Dimensionality Reduction From Several Angles

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http://www.cs.ubc.ca/~tmm/talks.html#sydney15
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Dimensionality Reduction

- what is it?
  - map data from high-dimensional measured space into low-dimensional 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
- how can you tell when you need it?
  - could estimate true dimensionality

Estimating true dimensionality

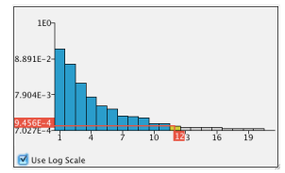
- error for low-dim projection vs high-dim projection
- no single correct answer; many metrics proposed
  - cumulative variance that is not accounted for
  - strain: match variations in distance (vs actual distance values)
  - stress: difference between interpoint distances in high and low dims

$$stress(D, \Delta) = \sqrt{\frac{\sum_{ij}\left(d_{ij} - \delta_{ij}\right)^2}{\sum_{ij}\delta_{ij}^2}}$$

- D: matrix of lowD distances
- Δ: matrix of hiD distances δ_{ij}

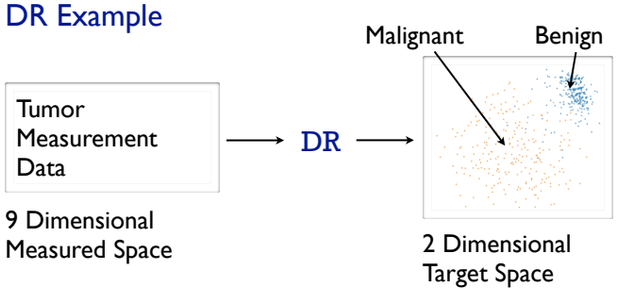
Showing dimensionality estimates

- scree plots as simple way: error against # attribs



  - original dataset: 294 dims
  - estimate: almost all variance preserved with < 20 dims
  -

DR Example



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

Visualizing Dimensionally-Reduced Data:

Interviews with Analysts and a Characterization of Task Sequences

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

http://www.cs.ubc.ca/labs/imager/tr/2014/DRVisTasks/

Visualizing Dimensionally-Reduced Data:
Interviews with Analysts and a Characterization of Task Sequences
Brehmer, Sedlmair, Ingram, and Munzner.
Proc. Beyond Time & Errors: Novel Evaluation Methods For Information Visualization (BELIV) 2014, p. 1-8.

Motivation

- 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?
- why and how do people use DR?
  - overarching question weaving through projects in this talk
  - preliminary results from study informed many of them

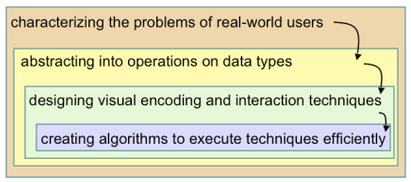
Two-Year Cross-Domain Qualitative Study

- in the wild
  - HCI 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
- five abstract tasks
  - naming synthesized dimensions
  - mapping synthesized dimension to original dimensions
  - verifying clusters
  - naming clusters
  - matching clusters and classes

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!



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

domain situation:
observe target users using existing tools

data/task abstraction:

encoding/interaction idiom:
justify design wrt alternatives

algorithm:
measure system time
analyze computational complexity

analyze results qualitatively
measure human time with lab experiment ("user study")

observe target users post-deployment ("field study")

measure adoption

- mismatch: cannot show idiom good with system timings
- mismatch: cannot show abstraction good with lab study

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

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

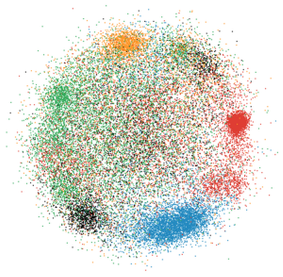
- benefits of multiple angles
  - parallax view of what's important
  - outcomes cross-pollinate

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/

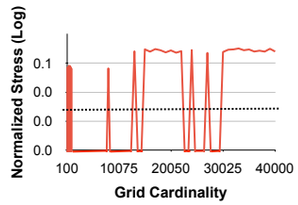
Glimmer: Multilevel MDS on the GPU.
Ingram, Munzner, Olano. IEEE TVCG 15(2):249-261, 2009.

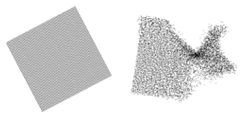
MDS: Multidimensional Scaling

- 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]
  - –limitations: quality for very high dimensional sparse data
- distance scaling: minimize stress
  - –nonlinear optimization: $O(N^2)$
    - SMACOF [de Leeuw 1977]
  - –force-directed placement: $O(N^2)$
    - 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

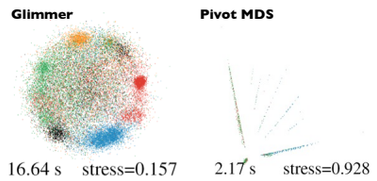


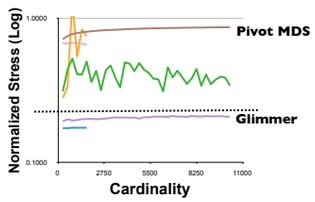


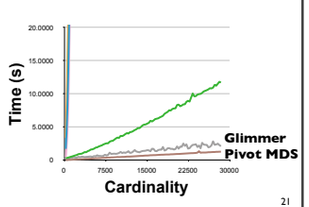
- Use as subsystem within new multilevel GPU alg with much better convergence properties

