#### Dimensionality Reduction From Several Angles

#### Tamara Munzner

Department of Computer Science University of British Columbia

FODAVA Distinguished Lecture Georgia Tech 7 Dec 2012

http://www.cs.ubc.ca/~tmm/talks.html#fodava12

#### 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

# Why use DR? Tumor Measurement Data 9 Dimensional Measured Space Alignant Benign DR DR 2 Dimensional Target Space

#### 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
- 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

#### Questions and Answers

- 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 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!

## designing visual encoding and interaction techniques creating algorithms to execute techniques efficiently A Nested Model

characterizing the problems of real-world users
abstracting into operations on data types

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

#### Matching Validation With Design Level

threat: wrong problem
validate: observe and interview target users

threat: bad data/operation abstraction

threat: ineffective encoding/interaction technique
validate: justify encoding/interaction design

threat: slow algorithm
validate: analyze computational complexity

implement system
validate: qualitative/quantitative result image analysis
[test on any users, informal usability study]
validate: lab study, measure human time/errors for operation
validate: test on target users, collect anecdotal evidence of utility
validate: field study, document human usage of deployed system
validate: observe adoption rates

#### 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/ Glimmer: Multilevel MDS on the GPU. Ingram, Munzner, Olano. IEEE TVCG 15(2):249-261, 2009. 17

#### 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

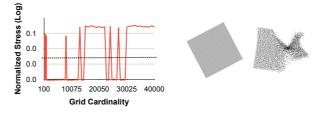
Glint: An MDS Framework for Costly Distance Function

Ingram, Munzner. Proc. SIGRAD 2012.

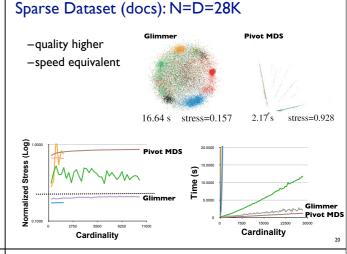
- -limitations: quality for very high dimensional sparse data
- distance scaling: minimize stress
- -nonlinear optimization: O(N2)
  - SMACOF [de Leeuw 1977]
- -force-directed placement: O(N2)
- Stochastic Force [Chalmers 1996]
- limitations: quality problems from local minima
- Glimmer goal: O(N) speed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



#### 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

#### MDS Algorithm Speeds

• newer algorithms linear, but...

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

Shuttle benchmark

N = 43K

D = 9

Classic MDS SMACOF

Pivot MDS Glimmer LAMP

Hours

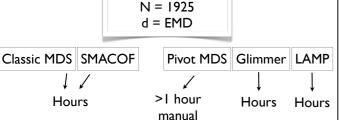
I Second

to Compute

MDS Speed on Coordinate Data

time to calculate distance between two points
 -0.00001 second

#### MDS Speed on Distance Matrix Data



Quality

Glimmer Original

Glimmer w/ Glint

time to calculate distance between two points
 -0.01 second

Force-Directed Instantiation Results

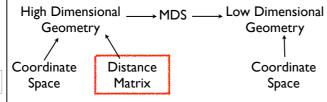
Speed

Cheap

dist

#### MDS Input: Coordinates vs Distances

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



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

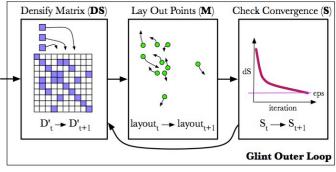
 $\bullet$  DR in the Wild revealed many real-world examples

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	Euclidean on 9-D data  0.00001  Database Query  0.001  Earth Mover Distance  0.01  Euclidean on 4M-D data  1.0

#### Glint Framework

to Compute

- 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

#### 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?
- can we build a DR system for real people?

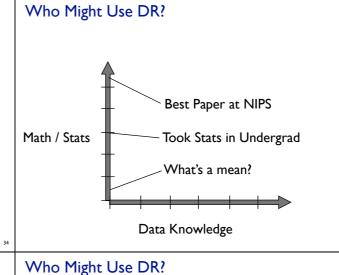
-next: how do we get people to use DR properly?

