Multidimensional Visualization and Clustering

Presentation for Visual Analytics
of Professor Klaus Mueller

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Paper List

- HD-Eye: Visual Mining of High-Dimensional Data
- Value and Relation Display for Interactive Exploration of High Dimensional Datasets
- PointCloudXplore: Visual Analysis of 3D Gene Expression Data Using Physical Views and Parallel Coordinates

HD-Eye: Visual Mining of High-Dimensional Data

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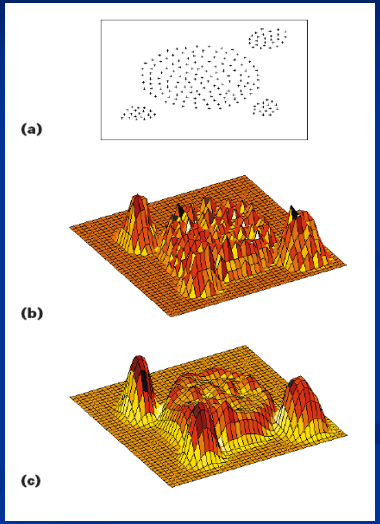
Introduction

- Motivation:
  - Efficient clustering for high-dimensional data under noise
- Key:
  - Interactive !
  - advanced clustering algorithm + new visualization methods → interactive clustering tool

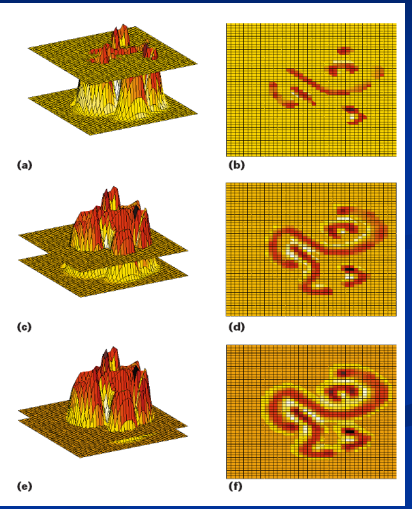
What is a cluster?

- Local maxima of density function



What is a cluster?

- Uni-centered vs multi-centered



How to cluster?

- Idea
  - First, project to lower dimension
  - Second, build separators and multidimensional grid in projected space

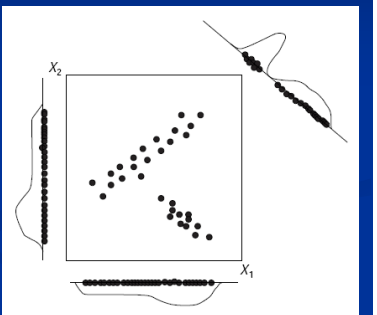
  Lemma:

  separation in contracting projection (w/ small error) →

  separation in original data space (w/o large error)
- Hierarchically
  - Independent choice of projections and separators in different nodes of the hierarchy
- Difficulty:
  - Choosing good projections
  - Choosing good separators
  - ***Need visual assistance!***

