## Visual Analytics for Large-scale High Dimensional Data: from Algorithms to Software Systems

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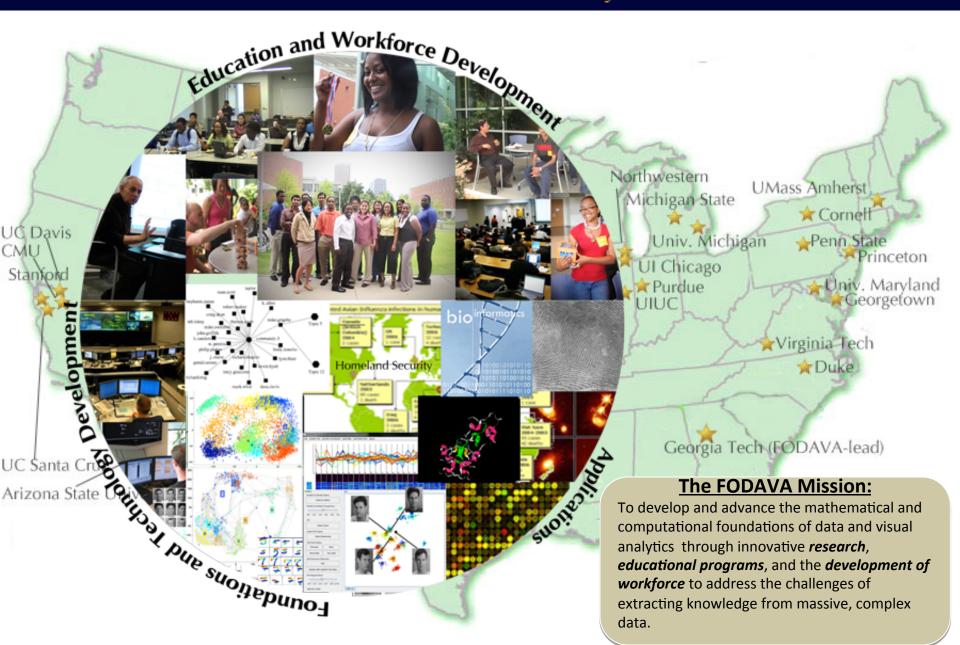
CSoI Big Data Workshop, March 18, 2013 This work is supported in part by NSF and DHS.



## Contributors

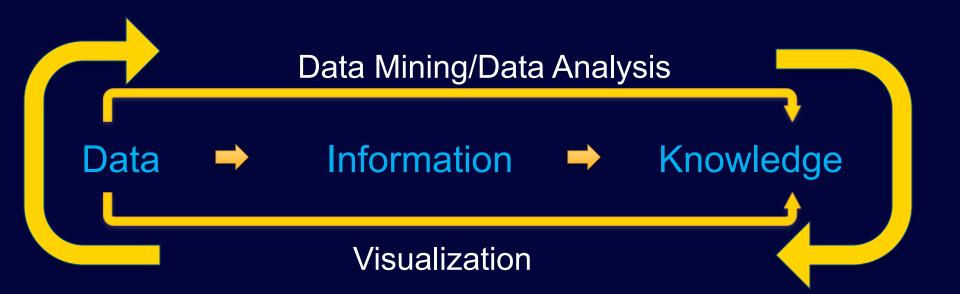
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- Ed Clarkson (Georgia Tech Research Institute)
- Polo Chau (Georgia Tech)
- Alexander Gray (and many of his students, Georgia Tech)
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- Jieping Ye (Arizona State University)

FOUNDATIONS OF Data and Visual Analytics



## **Data and Visual Analytics**

The Science of Analytical Reasoning facilitated by Automated Methods for Data Analysis and Interactive Visual Interfaces. (based on Thomas and Cook, Illuminating the Path: the research and development agenda for visual analytics, 2005)



"Solving a problem simply means representing it so that the solution is obvious." Herbert Simon, 96

#### Challenges and our Approaches for Interactive Analysis of *High Dimensional Large-scale Data*

#### • Challenges:

- Data are Massive, High-dimensional, Nonlinear, Unstructured, Imperfect, Heterogeneous, Time-varying, ...
- Limited Screen Space and Limited Visual Perception
- Need for real-time Interaction

#### • Our Approaches:

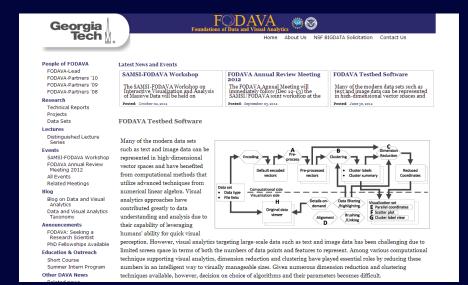
– Scalable and Robust algorithms:

works even when parts of the data are missing

- Integrated analysis: Representation of heterogeneous data on one map
- Fast Interaction: scalable, real-time, adaptive, on-line algorithms
- Severe dimension reduction: but key info preserved as much
- Informative representation of large volume of data

