Dimensionality Reduction From Several Angles

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Johannes Kepler University, Linz Austria 27 May 2014

http://www.cs.ubc.ca/~tmm/talks.html#linz14

Dimensionality Reduction

- · what is it?
- -map data from high-dimensional measured space into lowdimensional target space
- when to use it?
- -when you can't directly measure what you care about
- true dimensionality of dataset conjectured to be smaller than dimensionality of measurements
- · latent factors, hidden variables

DR Example Malignant Benign Tumor Measurement DR Data 9 Dimensional 2 Dimensional Measured Space Target Space

Dimensionality Reduction

- why do people do DR?
- -improve performance of downstream algorithm
 - · avoid curse of dimensionality
- -data analysis
 - if look at the output: visual data analysis

Angles of Attack

- · design algorithms
- design systems
- design tools to solve real-world user problems
- evaluate/validate all of these
- create taxonomies to characterize existing things
- benefits of multiple angles
- -parallax view of what's important
- -outcomes cross-pollinate

Questions: A Progression

- can we design DR algorithms/techniques that are better than previous ones?
- can we build a DR system that real people use?
- when do people need to look at DR output? - how can we figure out what people need?
- how should people look at DR output?
- how can we tell if we're drawing the right picture?
- do metrics match up with human perception?
- why and how do people use DR?

Even More Questions

- open questions
 - -how are real people actually using DR tools/techniques?
 - · does it match up with what we think/hope/assert/assume?
 - -why are they using it?
 - what are their goals and tasks, at abstract level?
 - —is it working?
 - · how do their goals match up with implicit assumptions behind different benchmarks?
 - do current state of the art tools meet their needs?

Dimensionality Reduction In the Wild

Tasks and Challenges

joint work with: Michael Sedlmair, Matthew Brehmer, Stephen Ingram

work in progress

Two-Year Cross-Domain Qualitative Study

- in the wild
- -HCl term for work in the field with real users
- vs controlled lab setting
- interviewed two dozen high-dim data analysts
- -across over a dozen domains and past several years
- final results coming soon
- -taxonomy of abstract tasks for DR
- -identified significant unmet user needs
- why and how do people use DR?
- -overarching question weaving through projects in this talk -preliminary results from study informed many of them

• can we design DR algorithms/techniques that are

Questions and Answers

- better than previous ones?
- can we build a DR system that real people use?
- when do people need to look at DR output?
- how should people look at DR output?
- why and how do people use DR?
- so... how do we answer these questions?
- -many validation methods to choose from!

abstracting into operations on data types designing visual encoding and interaction techniques creating algorithms to execute techniques efficiently

characterizing the problems of real-world users

A Nested Model

of Visualization Design and Validation

http://www.cs.ubc.ca/labs/imager/tr/2009/NestedModel

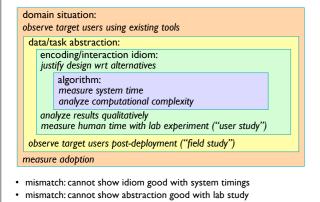
A Nested Model of Visualization Design and Validation. Munzner. IEEE TVCG 15(6):921-928, 2009 (Proc. InfoVis 2009).

Four Levels of Design and Validation

- four levels of design problems
- -different threats to validity at each level

problem characterization: you misunderstood their needs data/task abstraction: you're showing them the wrong thing visual encoding / interaction techniques: the way you show it doesn't work algorithm: your code is too slow

Nested Levels of Design and Validation



Where Do We Go From Here?

- no single paper includes all methods of validation -pick methods based on angle of attack
- in this talk
 - -cover many different methods and kinds of questions they can help with answering

Outline

- can we design better DR algorithms?
- can we build a DR system for real people?
- how should we show people DR results?
- when do people need to use DR?

Outline

- can we design better DR algorithms?
- -algorithm for GPU MDS: Glimmer
- -algorithm for MDS with costly distances: Glint
- can we build a DR system for real people?
- how should we show people DR results?
- when do people need to use DR?