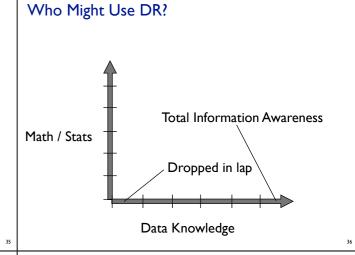
-move emphasis from solo algorithms to entire system

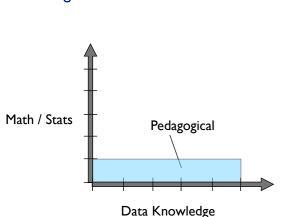
- -system that provides guidance: DimStiller
- when do people need to use DR?
- how should we show people DR results?
- why and how do people use DR?

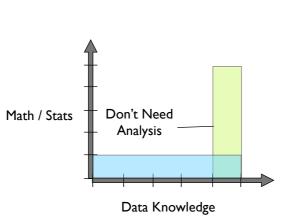
## Costly dists Costly major speed improvements while quality maintained

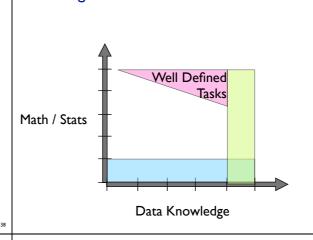
#### 

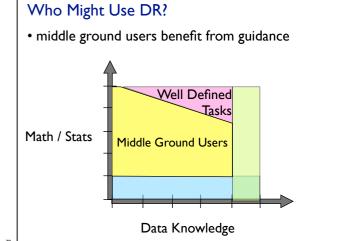


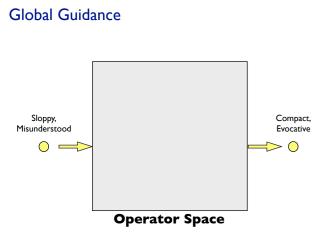


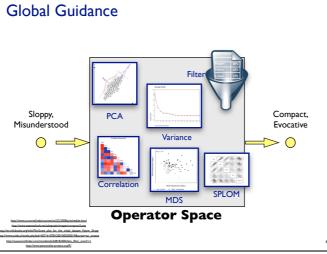


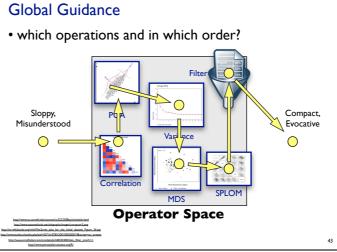


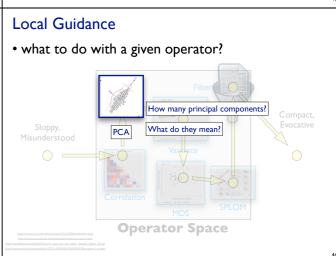












### 

#### 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!

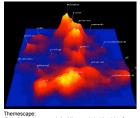
#### Outline

- 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
- visual Cluster Separation racto
- when do people need to use DR?



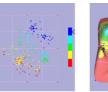
#### Information Landscapes

- 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





#### • abstract: search involving spatial areas and estimation Estimate which grid cell has the most points of the target color





domain-specific examples

Simple Idea

**Understanding User Task** 

- "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

**Cluster Separation:** 

• frequent subtask in pilot test of real data analysis

adjacent

#### Visual Cluster Separation Measures

(color + height redundantly encoded)

-points are better than landscapes

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

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

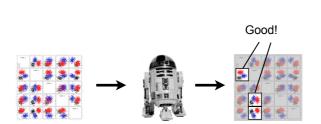
-2D landscapes (color only) better than 3D landscapes

• 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!



#### **Separation Factors** ioint work with:

A Taxonomy of

, Michael Sedlmair, Andrada Tatu, Melanie Tory

User vs. Data Study

-many users, few datasets

-few users, many datasets

-missing: dataset variety

user study

data study

**Visual Cluster** 

-previous work on validating cluster

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).

