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Módulo IV

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Outline

Part I – Concepts and Techniques
Rosane Minghim

Part II – Applications
Post-grad students CCMC - ICMC

Part III – Similarity-Based Visualization
Emilio Vital Brazil - IBM

Part IV – Visualization Case Studies
Vagner Santana – IBM

Outline Part I

- Context and Resources
- Data
- Point-centered Visualization
- Attribute-centered Visualization
- Relationship-centered Visualization
- Visualization and Mining

Our research at VICG Visualization, Imaging and Computer Graphics Lab vicg.icmc.usp.br

- Visual Data Mining
- Visual Analytics
- Visualization



Motivation

Context: Abstract Data Analysis

• Why Visualize?

How not visualize?

• When Visualize?

• Analysis, Illustration, Demonstration

Classification Results - Why





Classification Results - Why



Classification Results – How not



Before we continue...

Scientific Visualization



http://www.cs.rug.nl/svcg/SciVis/DTIVis

- Medicine
- Simulation
- Engineering
- Etc.



Fonte: Poco et al. 2012

Visualization for Data Science and Big Data What does it take?

- Algorithms
- Statistics essential
 - Alone will not do the job
- Mining essential
 - · Will not do the whole job, even with statistics
- Visualization exploratory situations and user centric decision
- Certain skills from complex reasoning to complete programming to innovative and daring goals. But mostly: Undestand the data

Companies all around the world know the value of Big Data

See, for instance:



Resources - books



Ward, Grinstein, Keim, 2015



Munzner, 2014



Telea, 2014



McDaniel & McDaniel, 2012

Resources - software

- Most data analytics tools have some sort of visualization capability.
 - Phyton
 - R
 - Javascript (d3.js)
 - VTK + (3D scientific)
 - TensorFlow
 - etc..
 - Watson[™]
 - Tableau[™]
 - etc..

Links to sources of data visualization tools and data

• HDR (ONU):

- (data) http://hdr.undp.org/en/composite/GII
- (vis) <u>http://hdr.undp.org/en/data-explorer/</u>

- <u>D3:</u>
 - https://d3js.org/
 - (gallery) <u>https://github.com/mbostock/d3/wiki/Gallery/</u>

What does your data tell

People trying to make sense of data

ímessyí data





Data

- Item
- Attribute
- Reference (index, position, location)
- Relationship
- Collection (data set/table, item, network)

Techniques

Point placement: 2D or 3D similarity-based layouts



pairwise distances

	5	12	15	2	7	5	0	12	9	0	8
-	12	5	0	12	12	12	12	12	18	12	12
-	0	1	05	10	15	12	8	12	9	11	5
No.	0	12	01	12	9	0	12	10	5	5	12
-	12	8	05	12	12	12	8	12	9	12	12
2	10	12	0	11	10	2	7	12	2	16	7
2	5	6	8	12	12	15	12	6	9	17	0
	7	12	05	0	12	12	10	17	9	12	12
	2	10	05	15	12	1	12	10	9	8	2
2	12	12	7	12	0	12	0	12	10	12	12
2	6	12	05	17	12	10	12	12	9	12	8
A	12	10	2	12	1	12	12	11	6	0	12
2	1	12	05	12	12	16	2	12	9	12	0
2	10	0	12	12	9	12	0	10	12	12	8
1	0	12	1	12	12	5	1	7	11	12	12
	8	2	11	10	7	12	5	12	15	10	0

and/or dimensional embedding (feature space)

Visualizations

Point-Based



source : Paiva et al.

Relationship Based

Attribute Based



source: Ward et al.