#### FODAVA Research Test-bed for Visual Analytics of High Dimensional Data http://fodava.gatech.edu/fodavatestbed-software

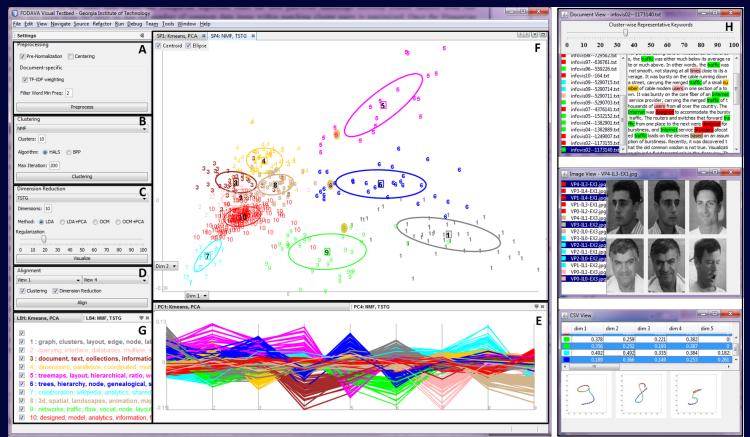
- Library of key computational methods for visual analytics of high dimensional data
- Modular: A base for specialized VA systems
- Supports various dimension reduction, clustering, and their visual representations and comparisons through alignments
- Application domains: document analysis, bioinformatics, healthcare, computer vision, ...
- Languages: backend library in Matlab, GUI in JAVA (no need for Matlab installed)
- System support: Windows 32/64 bit, Linux 32/64 bit



### **Testbed Modules and Overview**

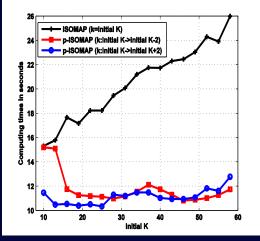
- Computational modules
  - Vector encoding
  - Pre-processing
  - Clustering
  - Dimension reduction

- Interactive visualization modules
  - Scatter plot
  - Parallel coordinates
  - Cluster summary
  - Raw data view
  - Brushing and Linking
  - Space alignment



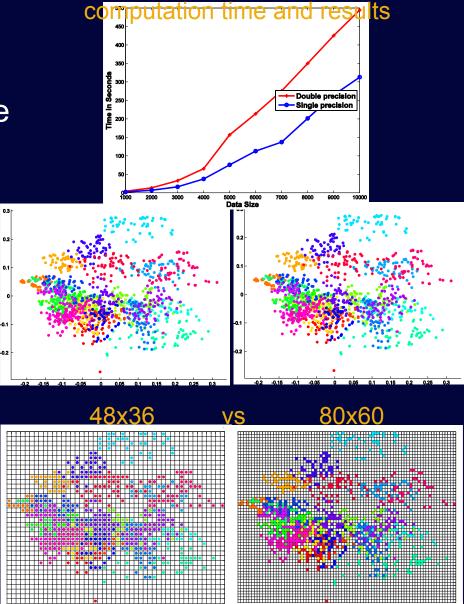
## Fast Comp. Modules for Interactive Vis.

- Essential for real-time interaction
- Let computational precision be governed by visual precision/ resolution
- Hierarchical refinement
- Adaptive algorithms



p-lsomap computing time vs. # of nearest neighbors





#### Dimension Reduction

- Linear and Nonlinear methods: PCA, FA, ProbPCA, LDA, OCM, NPE, LPP, LLTSA, NCA, MCML, MDS, Isomap, LLE, LTSA, Sammon, HessLLE, MVU, LandMVU, KernPCA, GDA, DiffMaps, SPE, AutoEnc, LLC, ManiChart, CFA, GPLVM, SNE, T-SNE
- Recursive dimension reduction: apply dimension reduction on userselected data

#### Clustering

- Hierarchical clustering, K-means, spherical K-means, GMM, NMF, constrained K-means, DisCluster/ DisKmeans [J. Ye]
- Cluster summary for document data
- Semi-supervised clustering
- Color-coded cluster/class labels

#### Classification

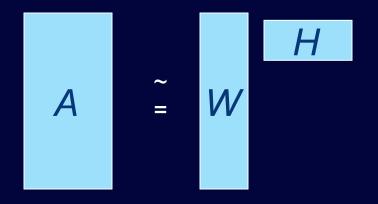
• *K*-nearest neighbors classifier, SVM, Logistic regression, Naïve Bayes