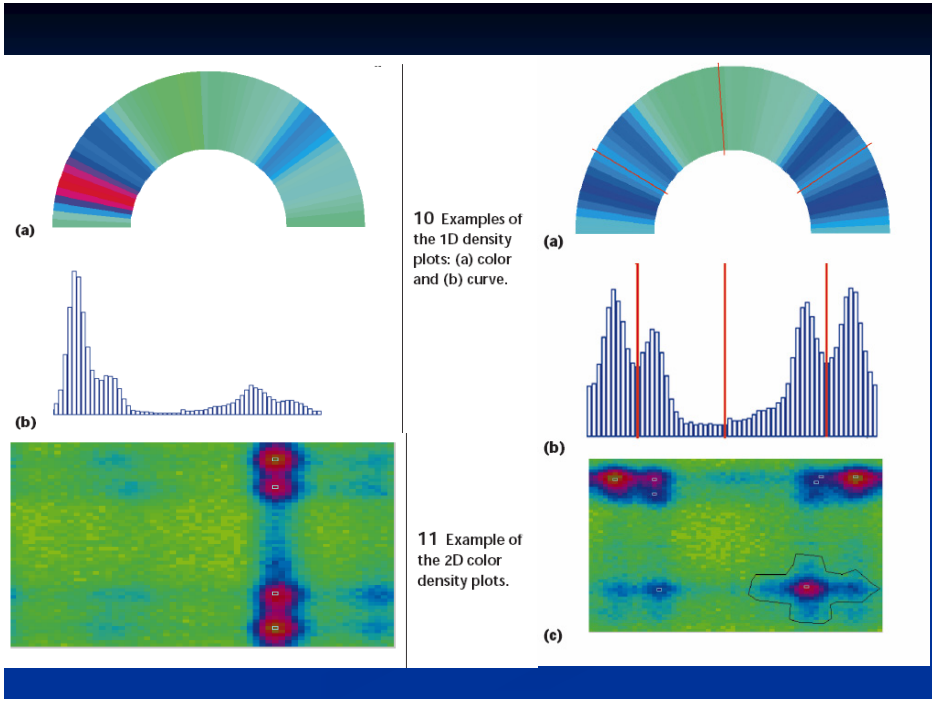
Visual Finding of Projections and Separators

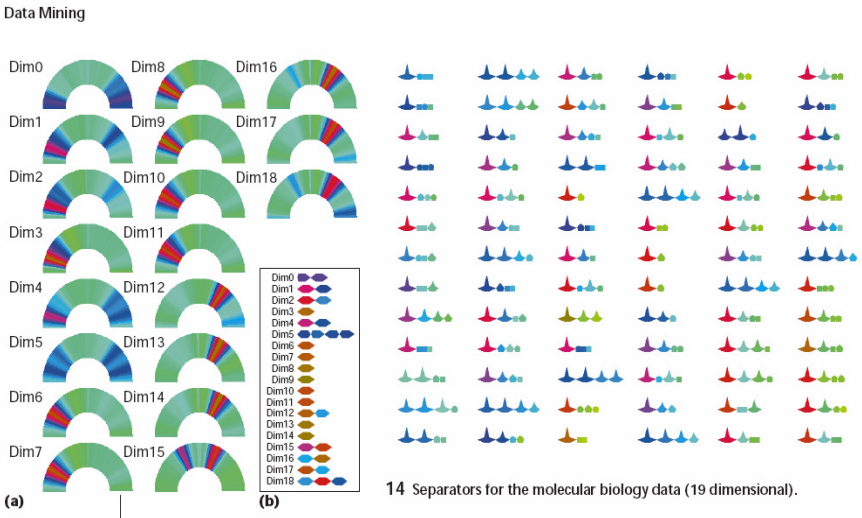
- Axes-parallel projection
  - only good for detecting center-defined clusters with no linear dependencies between the attributes.
- Good projections in general
  - Should contain well-separated clusters.
  - Do not require (like PCA) one projection separates all.



Visual Finding of Projections and Separators

- Finding projection
  - Initially, the HD-Eye system proposes some projections, like axes parallel projections, diagonal projections and etc.
  - Later on, the user can select the interesting projections, or generate other combinations from the selected ones.
- Finding separators
  - Put separators through low-density region
- After projection, how to visualize the clustering effect ?
  - abstract iconic display
  - color-based point density
  - curve-based point density