Glimmer Multilevel MDS on the GPU joint work with: Stephen Ingram, Marc Olano http://www.cs.ubc.ca/labs/imager/tr/2008/glimmer/

MDS: Multidimensional Scaling

- entire family of methods, linear and nonlinear
- classical scaling: minimize strain
- -Nystrom/spectral methods: O(N)
 - Landmark MDS [de Silva 2004], PivotMDS [Brandes & Pich 2006]

. 30h

Glint: An MDS Framework for Costly Distance Function

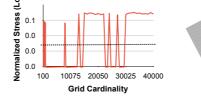
Ingram, Munzner. Proc. SIGRAD 2012.

- -limitations: quality for very high dimensional sparse data
- distance scaling: minimize stress
- -nonlinear optimization: O(N2)
 - SMACOF [de Leeuw 1977]
- -force-directed placement: O(N2)
- Stochastic Force [Chalmers 1996]
- limitations: quality problems from local minima
- Glimmer goal: O(N) speed and high quality

Glimmer Strategy

Stochastic force alg suitable for fast GPU port

 but systematic testing shows it often terminates too soon



 Use as subsystem within new multilevel GPU alg with much better convergence properties

Sparse Dataset (docs): N=D=28K -quality higher -speed equivalent 16.64 s stress=0.157 2.17 s stress=0.928 Pivot MDS Pivot MDS Gilimmer Pivot MDS O 10,000 Gilimmer Pivot MDS Cardinality Gilimmer Cardinality Gilimmer Cardinality

Methods and Outcomes

- methods
- quantitative algorithm benchmarks: speed, quality
 systematic comparison across 1K-10K instances vs a few spot
- -qualitative judgements of layout quality
- outcomes
- -characterized kinds of datasets where technique yields quality improvements

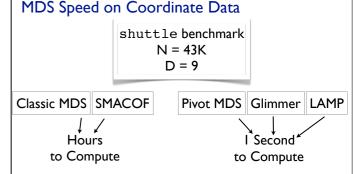
flickr benchmark

- then what?
- -saw what real users could do with it after release
 identified limitations
- identified illification.

MDS Algorithm Speeds • newer algorithms linear, but...

• newer algorithms linear, but...

Age	Algorithm	Author/Year	Complexity
ĺ	Classic MDS	Torgersen '52	$O(N^3)$
	SMACOF	de Leeuw '77	O(N³)
	Pivot MDS	Brandes '07	O(kN)
	Glimmer	Ingram '09	O(cN)
	LAMP	Joia 'I I	O(kN)



time to calculate distance between two points
 -0.00001 second

MDS Speed on Distance Matrix Data

N = 1925
d = EMD

Classic MDS SMACOF

Pivot MDS Glimmer LAMP

Hours

I hour Hours Hours

M = 1925
Hour Hours

 time to calculate distance between two points -0.01 second

MDS Input: Coordinates vs Distances

http://www.cs.ubc.ca/labs/imager/tr/2012/Glint/

High Dimensional ______ MDS _____ Low Dimensional Geometry Geometry Coordinate Space Coordinate Space

An MDS Framework for Costly Distance Functions

- some systems intrinsically require coordinates
 –fundamental to LAMP speedup approach
- some handle both
 including Glimmer

Glint

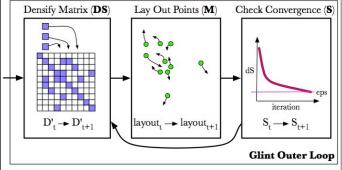
Costly Distances

• DR in the Wild revealed many real-world examples

Distance function	Cost (seconds)
Euclidean on 9-D data	0.00001
Database Query	0.001
Earth Mover Distance	0.01
Euclidean on 4M-D data	1.0
Human-in-the-loop	10.0
	Euclidean on 9-D data Database Query Earth Mover Distance Euclidean on 4M-D data

Glint Framework

- calculate as few distances as possible, maintain quality
- three-stage architecture