## **Key Computational Methods**

- NMF (Nonnegative Matrix Factorization) and its variations: for dimension reduction and clustering
- LDA/GSVD (Linear Discriminant Analysis) and its variations: for informative 2D representation of clustered and large scale data
- Orthogonal Procrustes and MDS (Multi-Dimensional Scaling): for space alignment and comparisons of visual representations

## **Nonnegative Matrix Factorization (NMF)**

(Paatero&Tappa 94, Lee&Seung NATURE 99, Pauca et al. SIAM DM 04, Hoyer 04, Lin 05, Berry 06, Kim and Park 06 Bioinformatics, Kim and Park 08 SIAM Journal on Matrix Analysis and Applications, …)



 $\rightarrow$  min || A – WH ||<sub>F</sub> W>=0, H>=0

Why Nonnegativity Constraints?
 Better Approx. vs. Better Representation/Interpretation
 *Nonnegative Constraints often physically meaningful, interpretable*

Fast Algorithms for NMF, with theoretical convergence (J. Kim and H. Park, IDCM08)
 NMF/ANLS: Iterate the following with Active Set-type Method (ANLS/BPP) fixing W, solve min<sub>H>=0</sub> || W H – A||<sub>F</sub> fixing H, solve min<sub>W>=0</sub> || H<sup>T</sup> W<sup>T</sup> – A<sup>T</sup>||<sub>F</sub>
 \* Software available at www.cc.gatech.edu/~hpark

 NMF variants developed for clustering, topic modeling, and graph clustering (sNMF, tNMF, SymNMF, hierarchicalNMF, BMF for recommender system,...)

## **NMF and K-means**

- Clustering and Lower Rank Approximation are related.
  - NMF for Clustering: (Ding et al. SDM 05; Kim & Park, TR 08)
  - Document (Xu et al. SIGIR 03), Image (Cai et al. ICDM 08), Microarray (Kim & Park, Bio 07), etc.
  - min  $\sum_{1 \le i \le n} ||a_i w_{\sigma i}||^2 \implies \min ||A WH||_F^2$  $\sigma_i = j$  when *i*-th point is assigned to *j*-th cluster ( $j \in \{1, ..., k\}$ )

<u>K-means</u>: *W*: *k* cluster centroids,  $h_i$ : cluster membership indicator <u>NMF</u>: *W*: basis vectors for rank-*k* approx.,  $h_i$ : *k*-dim rep. of  $a_i$ <u>Sparse NMF</u> (for sparse *H*) (H. Kim and Park, Bioinformatics, 07) min<sub>*W*, *H*</sub> {  $||A-WH||_F^2 + \eta ||W||_F^2 + \beta \sum_{1 \le j \le n} ||H(:, j)||_1^2$  },  $\forall i, j, W_{ij}, H_{ij} \ge 0$ 

 Obj. fun. of K-means and NMF are related when H ∈ E and A ≥ 0, but their performances may be very different.

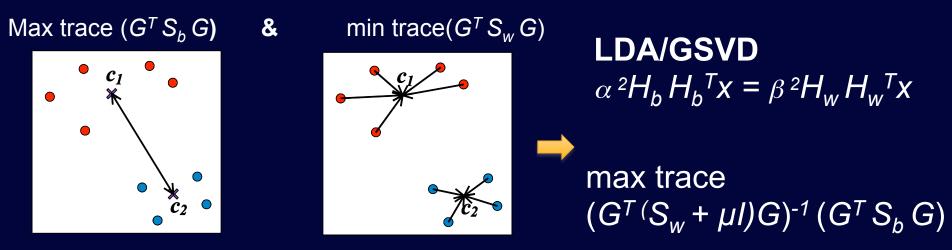
## **NMF for Clustering**

7	#clusters	2		6		10	1	14		18		Clustering Accurac on Reuters-21578	
	K-means	0.7867	0.5	137	0.	4191	0.4	4529	0.	3403			
Ν	IMF/ANLS	0.9257	0.6	934	0.	5568	0.5	5654	0.4	3130		and TCT2	
	#cluster	s 2		6		10		14		18		NMF is faster by factor of 2 at least	
	K-means	s 0.80	99	0.72	95	0.701	5	0.667	'5	0.667	5		
	NMF/ANL	.S 0.99	90	0.87	17	0.743	86	0.702	21	0.716	0		
	SNMF/AN	LS 0.99	91	0.87	70	0.751	2	0.726	9	0.727	8		
Data	a set	TDT2	TDT2		Reuters		NIPS			ORL	Ext Yale		
Dimension		26,618			12,998			17,583			69x84	56x64	
# data points		8,741			8.095		420	420			400	2.414	