Geo



sources : treevis.net e www.caida.org





sources: Google Maps e CartoDB

POINT-BASED TECHNIQUES

Scatterplots Multidimensional projections Similarity trees

Scatter Plots



Fonte: HDR (ONU)

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Technique: Scatter Plot Matrix



https://bl.ocks.org/mbostock/4063663

Advanced Visual Data Analysis via Point Placement and Dimension Reduction

Projection-based

 variations on MDS or other dimension reduction approaches to map data to visual space

- Tree-based
 - hierarchy of similarity relations
 - variations on tree layouts



Projection Techniques:

Mapping data set on the plane, allowing direct exploration

Ex: Patents surgery, drugs, molecular bio





$$\begin{split} & \delta : x_i, x_j \rightarrow R, x_i, x_j \in X \\ & \bullet d : y_i, y_j \rightarrow R, y_i, y_j \in Y \\ & \bullet f : X \rightarrow Y, |\delta(x_i, x_j) - d(f(x_i), f(x_j))| \approx 0, \ \forall \ x_i, x_j \in X \end{split}$$

Problems PCA



Projection as dimension reduction

Classical

- PCA (Principal Component Analysis)
- Classical Scaling
- LLE (Local Linear Embedding)
- ISOMAP
- Sammon's mapping



Classical Scaling



Force Based Point Placement











- 1. Map each point X to the plane (fastmap, nnp, etc.)
- 2. For each projected point x
 - 1. For each projected point $q' \neq x'$
 - 1. Compute the vector \mathbf{v} of $\langle x'$ to $q' \rangle$
 - 2. Move q' in direction of \mathbf{v} , one fraction of Δ

$$\Delta = \frac{\delta(x,q) - \delta_{\min}}{\delta_{\max} - \delta_{\min}} - d(x',q')$$

3. Normalize the coordinates between [0,1]

LSP [Paulovich et al., 2006/2008]

- Least-Square Projection (LSP)
- Core idea: project a sub-set of points and interpolate the rest.
- Interpolation seeks to preserve the neighborhood between points.
- Each point is mapped within the convex hull of its neighbors.

LSP [Paulovich et al., 2006/2008]

- Three main steps:
 - 1. Select a subset of points(control points) and Project these in R^p
 - 2. Determine the neighborhood of points
 - 3. Create a linear system whose answers are the Cartesian coordinates of points p_i in R^p

LSP: Laplacian Matrix

 Let V_i = {p_{i1},...,p_{iki}} be the neighborhood of a point p_i and c_i the coodinates of p_i in R^p

$$c_i - \frac{1}{ki} \sum_{p_j \in V_i} c_j = 0$$



• Each p_i will be the centroid of points in V_i


$$Lij = \begin{cases} 1 & i = j \\ -\frac{1}{ki} & p_j \in V_i \\ 0 & \text{otherwise} \end{cases}$$



LSP: Adding control points

$$A = \begin{pmatrix} L \\ C \end{pmatrix} \qquad Cij = \begin{cases} 1 & p_j \text{ is a control point} \\ 0 & otherwise \end{cases}$$

$$b_i = \begin{cases} 0 & i \le n \\ x_{p_{c_i}} & n < i \le n + nc \end{cases}$$



LSP: Solving the system

- It is necessary to solve Ax = b
- The system is solved by using least squares

$$\left\|Ax-b\right\|^2$$

The analytical solution is

$$A^T A \mathbf{x} = A^T \mathbf{b} \implies \mathbf{x} = (A^T A)^{-1} A^T \mathbf{b}$$

 A^TA is symmetric and sparse and can be solved using the factorization of Cholesky

LSP: Overview



LAMP, 2011 LSP, 2008 Slide show compiled based on the relations given by the final projection User manipulation making explicit relations between groups of images and musics (information, retrieval) (audio,music,computer,processing) outron Diverse (learning,logic,programming,inductive) rock/sports 17 classical/news (case,based,reasoning) min max NJ trees, 2007,2011 HiPP, 2008 [88]: [77]: mosque, suicide [66] immigration, senate PLP 2011 [69] baghdad, mosque [83]: hamas, palestinian [76]: bu 0 PLMP, 2010