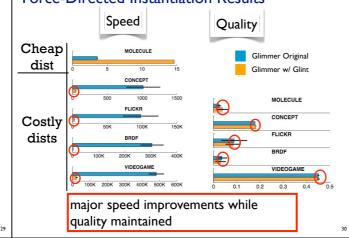


Glint Instantiations

- framework accommodates broad spectrum of algorithm types
- -three instantiations provided

MDS Algorithm Type	Chosen Algorithm
Gradient-based Optimization	SMACOF
Spectral/Analytic	Pivot MDS
Force-Directed	Glimmer

Force-Directed Instantiation Results



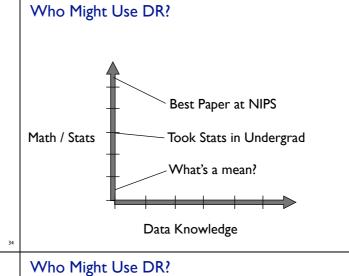
Methods and Outcomes

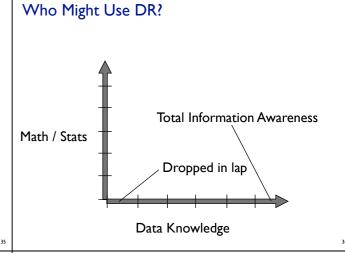
- methods
- -algorithm benchmarks
- outcomes
- -dataset characterization different from previous work motivated by needs of real-world users
- -characterized distance metrics where architecture yields speed improvements
- then what?
- keep talking to real users as way to discover more unmet needs

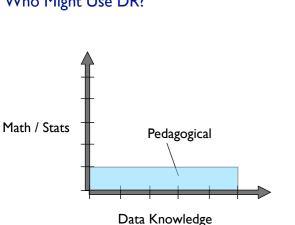
Outline

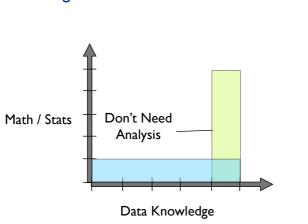
- can we design better DR algorithms?
- -next: how do we get people to use DR properly?-move emphasis from solo algorithms to entire system
- can we build a DR system for real people?
 system that provides guidance: DimStiller
- when do people need to use DR?
- how should we show people DR results?
- why and how do people use DR?

Who Might Use DR? • DR in the Wild revealed broad set of users **DimStiller** Math / Stats Workflows for Dimensional Analysis and Reduction , Stephen Ingram, Veronika Irvine, Melanie Tory, Steven Bergner, Torsten Möller http://www.cs.ubc.ca/labs/imager/tr/2010/DimStiller/ DimStiller:Workflows for dimensional analysis and reduction. Ingram, Munzner, Irvine, Tory, Bergner, Moeller. Proc. VAST 2010, p 3-10. Data Knowledge Who Might Use DR? Who Might Use DR?

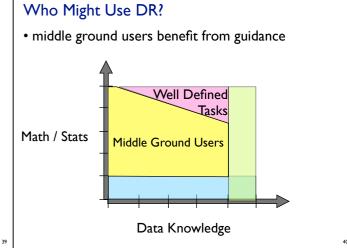


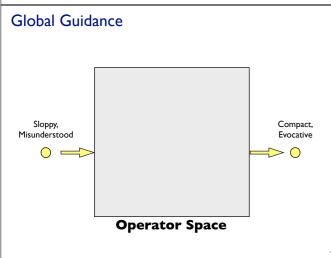


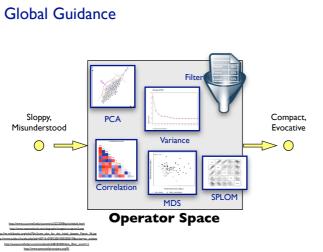


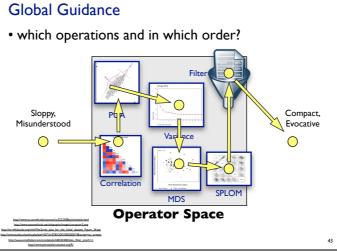


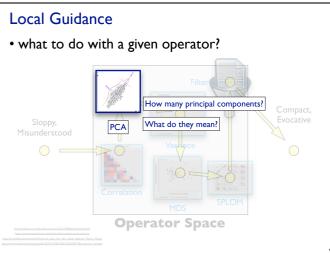
Well Defined **Tasks** Math / Stats Data Knowledge