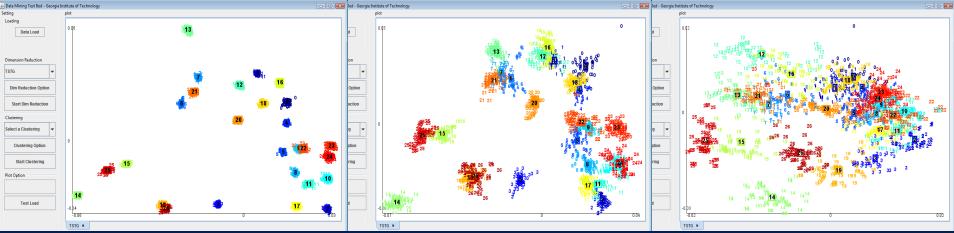
Data set	TDT2	Reuters	NIPS	ORL	Ext YaleB
Dimension	26,618	12,998	17,583	69x84	56x64
# data points	8,741	8,095	420	400	2,414
# clusters	20	20	9	40	38
Kmeans	0.6734	0.4289	0.4650	0.6499	0.0944
Ker. Kmeans	0.6789	0.3455	0.5071	0.6858	0.1692
NMF	0.8534	0.3770	0.4877	0.7020	0.1926
GNMF	0.8077	0.4441	0.4894	0.7282	0.2109
SymNMF	0.8979	0.5305	0.5129	0.7798	0.2307

#### Linear Discriminant Analysis for 2D/3D Representation of Clustered Data

(J. Choo, S. Bohn, HP, VAST09)



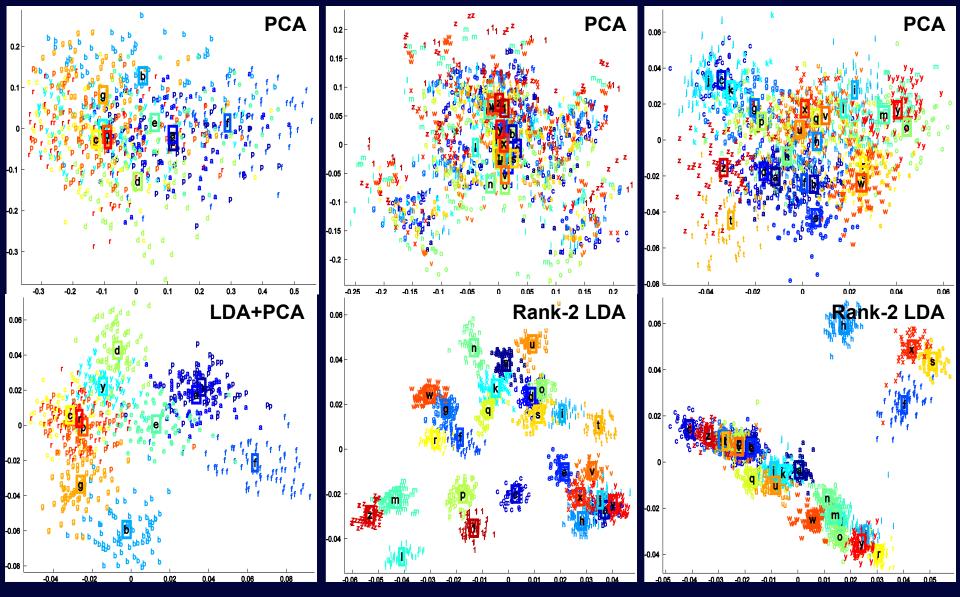
#### Regularization in LDA for Computational Zooming-in



#### Small regularization

#### Large regularization

## 2D Visualization of Clustered Text, Image, Audio Data



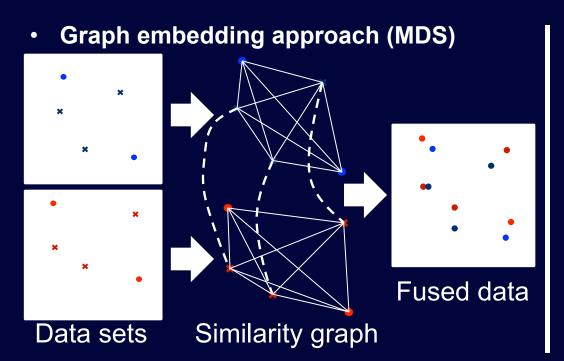
20news Data (Text)

Facial Data (Image)

Spoken Letters (Audio)

#### Information Fusion and Visual Comparisons based on Space Alignment (J. Choo, S. Bohn, G. Nakamura, A. White, HP)

- Want: Unified visual representations of different results
- Assume: Reference correspondence information between data pairs or cluster correspondence
- Two conflicting criteria: maximize alignment and minimize deformation