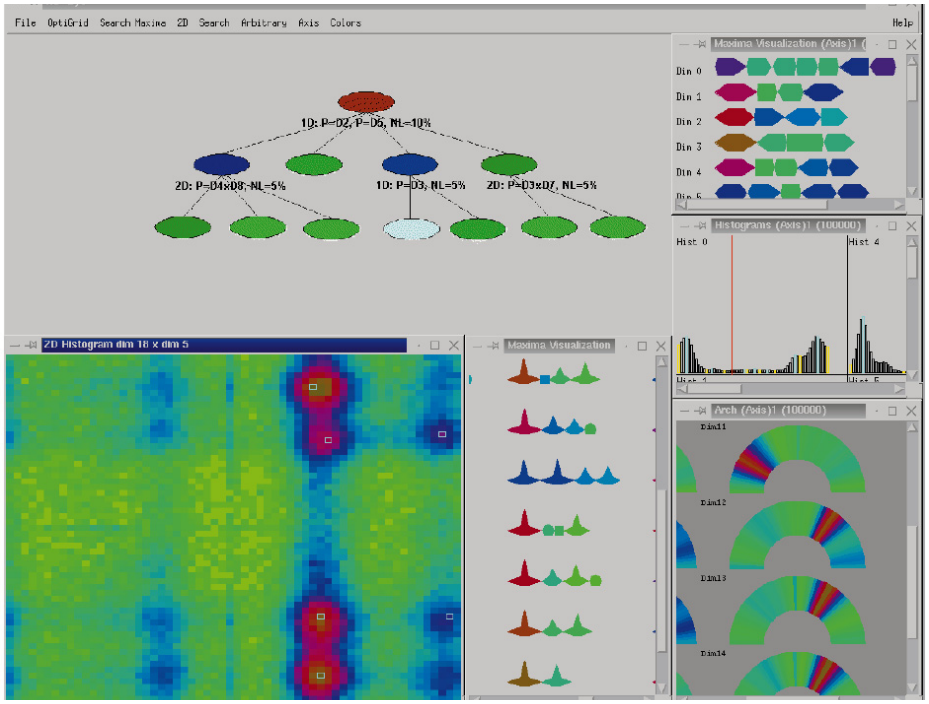




14 Separators for the molecular biology data (19 dimensional).

Overall Pipeline

- 1. Initialize the cluster hierarchy with *root* = *D*
  - *Note:*
    - *node in hierarchy* ←→ *a region in the original space*
    - *Going down the hierarchy, regions are subdivided iteratively*
- 2. While a node *v* with the data set *Dv* can be split
  - Visually find projections $P = \{ P1, \ldots, Pk \}$
  - Visually find separators $H = \{ H1, \ldots, Hr \}$
  - Partition the region (associated with node *v*) into a multidimensional grid *G*, and insert data points of *Dv* into *G*
  - pick highly populated grid cells in *G* (i.e. containing clusters), add the cells as child nodes of *v* in the hierarchy



Value and Relation Display for Interactive Exploration of High Dimensional Datasets

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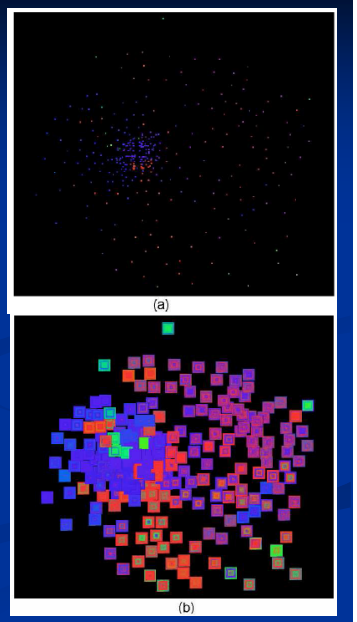
- VaR
  - A new multi-dimensional visualization technique
- At high level:
  - map dimensions to a 2D space
- At low level:
  - map data value within a single dimension into a "glyph" (subwindow)
- Interactive tools:
  - For navigation:
  - For selection:



