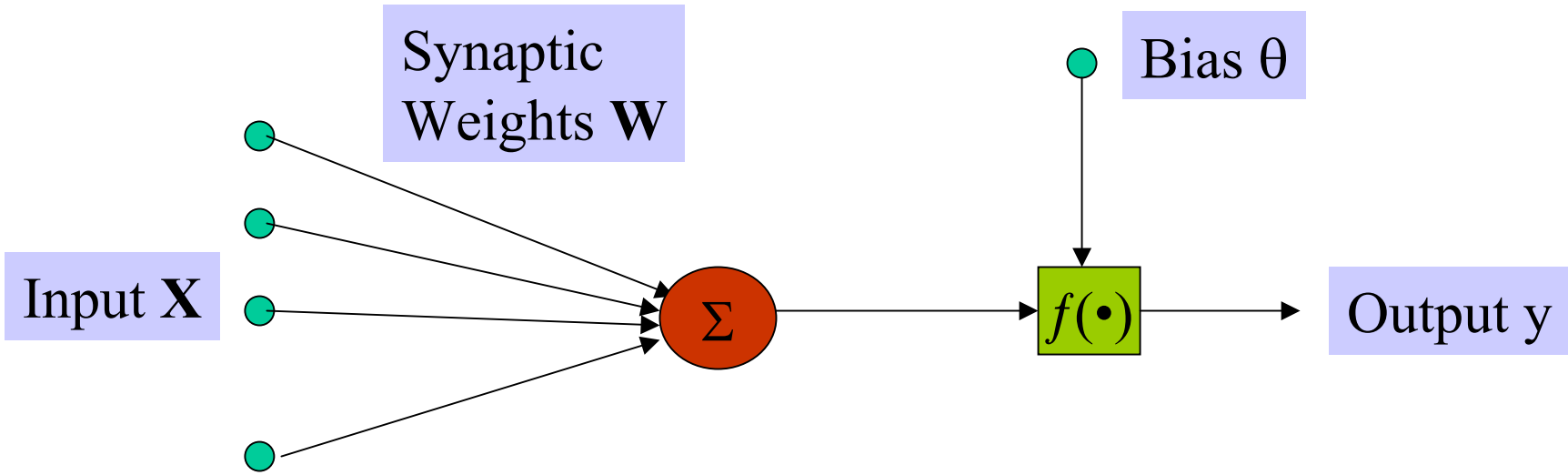
Viewing SOM Clusters on PCA axes



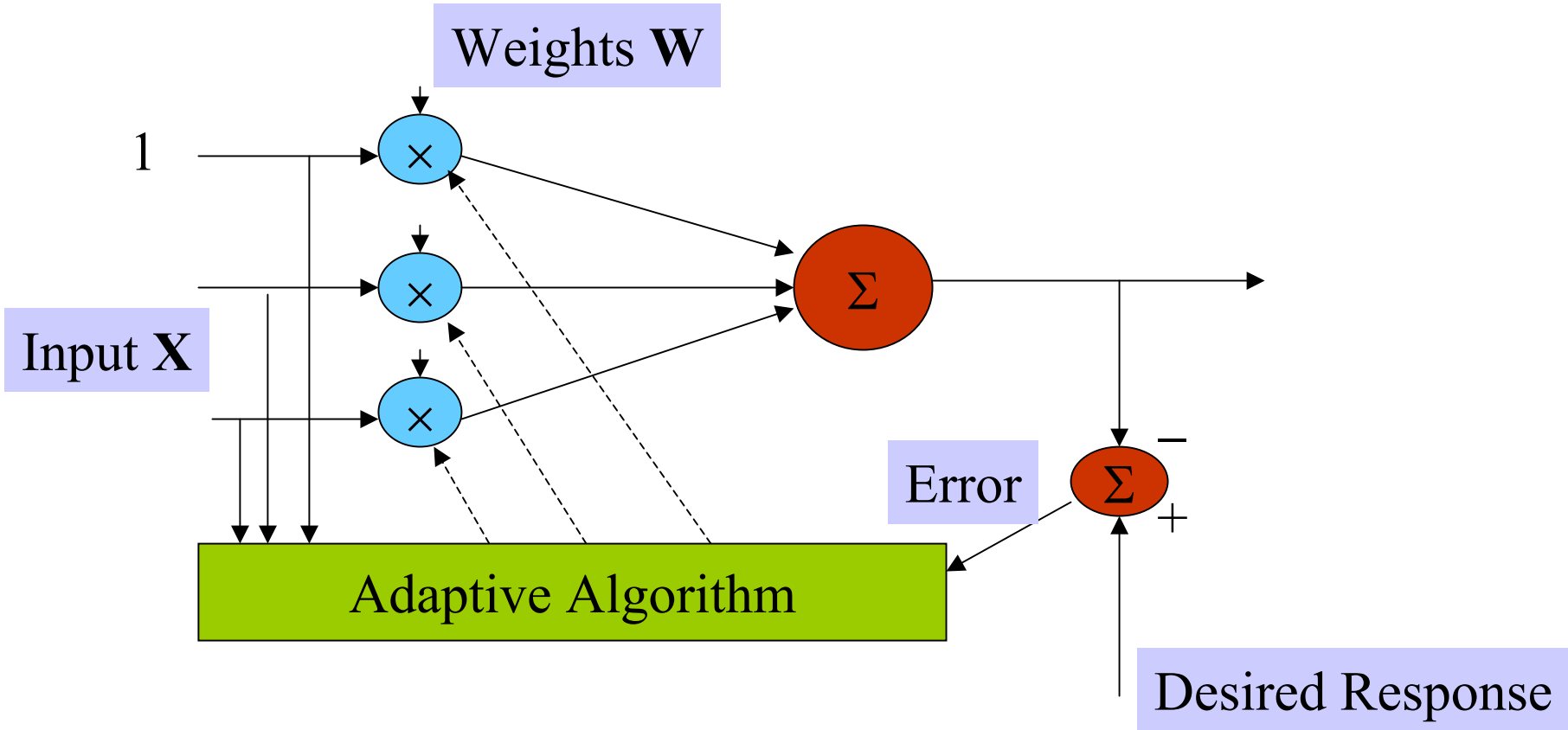
SOM Example [Xiao-rui He]



Neural Networks



Learning NN


Weights W
1
Input X
Σ
Error
Σ
−
+
Adaptive Algorithm
Desired Response

Types of NNs

- Recurrent NN
- Feed-forward NN
- Layered

Other issues

- Hidden layers possible
- Different activation functions possible

Application: Secondary Structure Prediction