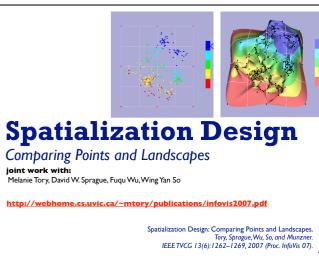


DimStiller Methods and Outcomes

- methods
 - -usage scenarios: workflows
 - identified several (preliminary DRITW results)
 - · built system to accommodate new ones as they're uncovered
- outcomes
- -prototype system: "DR for the rest of us"
- then what?
- -who else needs guidance? not just end users!

Outline

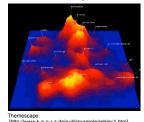
- can we design better DR algorithms/techniques?
- can we build a DR system for real people?
- -next: more guidance about visual encoding
- how should we show people DR results?
- -visual encoding guidance for system developers: Points vs Landscapes
- -visual encoding guidance for metric developers wrt human perception:
 - **Visual Cluster Separation Factors**
- when do people need to use DR?



- local guidance for each operator
- example: estimate true dimensionality with scree plot

Information Landscapes

- 2D or 3D landscape from set of DR points
- -height based on density
- oddly popular choice in DR
- -despite known occlusion/distortion problems with 3D
- -assertions: pattern recognition, spatial reasoning, familiar





Understanding User Task • abstract: search involving spatial areas and estimation

Estimate which grid cell has the most points of the target color

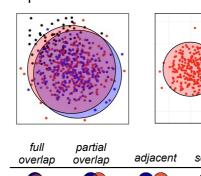




- domain-specific examples
 - "Where in the display are people with high incomes?"
 "Does this area also have high education levels?"
 - 'Does this area correspond to a particular work sector?
- non-trivial complexity yet fast response time
- frequent subtask in pilot test of real data analysis

Cluster Separation

• simple idea



Visual Cluster Separation Measures

(color + height redundantly encoded)

-points are better than landscapes

hypotheses

• result: yes!

result: yes

• Many cluster separation measures proposed for semi-automatic guidance in high-dim data analysis

• much better: 2-4 × faster, 5-14 × more accurate

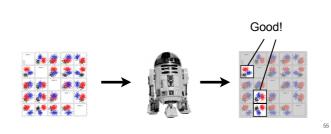
-2D landscapes (color only) better than 3D landscapes

• significantly faster, no significant difference in accuracy

Sips et al.: Selecting good views of high-dimensional data using class consistency

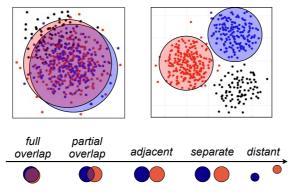
Lab Study: Test Human Response Time and Error

Tatu et al.: Combining automated analysis and visualization techniques for effective xploration of high-dimensional data [VAST 2009]



Methods and Outcomes

- methods
- -lab study: controlled experiment
 - outcomes
 - -prescriptive advice at visual encoding level avoid 3D landscapes
 - then what?
 - -yet more guidance from user studies? not so fast...



Visual Cluster Separation Measures

- goal: number captures whether human looking at layout sees something interesting
- -after computation is done, not to refine clustering
- measures checked with user studies

Tatu et al.: Visual quality metrics and human perception: an initial study on 2D projections of large multidimensional data [AVI 2010]

 but our attempt to use for guidance showed problems No!



User vs. Data Study

, Michael Sedlmair, Andrada Tatu, Melanie Tory

A Taxonomy of

ioint work with:

- user study
- -previous work on validating cluster

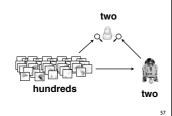
Visual Cluster

Separation Factors

http://www.cs.ubc.ca/labs/imager/tr/2012/VisClusterSep

A Taxonomy of Visual Cluster Separation Factors. SedImair, Tatu, Munzner, Tory. Computer Graphics Forum 31(3):1335-1344, 2012 (Proc. EuroVis 2012).