Glyph Positioning

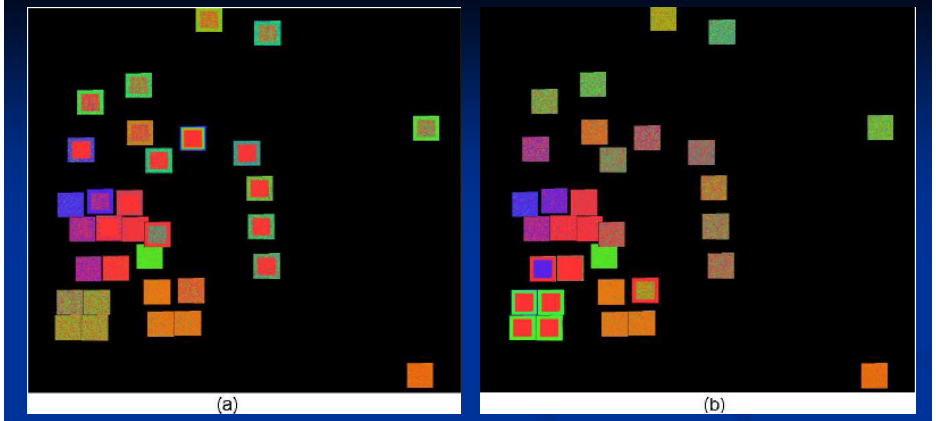
- Where to put glyphs ?
  - Step1: Build a *distance matrix* that captures the correlation between each pair of dimensions in the dataset.
  - Step2: Apply MDS on the distance matrix to get a set of positions in a 2D space, where each position corresponds to a dimension.
- How to build the "distance matrix" ?
  - Determined by certain *correlation measures*
  - a good *correlation measures* should keep most (least) related dimensions close to (far from) each other;
  - That is, the *distance matrix* should have maximum variance among all non-diagonal elements.

Glyph Positioning

- A de facto problem …
  - Two dimensions might be closely related only in part of the data items.
  - Need build histogram of the data value difference s between each pair of dimensions,
  - and partition each histogram into "bins".

Pixel Arrangement in Glyphs

- Idea
  - Use 2D texture to reveal data patterns in each dimension
- VaR uses "spiral arrangement"
  - Map each *data item* to a *pixel*
  - *Order* the data items by their values in a certain *base dimension*
  - place the ordered pixels from the center to the outside of a square *spirally*

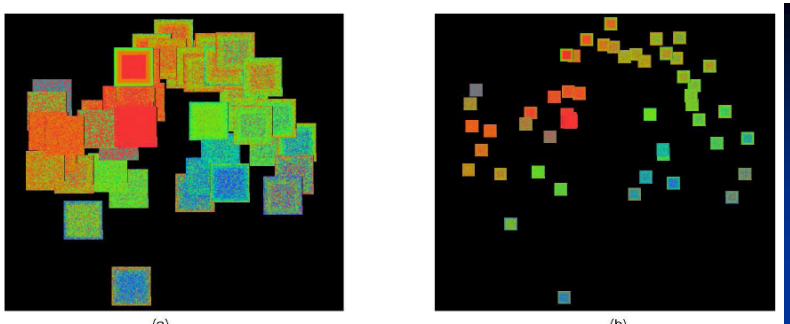


- Different choice of base dimension → different information conveyed by VaR
  - (a): dimensions in the top are closely related to base dimension a.
  - (b): dimensions in the bottom left are closely related to base dimension b.

Interactive Tools

- Navigation Tools
  - Goal
    - To solve the "overlapped glyphs" problem
  - Operations:

    Showing name, layer reordering, manual relocation, extent scaling, dynamic masking, automatic shifting, distortion, zooming and panning, manual pixel reordering, comparing, refining …
  - Example …
    - Oringinal, extent scaling, automatic shifting, distortion