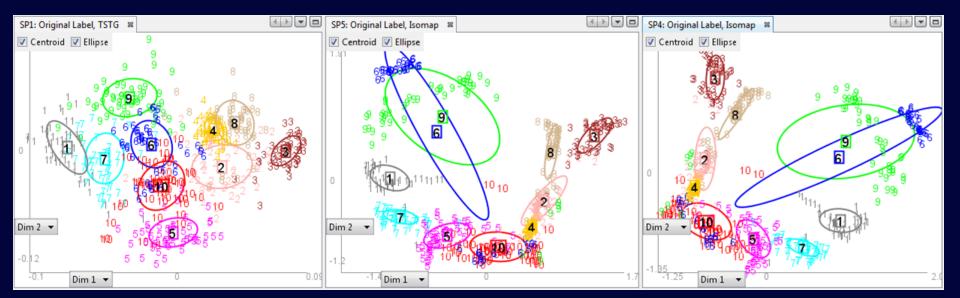


• Procrustes analysis min ||  $(A-\mu_A 1^T)-kQ(B-\mu_B 1^T)||_F$  $Q^TQ=I$ 

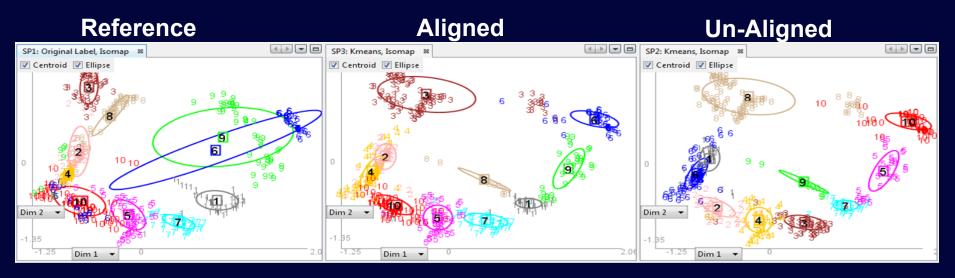
## Space Alignment by Orthogonal Procrustes

min  $|| (A - \mu_A 1^T) - kQ(B - \mu_B 1^T) ||_F$ , where  $Q^TQ = I$ 

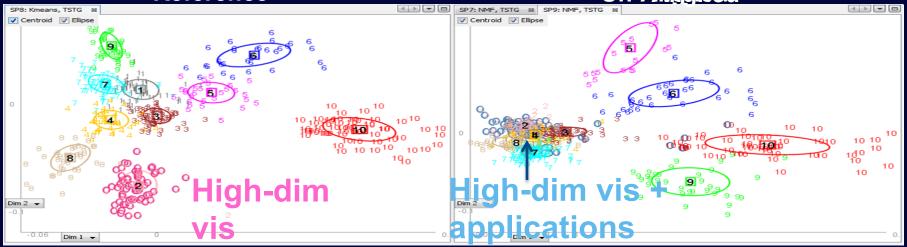
# Alignment of Dimension Reduction ResultsReferenceAlignedUn-Aligned



## Cluster Alignment: Label Matching and Space Alignment



Reference



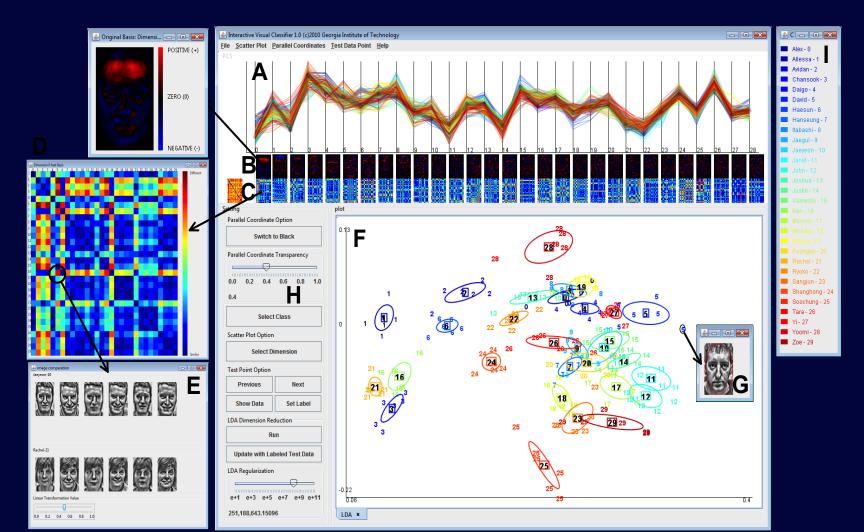
Un-Aliboneed

- InfoVis and VAST paper data set
- Help refine cluster results and obtain consensus clustering

#### **iVisClassifier**

(J. Choo, H. Lee, J. Kihm, HP, VAST10)