- -many users, few datasets
- -missing: dataset variety
- data study
- -few users, many datasets



816 Dataset Instances

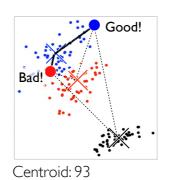
- 75 datasets
- -31 real, 44 synthetic
- -pre-classified
- 4 DR methods
- -PCA
- -Robust PCA
- -Glimmer MDS
- -t-SNE
- 3 visual encoding methods
- -2D scatterplots, 3D scatterplots, 2D SPLOMs
- -color-coded by class







Centroid Measure



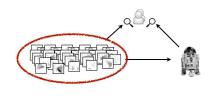
Analysis Approach

- · qualitative method out of social science: coding -open coding: gradually build/refine code set
- -axial coding: relationships between categories

Charmaz, K. Constructing Grounded Theory: A Practical Guide through Qualitative Analysis. 2006. Furniss, D., Blandford, A., Curzon, P. and Mary, Q. (2011). Confessions: PhD: experiences and lessons learnt. Proc. ACM CHI 2011, p 113-122.

- evaluating the measures
- -metric aligns with human judgement?
- -if not: what are the reasons?

Qualitative Analysis I: Cluster Separation Factors













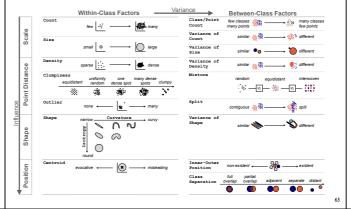
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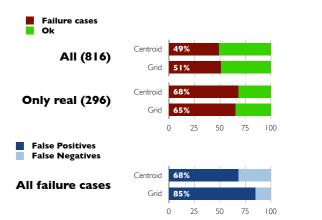
Furniss, D., Blandford, A., Curzon, P. and Mary, Q. (2011). Confessions PhD: experiences and lessons learnt. Proc. ACM CHI 2011, p 113-122

- · evaluating the measures
- -metric aligns with human judgement?
- -if not: what are the reasons?
- building taxonomy of factors from reasons
- mapping measure failures onto taxonomy

A Taxonomy of Cluster Separation Factors



High-Level Results



Centroid Failure Example

• big classes overspread small ones

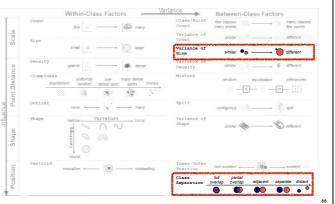


Problem: FP

Red: 77 (Good)

Data: Gaussian, synthetic DR: MDS

Relevant Taxonomy Factors



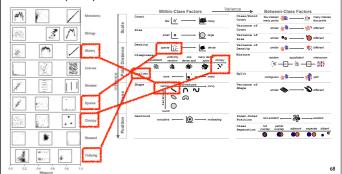
Centroid: Mapping Assumptions Into Taxonomy

- centroid only reliable if
 - -round-ish clusters
 - -not more than one dense spot
 - -no outliers
 - -similar sizes & number of points
- rarely true for real datasets

Related Work

×

- Scagnostics [Wilkinson et al. 2005]
- -mathematical description and algorithmic instantiation vs human perception



Methods and Outcomes

- methods
- -qualitative data study
- · we encourage more work along these lines
- outcomes
- -taxonomy to understand current problems
- measures
- -taxonomy to advise future development
- measures, techniques, systems
- then what?
- -from how to help them do DR better to understanding when they need to do it at all

Outline

- how can we design better DR algorithms/techniques?
- how can we build a DR system for real people?
- how should we show people DR results?
- -next: continue figuring out what people need
- when do people need to use DR?
- -sometimes they don't: QuestVis
- -how to figure out when they do or don't: Design Study Methodology



A Visualization System for an Environmental Sustainability Model

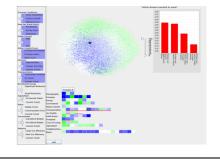
ioint work with Aaron Barsky, Matt Williams

http://www.cs.ubc.ca/labs/imager/tr/2011/QuestVis/

Reflections on QuestVis:AVisualization System for an Environmental Sustainability Model munzner, Barsky, Williams.
Scientific Visualization: Interactions, Features, Metaphors. Dagstuhl Follow-Ups 2, 2011, Chapter 17, p 240–259.