#### 816 Dataset Instances

partial

overlap

• 75 datasets

full

overlap

- -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



distant



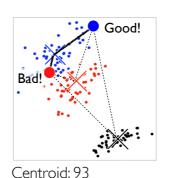


#### Centroid Measure

hypotheses

• result: yes!

result: yes



#### **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.

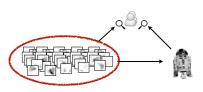
evaluating the measures

**High-Level Results** 

All failure cases

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

#### Qualitative Analysis I: Cluster Separation Factors













points

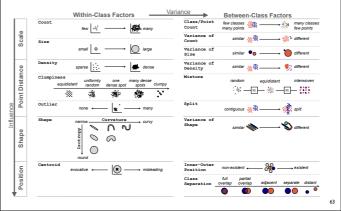
#### Analysis Approach

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

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

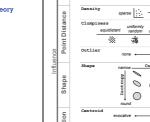
- · evaluating the measures
- -metric aligns with human judgement?
- -if not: what are the reasons?
- building taxonomy of factors from reasons
- mapping measure failures onto taxonomy

#### A Taxonomy of Cluster Separation Factors



#### Failure cases AII (816) Only real (296) False Positives False Negatives

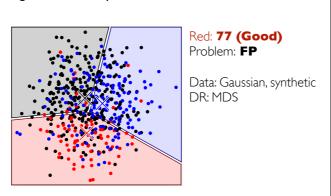
25 50



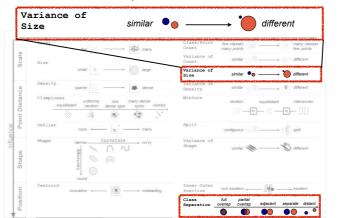
Using Taxonomy To Explain Measure Failures

#### Centroid Failure Example

• big classes overspread small ones

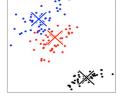


#### Relevant Taxonomy Factors



#### Centroid: Mapping Assumptions Into Taxonomy

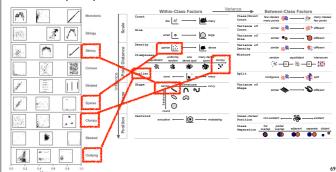
- · centroid only reliable if
- -round-ish clusters
- -not more than one dense spot
- -no outliers
- -similar sizes & number of points



rarely true for real datasets

#### Related Work

- Scagnostics [Wilkinson and Anand 2005]
- -mathematical description and algorithmic instantiation vs human perception



#### Methods and Outcomes

- methods
  - -qualitative data study
  - we encourage more work along these lines
- - -taxonomy to understand current problems
- -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

#### Reflections on **QuestVis**

A Visualization System for an Environmental Sustainability Model

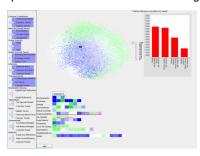
ioint work with: Aaron Barsky, Matt Williams

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

Reflections on QuestVis: A Visualization System for an Environmental Sustainability Mode 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 driving examples behind development of 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

#### **Design Study** 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. SedImair, Meyer, Munzner. IEEE TVCG 18(12): 2431-2440, 2012 (Proc. InfoVis 2012).

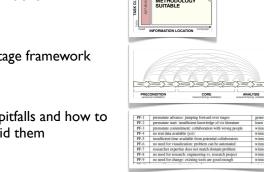
DESIGN STUDY METHODOLOGY SUITABLE

#### **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

Must be first!



Am I ready?



#### Methods and Outcomes

- -introspection on lessons learned as authors and reviewers
- 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
- -final results coming soon
- DR for journalism
- -Overview project http://overview.ap.org
- -funded by Knight Foundation, collaboration with AP
- starting point: Glimmer meets WikiLeaks
- -led us to identify and address more unmet real-world analysis needs - new technique developed and partially deployed
- end point: stay tuned

#### 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#fodava12
- http://www.cs.ubc.ca/~tmm/papers
- 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
- · hiring opportunity
- Stephen Ingram (DimStiller, Glimmer, Glint) will finish PhD soon
- http://www.cs.ubc.ca/~sfingram
- available for hacker-analyst job in industry or research lab
- in spring 2014 after postdoc