Interactive visual analytics system for **classification** of high-dim. data (image, text, etc) and **search space reduction** 



#### VisIRR: Visual Information Retrieval and Recommendation System for Document Discovery

#### Our differentiators:

- Improves personalization and understandability via integrated visualizations of document retrieval and recommendation
- Visual IR: beyond Google-like keyword search:
  - See **more** relevant documents
  - See **relationships**: topical, inter-document
  - Whole **content**-based, not keyword-based
- Visual Recommendation: enables discovery
  - Personalized based on user feedback, persistent
  - Understand "why" due to visualized relationships
- Only possible due to **new/fast ML** algorithms

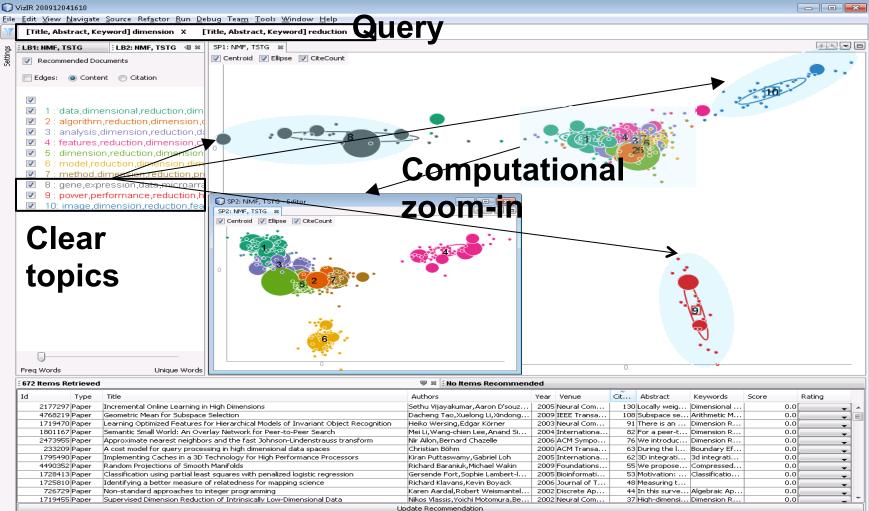
## **VisIRR**

## An interactive visual information retrieval and recommender system for large-scale document data

VizIR 200912041610							
File Edit View Navigate Source Refactor Run Debug Team Tools Window Help							
[Title] disease X							
: Settings 4	SP1:NMF,TSTG m						
Grouping Options	V Centroid V Ellipse V CiteCount						
NMF •		·· · · · · · · · · · · · · · · · · · ·					
Clusters: 10		· · · · · /					
Algorithm:  Algori							
Max Iteration: 200							
Visualization Options							
#Dimensions: 2		Chater-vise Representative Keywords					
Option: 1		0 10 20 30 40 50 60 70 80 90 100					
Regularization		2181099 Marc Schaub,Irene Kaplow,Marina Sirota,Chuong Do,Atul					
UI:    Slidebar   Textbox		6079204 Butte.Serafim Batzoglou, A Classifier-based approach to 13005577 identify genetic similarities between diseases.					
		6025520 1866732 Bioinformatics/computer Applications in The Biosciences, 2009, 1866732 Keywords: Cenetic Similarity Genetic Variation Rheumatold					
0 10 20 30 40 50 60 70		<ul> <li>4279661 Arthritis, Single Nucleotide Polymorphism, type 1 diabetes, Decision Tree Classifier Genome Wite Association Study</li> </ul>					
		Abstract: Motivation: Genome-wide association studies are commonly used to identify possible associations between menetic					
Regularization Value: 10 <sup>^</sup> 0		variations and diseases. These studies mainly focus on [centifying Individual sincle nucleotide polymorphisms (SNPs) potentially					
Perform Visualization		linked with one <u>bisense</u> of interest. In this work, we introduce a novel methodology that <u>items</u> in this work, we introduce a					
Re-grouping Visualize		using information from a large number of SNPs. We separate the diseases for which we have individual genotype data into one					
Recommendation Options		reference <b>Incente</b> and several query diseases. We train a <b>Classifier</b> that distinguishes between individuals that have the					
Based on:  Content  Citation  Co-authorship		SP1: NMF, TSTG - Editor					
#Interations: 3		V Centroid V Elipse V CiteCount					
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i LB1: NMF, TSTG 📲 🕷							
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🖉 Edges: 💿 Content 💿 Citation 💿 Co-authorship							
1 : disease,study,based,data,system,heart,information							
2 : gene,disease,expression,human,network,method,		0					