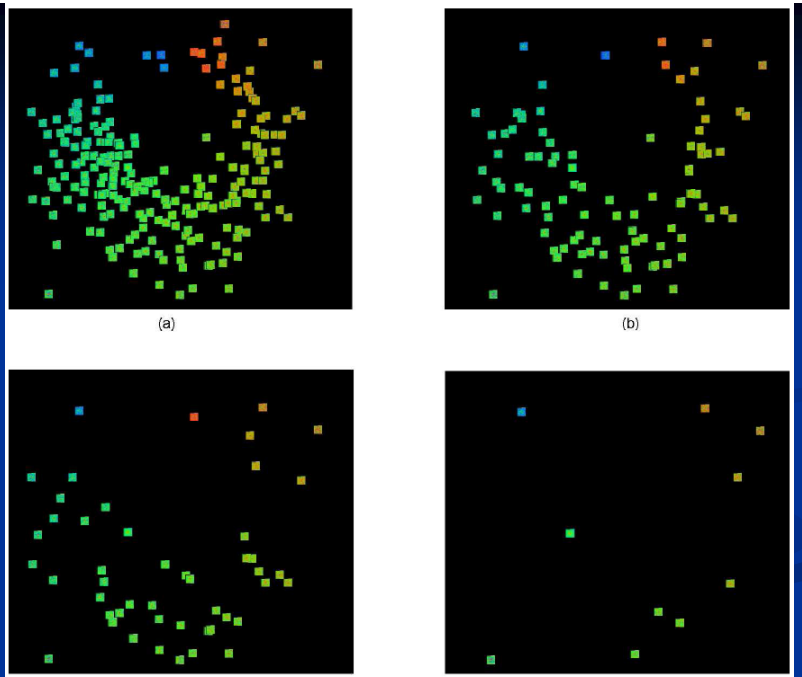
Interactive Tools

- Selection Tools
  - Goal
    - Allow users to select dimensions of interests for further exploration.
    - i.e. dimension reduction
  - Operations:

    Automatic selection of related dimensions

    Automatic selection of separated dimensions

    Manual selection of arbitrary dimensions
  - Example …
    - Automatic selection of separated dimensions with increasing correlation thresholds



PointCloudXplore: Visual Analysis of 3D Gene Expression Data Using Physical Views and Parallel Coordinates

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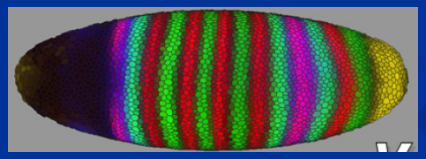
Motivation

- Objects under Study
  - An *embryo surface* has multiple *cells*
  - Each cell has n *genes* (each of which has a value of *gene expression level*)



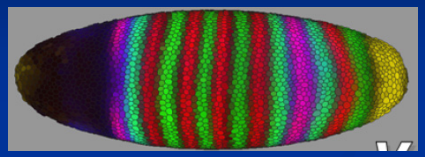
  - *Therefore each cell is assigned with a n-tuple (l1, l2, … ln);*
  - *The set of n-tuples from all cells constitute a gene expressions pattern for the whole embryo surface*

Motivation

- Goal:
  - Visualizing the gene expression pattern for a given embryo surface
  - That is, visualizing the set of (l1, l2, …, ln) values of all the cells on the embryo surface.
- Approaches:
  - Visualize in the *physical space*
  - Visualize in the *gene expression space*
  - Build *link* between these two spaces

Physical Space

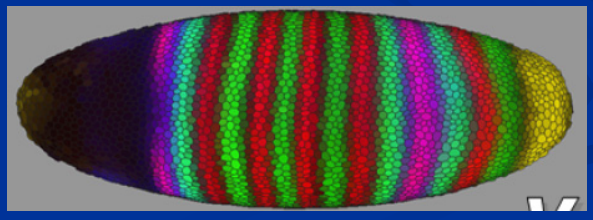
- Physical Space
  - Data space:
    - 3D space, one dim per gene
  - Data point:
    - A 3D position
    - with coordinate (x, y, z)
  - Sample point:
    - a cell (or its nucleus) on the embryo surface
    - whose coordinate (x, y, z) is the physical position of the cell (or of its nucleus)



- Visualization Techniques
  - Color encoding
  - Multi-views (orthographic or unrolled)
  - Expression surfaces