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Stochastic Neighborhood Embedding sne and t-sne

Distance in original space

$$p_{j|i} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)},$$

Distance in projected space

$$q_{j|i} = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{k \neq i} \exp(-\|y_i - y_k\|^2)}$$

Cost function

$$C = \sum_{i} KL(P_i||Q_i) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}$$

Non-gaussian neighborhoods: t-sne

L.J.P. van der Maaten and G.E. Hinton. **Visualizing High-Dimensional Data Using t-SNE**. *Journal of Machine Learning Research* 9(Nov):2579-2605, 2008

T-sne Examples



Source: https://www.slideshare.net/xuyangela/an-introduction-to-tsne

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RadViz



P. Hoffman, G. Grinstein, K. Marx, I. Grosse, and E. Stanley. DNA visual and analytic data mining. In Proceedings of the 8th conference on Visualization '97, VIS '97, pages 437–441, Los Alamitos, CA, USA, 1997. IEEE Computer Society Press.

Analysis Examples

- Fluid Samples
- Text
 - Papers
 - News feeds
- Biomarkers
- GPS samples
- Images

Projection: Voting



LSP mapping of music features



Similarity map of 1,300 songs of 3 genres plus music icons relative to the selections (LSP + DTW, features extracted from MIDI)

Vargas et al. Visualizing music collections based on structural similarity. SIBGRAPI Conf. Graphics, Patterns and Images 2014

Sammon's Mapping of combined responses of four nanosensors



Perinotto et al., *Anal. Chem.* 2010 Paulovich et al., *Anal. Bioanal. Chem.* 2011



Topic detailing



SOM-based projection



Skupin, A. 2004 - The world of geography: Visualizing a knowledge domain with cartographic means, PNAS, vo. 101.

Coordinating





Surface-based – Landscape Views

• Building a Surface













RSS News Flash



Bird and Flu



Palestinian



Bush



Iraq







Curvas de Nível



Siqueira, P. H. ; <u>Telles, G. P.</u> ; **MINGHIM, R.** . Revisiting Landscape views in Information Visualization. In: Bruno Lopes; Talita Perciano. (Org.). Learning and Infering. Festschrift for Alejandro C. Frery on the Occasion of his 55th Birthday. 1ed.Londres: College Publications, 2015, p. 131-152.

More Applications – Fiber Tracking

- Projection from fiber features
- Interaction through fast and reconfigurable projections (LAMP)
- Lines, Tubes and Surface Views



Poco, Eler, Paulovich, Minghim - Employing 2D projections for fast visual exploration of large fiber tracking data, **Computer Graphics Forum**, **Eurovis** 2012.











- Specific issues
 - How do users perceive point-placement layouts?
 - What are such layouts good for?
 - Which techniques do best in which situations? How do they compare?
 - Measures from a controlled user study
 - Numerical measures

- Study with 61 subjects aimed at comparing how different layouts are perceived
- 5 point-placement techniques (NJ tree, Glimmer, LSP, ISOMAP and PCA) compared for segregation, precision and clutter avoidance capabilities
- Hypotheses
 - H1 Different projections perform better on different tasks
 - H2 Performance of projections is task dependent
 - H3 Performance of projections depends on data characteristics
 - H4 User preferences for projections are governed by good segregation capability
- Tasks: cluster and outlier perception, neighborhood perception, density perception
- Data sets: image and text collections

- Hypotheses
 - H1 Different projections perform better on different tasks Yes!
 - H2 Performance is task dependent

Partly!

- H3 Performance depends on data characteristics Yes!
- H4 User preference is governed by good segregation
 No!