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6 : patient,disease,control,test,based,analysis,brain,c		Venue CiteCnt Abstract Keywords Score Rating					
7 : system,disease,based,support,medical,heart,data		9/IEEE International Confer 0/Inspired by Genetic Dise 9.193					
8 : liver,disease,diagnosis,features,case,based,select		6 Bioinformatics/computer 17 Over 1600 Comparativ 8.674 Highly Like (5)					
9 : network,disease,neural,classification,model,feature	2529942 Paper A partially supervised classification approach to dominant and recessive human diseas Borja Calvo, Núria López-bigas, Simon Furney, Pe 2007 4754384 Paper A lan human interactione with observative causa two censes and networks und Xuebing Wu, Offang Lu, Ruji Jiang 2009	Computer Methods and P     8 The discove Computatio     8.545     Bioinformatics/computer     8 Motivation: Gene Netwo     8.534     Highly DisLike (1)					
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	4755093 Paper Gene-disease relationship discovery based on model-driven data integration and data 5. Yilmaz, P. Jonveaux, C. Bicep, L. Pierron, Malika 2009	9 Bioinformatics/computer 2 Motivation: Data Integrity 6.052 Weakly Like (4)					
		7 Soft Computing 5 The genetic Combinatori 5.677 4 IEEE Computer Society Bi 1 Constructin Colon Cance 5.070					
		8 International Conference 0 In the post Functional A 5.043 Weakly Like (4)					
	4428698 Paper Medical ontologies to support human disease research and control Maja Hadzic, Elizabeth Chang 2005	5 International Journal of 4 In this pape Human Dise 4.845					
		7 IEEE International Confer 1 Discovering Gene Predic 4.760 6 Bioinformatics/computer 51 Motivation: Cross Valida 4.363					
		9 Bioinformatics/computer 4 Motivation: Genetic Simil 4.295 No opinion (3)					
	6065805 Paper Phenotypic categorization of genetic skin diseases reveals new relations between phe Ruslan Sadreyev, Jamison Feramisco, Hensin Tsa 2009	9 Bioinformatics/computer 2 Motivation: Genetics, Ski 4.240					
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0	50643 Paper PTD Controller Ontimization Based on the Self-Organization Genetic Algorithm with Cvcl. Zhang Jiohua Zhuang Jian Du Haifeng Wang Su. 2007.	7 Mexican International Co. 2 In this name invaluation of 3.866					
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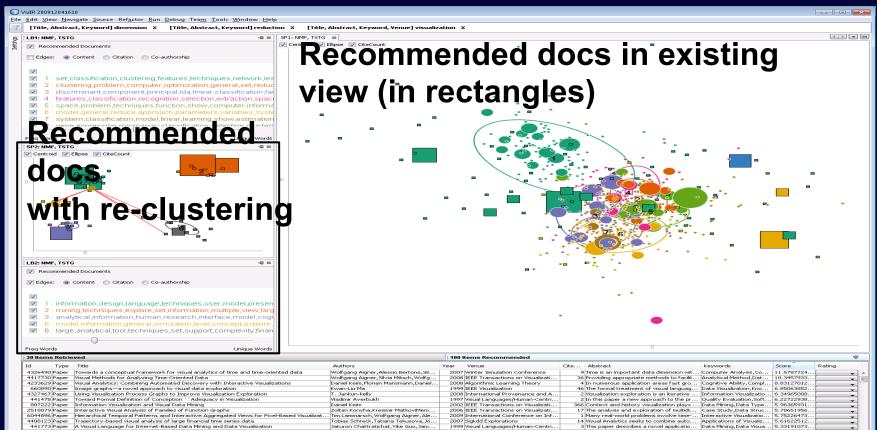
## **Visualization Example of Queried Set**

#### Keyword query, 'dimension reduction'



## **Recommendation Example**

Preference-assigned item as 'highly like' : 'Enhancing the visualization process with principal component analysis to support the exploration of trends'



2002 IEEE Visualization

nutor Crash

29 The current state of the art in visualiza.

Data Exploration, Gene

Jankun-Kelly,Kwan-Liu Ma,Michael.

660116 Paper

A model for the visualization exploration process

## **FODAVA Website** http://fodava.gatech.edu

- Dissemination of FODAVA results to user communities
  - FODAVA Tech Reports/Software
- FODAVA meeting/lecture materials
- Data Sets
- DAVA Taxonomy and course material
- DAVA community events and meeting information