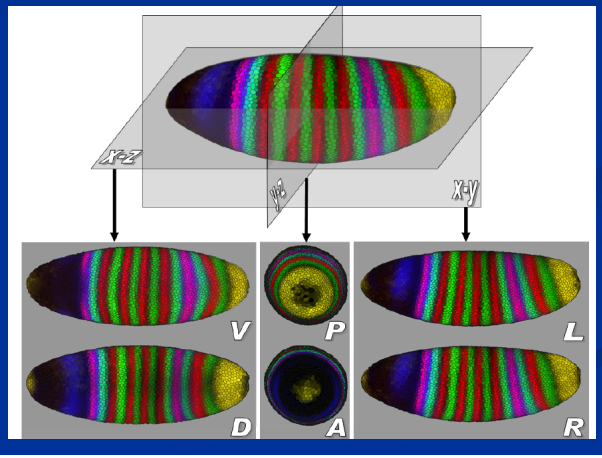
Representing expression with color

- Scheme:
  - One color for each gene,
  - expression values mapped linearly to brightness.
- Example:
  - expression patterns of four genes
  - eve (red), ftz (green), gt (blue), fkh (yellow).



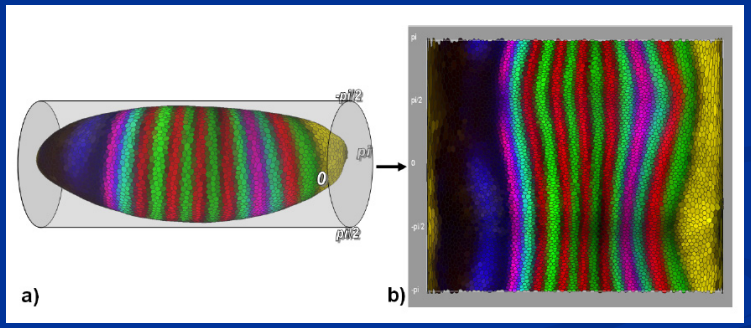
Orthographic views

- 3D → {2D}



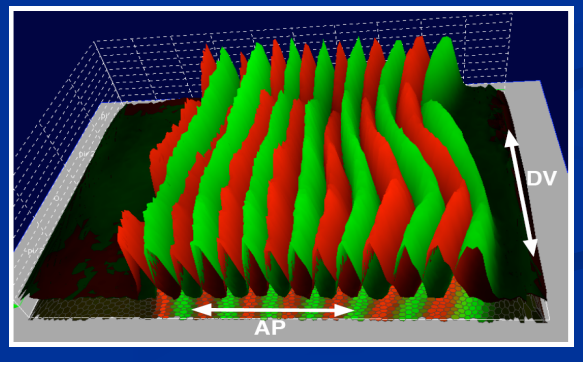
Unrolled Views

- 3D → 2D



Expression Surfaces

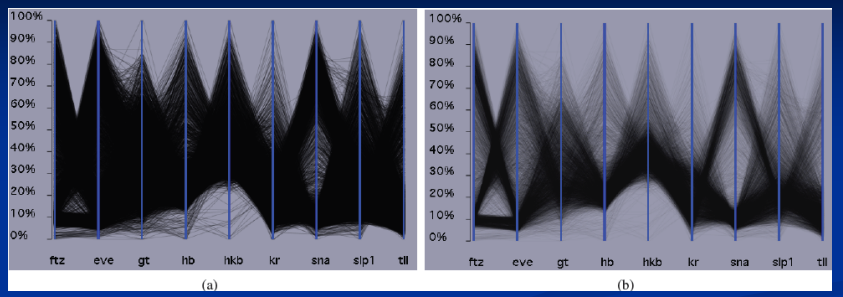
- One surface per gene
  - XY: 2D view (either orthographic or unrolled)
  - Z: value of gene expression level



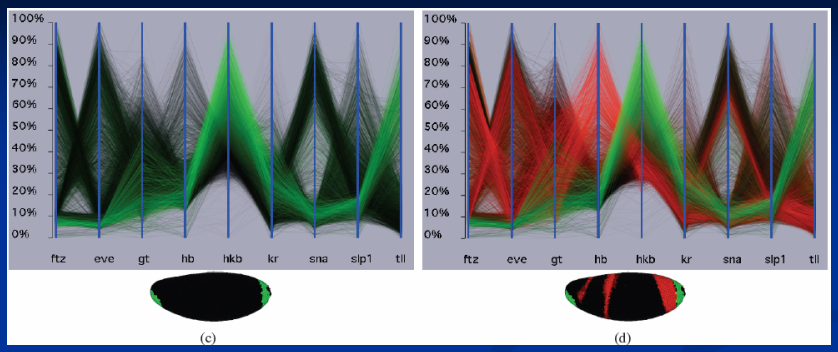
- Physical Space
  - Due to overlap between information from different genes
  - Only allow a few number of genes whose expression can be displayed at the same time
- Gene Expression Space
  - can show relationships between many genes' expression.