Etemadpour, R. ; Motta, R; Paiva, J.G.S; Minghim, R.; Oliveira, M. C. F., Linsen, L. Perception-Based Evaluation of Projection Methods for Multidimensional Data Visualization. IEEE Transactions on Visualization and Computer Graphics , v. 21, p. 81-94, 2015

- Numerical measures + contrasting with results from user study
 - Previous: Neighborhood Hit, Silhouette Coefficient, Distance Plots
 - New: topological measures defined on a similarity graph built from the projections
 - Class segregation
 - Group formation
 - Cluttering

Assessing projection mappings



Figure 10: LSP and t-SNE projections of *Optdigits*: (a) LSP with classes; (b) LSP mapping *Class Separation Validation*; (c) t-SNE with classes; (d) t-SNE mapping *Class Separation Validation* (darker is better). Summary measure for the projection is shown in parentheses.

R. Motta, A.A. Lopes, R. Minghim, M.C.F. Oliveira, Graph-based measures to assist user assessment of multidimensional projections. *Neurocomputing 150*: 583-598 (2015)

Point Placement by Phylogenetic Tree Construction Algorithms (N-J Trees)



Point Placement by Phylogenetic Tree Construction Algorithms (N-J Trees)

$$d_{AB} + d_{CD} \le \max(d_{AC} + d_{BD}, d_{AD} + d_{BC})$$



Algorithm Neighbor-joining

Input: distance matrix

- 1. Criate a star tree for n objects.
- 2. Iteration
 - 1. Select a node pair (i,j) with smaller Sij (branch size)

$$S_{ij} = \frac{1}{2(n-2)} \sum_{k=3}^{N} (D_{ik} + D_{jk}) + \frac{1}{2} D_{ij} + \frac{1}{n-2} \sum_{3 \le m < n} D_{ij}$$

2. Combine nodes i and j in a new node and calculate the branch size of the new node.

$$L_{ix} = \frac{D_{ij} + D_{iz} - D_{jz}}{2} \qquad \qquad L_{jx} = \frac{D_{ij} + D_{jz} - D_{iz}}{2}$$
Algorithm Neighbor-joining

3. Calculate new distance matrix, computing the new distances from the new node to the remaining nodes.

$$D_{(i-j),k} = \frac{(D_{ik} + D_{jk})}{2} \qquad (3 \le k \le N)$$

- 4. Eliminate previous nodes i and j
- 5. If n>2 then iterate again.

Initial view (N-J Tree)







- Cuadros, Paulovich, Minghim, Telles, Point placement by phylogenetic trees and its application to visual analysis of document collections, *IEEE VAST* 2007.
- Paiva, Florian-Cruz, Pedrini, Telles, Minghim, Improved Similarity Trees and their Application to Visual Data Classification, *IEEE Trans. Visualization and Computer Graphics*, 2011.

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Example: Images



Example: Images



Applications



Exploratory visualization of

- images
- text: news, scientific papers, web search results
- sensor measurements
- volumetric data: vector, scalar
- social networks
- neural fibers
- particle trajectories
- time series

VDM – Supervision in DR and Projections

- User feeds samples in small amounts
- Larger data sets are reduced in dimensions or projected via Partial Least Squares



Paiva, Schwartz, Pedrini, Minghim, Semi-Supervised Dimensionality Reduction based on Partial Least Squares for Visual Analysis of High Dimensional Data, **Computer Graphics Forum**, **Eurovis 2012.**



- Sheer volume
- Data transformation/formatting/structuring
- Ownership of the data
- Different types
- Spurious correlations
- Inespecificity of questions

Visualization examples: clutter





Paulovich and Minghim, HiPP: a novel hierarchical point placement strategy and its application to the exploration of document collections, *IEEE Trans. Visualization & Computer Graphics*, 2008

Poco; Etedmapour, Paulovich, Long, Rosenthal, Oliveira, Linsen, Minghim. A framework for exploring multidimensional data with 3D projections, *Computer Graphics Forum*, Eurovis 2011.

