Multidimensional Visualization and Clustering

Presentation for Visual Analytics of Professor Klaus Mueller

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HD-Eye: Visual Mining of High-Dimensional Data

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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

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

- Uni-centered vs multi-centered

How to cluster?

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

- Hierarchically
  - Independent choice of projections and separators in different nodes of the hierarchy

- Difficulty:
  - Choosing good projections
  - Choosing good separators
  - Need visual assistance

- 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
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

1. Initialize the cluster hierarchy with \( \text{root} = D \)
   - Note:
     - node in hierarchy \( \leftrightarrow \) 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 \( P = \{ P_1, \ldots, P_k \} \)
   - Visually find separators \( H = \{ H_1, \ldots, H_r \} \)
   - 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?
  - Step 1: Build a distance matrix that captures the correlation between each pair of dimensions in the dataset.
  - Step 2: 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 measure 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 differences 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 \textarrow{} 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 …
    - Original, 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 \((l_1, l_2, \ldots, l_n)\);
- The set of *n*-tuples from all cells constitute a *gene expressions pattern* for the whole embryo surface

Goal:

- Visualizing the gene expression pattern for a given embryo surface
- That is, visualizing the set of \((l_1, l_2, \ldots, l_n)\) 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

- $3D \rightarrow \{2D\}$

Unrolled Views

- $3D \rightarrow 2D$

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

- Data space:
  - n-dimensional space, one dim per gene
- Data point:
  - a combination of expression levels for the set of genes, with coordinate \((l_1, l_2, \ldots, l_n)\)
- Sample point:
  - a cell from the embryo surface, whose coordinate \((l_1, l_2, \ldots, l_n)\) 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