Gene Expression Space

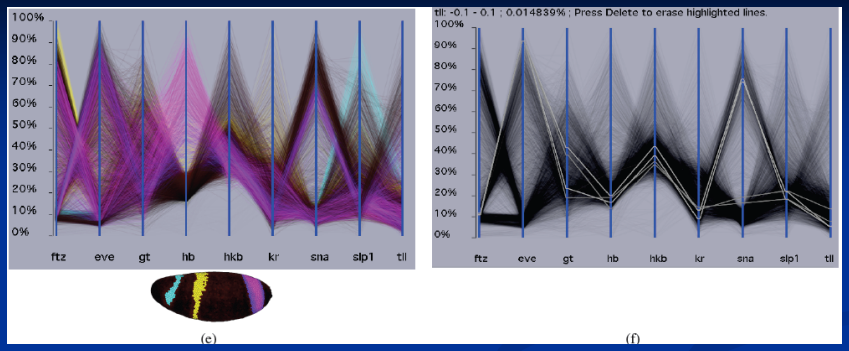
- Gene Expression Space
  - Data space:
    - n-dimesional space, one dim per gene
  - Data point:
    - a combination of expression levels for the set of genes,
    - with coordinate (l1, l2, … ln)
  - Sample point:
    - a cell from the embryo surface,
    - whose coordinate (l1, l2, … ln) is the gene expression levels for this cell
- Visualization Techniques
  - Parallel coordinates



- 2D Parallel Coordinate View for nine genes.
- (a) A view in which data lines have maximum opacity.
- (b) A view in which data line transparancy has been increased.

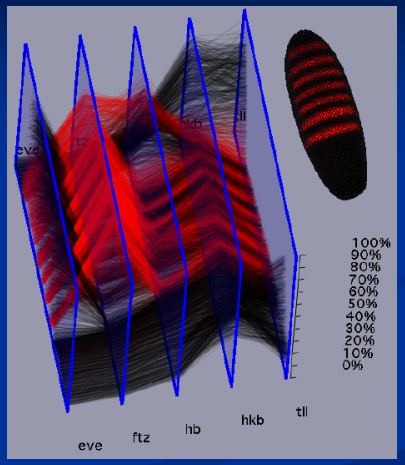


- (c) A view in which color from an Embryo View showing hkb expression (green) is shown.
- (d) A view in which colors from an Embryo view showing both hkb (green) and hb (orange)expression are shown.



- (e) A view showing two brushes drawn on an Embryo View to highlight distinguish between the three hb stripes of expression (light blue, yellow and pink).
- (f) A view showing line traces that highlight data associated with several cells.

- Coupling two spaces !!
- 3D parallel coordinates
  - Paths in red: cells with high expression level of ftz gene.
  - Stretching the 2D parallel coordinates along "anterior" → "posterior" direction



Conclusion

- *HD-Eye: Visual Mining of High-Dimensional Data*
  - Hierarchical clustering techniques with visual assistance
  - Project to low dim space, (visually choosing projections)
  - And partition there (visually choosing separators)
- *Value and Relation Display for Interactive Exploration of High Dimensional Datasets*
  - A new multi-dimensional visualization technique
  - At high level: capture inter-dimension correlation in a 2D space
  - At low level: capture data pattern in each dimension by a "glyph"
  - Interactive tools for navigation and selection
- *PointCloudXplore: Visual Analysis of 3D Gene Expression Data*
  - Application driven
  - Employing physical views and parallel coordinates