Handling scalability? The Visual Super Tree



More Data – Summarization

- Wordclouds
- Representative Images







Multi-level text

Multi-level images

ATTRIBUTE BASED VISUALIZATION

Table Views Parallel Coordinates Tag Clouds Time dependente and text

Stats









Data Matrix and Correlation Matrix view by heatmap



http://www.sthda.com/english/wiki/visualize-correlation-matrix-using-correlogram



Parallel Coordinates



https://www.gigawiz.com/parallelco3.html





0%

Pixel-based techniques



DOW JONES

Peano-Hilbert

Space-Filling Curves



DOW JONES

Morton (Z-Curve)



Tag-clouds and Theme River



Stacked graph aka Steam graph, Theme river



http://complexdatavisualized.com/time-series-visualizations-an-overview/

RELATIONSHIP – BASED VISUALIZATION

Graphs

Trees

Graphs and trees can be large



https://www.caida.org/research/performance/rtt/walrus0202/a-root-rtt-05-key.png

Graphs: Force-directed Graph Layout

http://bl.ocks.org/mbostock/4062045



Adjacency Matrix Graph Layout

https://bost.ocks.org/mike/miserables/



Clutter – graph bundling



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Readjusting Layouts on Cluster-based Readjustment

• 2D Abstraction: Gmap [Gansner et al. 2010]



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Readjusting Layouts on Cluster-based Readjustment

• **3D Abstraction:** Graph Cluster Surfaces [Balzer+Deussen 2007]



Density and attribute mapping





A hierarchy must be present, detected or imposed

Many layouts and applications: see http://treevis.net

Standard layout – link-node (nó e aresta)



Ward et al. 2015

Trees - Force Layout

http://mbostock.github.io/d3/talk/20111116/force-collapsible.html





Highlighted 9 protocols

Cone Tree



File system structure visualized as a cone tree

Animated 3D visualization of hierarchical data



http://mbostock.github.io/d3/talk/20111018/treemap.html



Trees – Sunburst and Curved Trees



M. Ali Rostami, Azin Azadi and H. Martin Bücker, <u>A new approach to visualizing general trees using thickness-adjustable quadratic curves</u>, GD'14: Proceedings of the International Symposium on Graph Drawing, pages 525-52.

Chen, Y., Zhang, X., Feng, Y. et al. Sunburst with ordered nodes based on hierarchical clustering: a visual analyzing method for associated hierarchical pesticide residue data. J Vis (2015) 18-237. Stasko, Catrambone, Guzdial, McDonald 2000: <u>An evaluation of space-filling information visualizations for depiction hierarchical structures</u>

Visualization for Clustering

- User: important role in cluster analysis
- User perspective is of importance in many applications
- IvisClustering (LDA-based clustering)
- JigsawCluster
- Kt-vis (keyterm-based clustering)

Visualization for Clustering kt-vis



Nourashrafeddin, Sherkat, Minghim, Milios – A Visual Approach for Interactive Keyterm-based Clustering - Submitted ACM TIIS

Visualization for Classification

- User: important role in building, applying and adjusting classifiers
 - Knowledge of the problem
 - Insertion of the classification process
- Insertion may be more effective: better data sets presentation
 - Data set structure and instances relationship understanding
 - Detection of specificities that justify classifiers behaviors

Paiva, J.G.S., Schwartz, W. R., Pedrini, H, Minghim, R. An Approach to Supporting Incremental Visual Data Classification. IEEE Transactions on Visualization and Computer Graphics, v. 21, p. 4-17, 2015
Similarity Organization





Similarity Organization





Selection of Representative Instances



Instances selected to train classification model

Classification using Created Model



Classification Results











Classification Model Upgrading

- Several upgrade strategies: Layout also works as a guide
 - Example: relabeling of strategic instances: adjustment to specific scenarios
- Successive iterations: classifiers adaptation
 - Insertion of user knowledge on the classification model
 - Convergence to desired results