Application Domain: Sustainability

- · user data: sustainability simulation model
- -high-dimensional inputs/outputs
- our decision: show relationship between input choices and output indicators with linked views including DR layout



Hammer Looking for A Nail

- wrong task abstraction: they didn't need DR!
- -goal mismatch
- discussion of issues and behavior change from general public
- not data analysis to understand exact relationships between input and output variables
- -this failure case was one of motivations for nested model
- how can we tell what users actually need?
- -talking to users: necessary but not sufficient
- -we now have some answers!
- · we have proposed a methodology for problem-driven research -design studies: build vis tools to solve user problems
- -DR as one of many possible techniques that might be used

DESIGN STUDY METHODOLOGY SUITABLE **Design Study** INFORMATION LOCATION Methodology

Reflections from the Trenches and from the Stacks

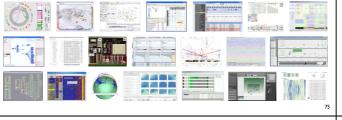
Michael Sedlmair, Miriah Meyer

http://www.cs.ubc.ca/labs/imager/tr/2012/dsm.

Design Study Methodology: Reflections from the Trenches and from the Stacks. Sedlmair, Meyer, Munzner. IEEE TVCG 18(12): 2431-2440, 2012 (Proc. InfoVis 2012).

Design Studies

- · long and winding road with many pitfalls
- -reflections after doing 21 of them
 - many successes, a few failures, many lessons learned



How To Do Design Studies

definitions

• 9-stage framework

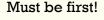
 32 pitfalls and how to avoid them



Pitfall Example: Premature Publishing

technique-driven

problem-driven



Am I ready?



Methods and Outcomes

- -introspection on lessons learned as authors and reviewers
- -extensive literature search
- outcomes
 - -prescriptive methodology advice
 - · here's a way to do design studies
 - · avoid these pitfalls
- exhortation
- -meta/how-to/reflection papers are worth doing
- -thinking about methods and methodologies is fruitful for any flavor of research!

Work in Progress

- DR in the Wild
- -end point: stay tuned
- DR for journalism
- -Overview project http://overview.ap.org
- -funded by Knight Foundation, collaboration with Stray@AP
 - starting point: Glimmer meets WikiLeaks -led us to identify and address more unmet real-world analysis needs
 - -iterative rounds of development, deployment, adoption
- end point: stay tuned
- -Pulitzer Prize finalist story used Overview for data analysis (Adam Playford, Newsday, For Their Eyes Only)

Conclusions

- cross-fertilization from attacking DR through different methodological angles
- -scratching own itches often leads to problems that are important and high impact
- outcomes of evaluation informs how to build
- grappling with issues of building informs what studies to run
- taxonomy creation informs what to build: unsolved problems
- finding mismatches
- -between principles and practice
- -between practice and needs
- need parallax view of principles, practices, and needs!

Thanks and Questions

- further info
- -http://www.cs.ubc.ca/~tmm/talks.html#linz14
- -http://www.cs.ubc.ca/group/infovis
- acknowledgements
- -funding: NSERC Strategic Grant
- -joint work: all collaborators
- Aaron Barsky, Steven Bergner, Matthew Brehmer, Stephen Ingram, Veronika Irvine, Miriah Meyer, Torsten Möller, Marc Olano, David W. Sprague, Melanie Tory, Michael Sedlmair, Wing Yan So, Andrada Tatu, Matt Williams, Fuqu Wu
- -feedback on this talk
- Matthew Brehmer, Joel Ferstay, Stephen Ingram, Torsten Möller, Michael Sedlmair, Jessica Dawson