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People of FODAVA	Latest News and Events	People of FODAVA		
FODAVA-Lead FODAVA-Partners '10	SAMSI-FODAVA Workshop	FODAVA Annual Review Meeting	FODAVA Testbed Software	FODAVA-Lead FODAVA-Partners '10
FODAVA-Partners 10 FODAVA-Partners 109	The SAMSLEODAVA Workshop on		Many of the modern data sets such as text	FODAVA-Partners '09
FODAVA-Partners '08	The SAMSI-FODAVA Workshop on Interactive Visualization and Analysis of Massive Data will be held on December	The FODAVA Annual Meeting will immediately follow (Dec 12-13) the SAMSI/FODAVA joint workshop at the	Many of the modern data sets such as text and image data can be represented in high-dimensional vector spaces and have	FODAVA-Partners '08
Research	Posted: October 02, 2012	Posted: September 05, 2012	Posted: June 30, 2012	Research
Technical Reports	Functi. October 02, 2012	Toste. Optimier 03, 2012	Tostel. June 30, 2012	Technical Reports
Projects		Projects		
Data Sets	About FODAVA			Data Sets
.ectures				Lectures
Distinguished Lecture Series	Enormous amounts of data are being generated		About fodava.gatech.edu	Distinguished Lecture Series
vents	00			Events
All Events	every day in health care,		Our goal is to keep you informed on	All Events
Related Meetings	computational biology,		the progress of the FODAVA initiative while being maintained as a	Related Meetings
Blog	homeland security,		base for further education and	Blog
Blog on Data and Visual	commerce, and many		outreach to the data and visual	Blog on Data and Visual Analytics
Analytics	other areas. Analyzing		analytics community.	Data and Visual Analytics
Data and Visual Analytics Taxonomy	these massive and			Taxonomy
Announcements	complex data sets is		Read more about FODAVA and view	Announcements
FODAVA: Seeking a	essential to achieve new	A STATE AND A STAT	a presentation on FODAVA's	FODAVA: Seeking a Research Scientist
Research Scientist	discoveries, but		Research, Education and Community Building!	PhD Fellowships Available
PhD Fellowships Available	extremely difficult. An		Building:	Education & Outreach
ducation & Outreach	emerging research field		Recently updated	Short Course
Short Course	known as data and visual		Recently updated	Summer Intern Program
Summer Intern Program	analytics is concerned with synthesizing	information and deriving insight from	Links	Other DAVA News
Other DAVA News	massive, dynamic, ambiguous and possi	bly conflicting digital data for increased		Related news
Related news	understanding and effective decision ma	king.	<ul> <li><u>Department of Homeland Security</u></li> <li>National Science Foundation</li> </ul>	
			Research, Education and	
			Community Building	
	The Foundations on Data Analysis and V			
	initiative is dedicated to both defining th			
		of-the-art. Established in 2008, the FODA		
	initiative is a collaborative effort funded			

<u>8</u> 🛞 Home About Us NSF BIGDATA Solicitation Contact Us Latest News and Events SAMSI-FODAVA Workshop **FODAVA Annual Review Meeting** FODAVA Testbed Software 2012 The SAMSI-FODAVA Workshop on Interactive Visualization and Analysis of Massive Data will be held on December The FODAVA Annual Meeting will immediately follow (Dec 12-13) the SAMSI/FODAVA joint workshop at the Many of the modern data sets such as text and image data can be represented in high-dimensional vector spaces and have Posted: October 02, 2011 Posted: September 05, 2012 Posted: June 30, 2011 FODAVA Testhed Software Many of the modern data sets such as text and image data can be represented in high-dimensional vector spaces and have benefited from computational methods that utilize advanced techniques from numerical linear algebra. Visual analytics approaches have contributed greatly to data understanding and analysis due to their capability of leveraging humans' ability for quick visual perception. However, visual analytics targeting large-scale data such as text and image data has been challenging due to

perception. However, visual analytics targeting large-scale data such as text and image data has been challenging due to limited screen space in terms of both the numbers of data points and features to represent. Among various computational technique supporting visual analytics, dimension reduction and clustering have played essential roles by reducing these numbers in an intelligent way to visually manageable sizes. Given numerous dimension reduction and clustering techniques available, however, decision on choice of algorithms and their parameters becomes difficult.

The FODAVA testbed system is an interactive visual testbed system for dimension reduction and clustering in a large-scale high-dimensional data analysis. The testbed system enables users to apply various dimension reduction and clustering methods with different settings, visually compare the results from different algorithmic methods to obtain rich knowledge for the data and tasks at hand, and eventually choose the most appropriate path for a collection of algorithms and parameters.

The testbed can load image, raw text, and vector-encoded data types. It offers 4 different clustering and 17 different dimension reduction methods. Furthermore, the FODAVA testbed system is implemented in a flexible and modular way so

The Georgia Institute of Technology, as the FODAVA-Lead institution will lead and

(NSF) and the Department of Homeland Security (DHS)

## **Concluding Remarks**

- Data and Visual Analytics is especially important for data understanding and question generation
- For Big data analytics, more integrated research that tie automated algorithms and interactive visualization needed
- Our Contributions:
  - Foundational algorithms for visual representations of high dimensional, large scale, heterogeneous data
  - Fast algorithms for real time interaction
  - Development of VA testbed and other VA systems

Thank you!