Misclassified Instances Relabeling











Classification Model Upgrading



Reclassification - Upgraded Model



Reclassification - Upgraded Model



Visual Classification Methodology



Analysis of the classification results



Analysis of the classification results



Matching instances :	598 - 85,4%
Non-matching instances :	102 - 14,6%
lon-corresponding instances :	0 - 0%
Accuracy:	97,16%
Precision :	86,55%
Recall :	85,43%
F1:	0,86

		Classification										
		0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	FNR
Ground Truth 6.0 7.0 8.1 7.0 8.1 8.1 8.1 8.1 8.1 8.1 8.1 8.1 8.1 8.1	0.0	57	1	6	0	0	2	0	0	0	4	18,57%
	1.0	2	35	21	2	0	3	1	0	6	0	50,00%
	2.0	0	4	63	0	0	0	0	0	2	1	10,00%
	3.0	0	0	1	69	0	0	0	0	0	0	1,43%
	4.0	1	0	0	0	62	0	0	2	3	2	11,43%
	5.0	1	1	9	0	0	52	0	5	0	2	25,71%
	6.0	0	0	0	0	0	0	70	0	0	0	0,00%
	7.0	1	0	2	0	0	0	0	66	0	1	5,71%
	8.0	2	5	3	0	0	4	0	0	56	0	20,00%
	9.0	0	0	1	0	0	0	0	0	1	68	2,86%
FPR		1,10%	1,72%	6,39%	0,32%	0,00%	1,41%	0,16%	1,10%	1,87%	1,56%	



- Layout: clues
 - Data set structure
 - Classifier behaviour
 - Classes 6 and 25: heterogeneous branches
 - Classification is mixing instances in these branches



- Layout: clues
 - Data set structure
 - Classifier behaviour
 - Classes 6: several branches
 - Class covers a wide range of features
 - Naturally heterogeneous: could be divided into more homogeneous subclasses



- Layout: clues
 - Data set structure
 - Classifier behaviour
- Neighborhood of classes 6 and 25
- Confusion Matrix
 - Class 25 instances → class 8
 - Class 6 instances → class 15



Several upgrade strategies

- Verification of branches with high misclassification rates
- Classmatch tree: 23 representative misclassified instances
 - Class 25: 8 instances
 - Class 6: 15 intances



class 6



	Initial Model	Upgraded Model		
	ETHZ-Reduced			
Matching Instances	1704 (88.1%)	1808 (93.4%)		
Non-matching Instances	231 (11.9%)	127 (6.6%)		
Accuracy	98.47%	99.14%		
Precision	89.05%	94.06%		
Recall	88.06%	93.44%		
	ALL-Reduced			
Matching Instances	1875 (67.7%)	1991 (71.9%)		
Non-matching Instances	894 (32.3%)	778 (28.1%)		
Accuracy	86.61%	88.45%		
Precision	71.98%	73.79%		
Recall	67.71%	71.90%		

Dynamic scenarios

Data Set	Content	Classes	Items	Attributes
NEWS2011	News	7	1018	3731

Instances

Training Set	Test Set
42	976

- Classification model: 7 classes
 - Greek Financial Crisis
 - Ratko Mladic judgment
 - Syria Conflicts
 - USA Crisis
 - Yemen Attacks
 - Afghanistan
 - AmyWinehouse Death





- Two heterogeneous branches
 - Unknown patterns



- Main topics per branch
- New topics
 - Norway bomb
 - Escherichia coli outbreak



 Instances of new topics are used to update the classification model

Norway bomb

Escherichia coli outbreak









Point placement Techniques Capabilities

- Projection techniques
 - Group shapes are mantained
 - Outliers are more evident
 - Clutter is higher

NJ Trees

- Capable of describing the organization of the similarity
- Similarity is consistent at the branches' ends
- Does not require any parameter

Final Remarks

- Processing scalability
- Data access scalability
- Visual scalability
- Partition Strategies
- Sampling Strategies
- Data Structures related to Analysis processes and tasks
- Integration with Mining, Learning, Data Analysis in General
- Applications

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