Sparse Dataset (docs): N=D=28K

- –quality higher
- –speed equivalent

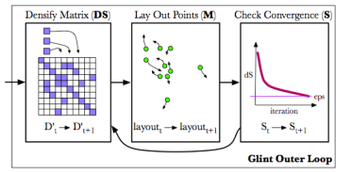






Methods and Outcomes

- methods
  - –quantitative algorithm benchmarks: speed, quality
    - systematic comparison across 1K-10K instances vs a few spot checks
  - –qualitative judgements of layout quality
- outcomes
  - –characterized kinds of datasets where technique yields quality improvements
- then what?
  - –saw what real users could do with it after release
    - identified limitations



Glint

An MDS Framework for Costly Distance Functions

joint work with:
Stephen Ingram

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

Glint: An MDS Framework for Costly Distance Functions.
Ingram, Munzner. Proc. SIGRAD 2012.

MDS Algorithm Speeds

- newer algorithms linear, but...

Age ↓

Algorithm	Author/Year	Complexity
Classic MDS	Torgersen '52	$O(N^3)$
SMACOF	de Leeuw '77	$O(N^3)$
Pivot MDS	Brandes '07	O(kN)
Glimmer	Ingram '09	O(cN)
LAMP	Joia '11	O(kN)

MDS Speed on Coordinate Data

`shuttle` benchmark
N = 43K
D = 9

Classic MDS	SMACOF	Pivot MDS	Glimmer	LAMP
Hours to Compute		1 Second to Compute		

- time to calculate distance between two points
  - –0.00001 second

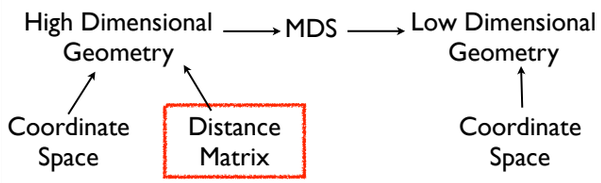
MDS Speed on Distance Matrix Data

`flickr` benchmark
N = 1925
d = EMD

Classic MDS	SMACOF	Pivot MDS	Glimmer	LAMP
Hours		>1 hour manual	Hours	Hours

- time to calculate distance between two points
  - –0.01 second

MDS Input: Coordinates vs Distances



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

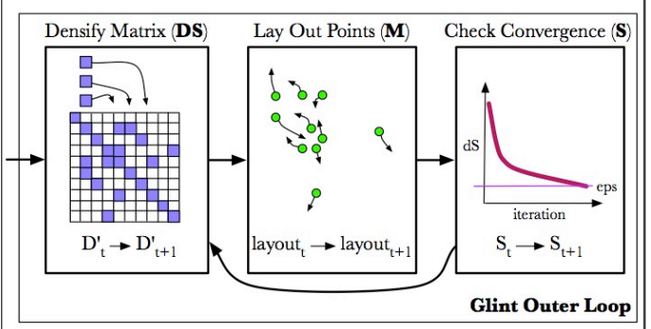
Costly Distances

- DR in the Wild revealed many real-world examples

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

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

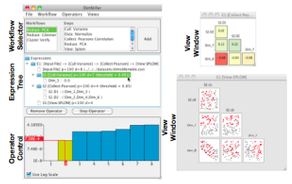
major speed improvements while quality maintained

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?



DimStiller

Workflows for Dimensional Analysis and Reduction

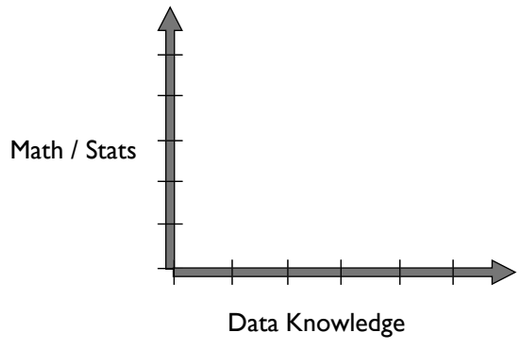
joint work with:
Stephen Ingram, Veronika Irvine, Melanie Tory, Steven Bergner, Torsten Möller

http://www.cs.ubc.ca/labs/imager/tr/2010/DimStiller/

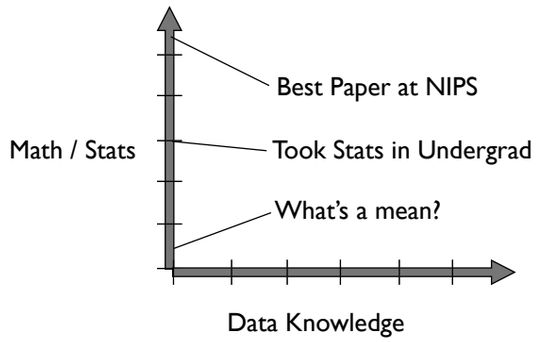
DimStiller: Workflows for dimensional analysis and reduction.
Ingram, Munzner, Irvine, Tory, Bergner, Moeller. Proc. VAST 2010, p 3-10.

Who Might Use DR?

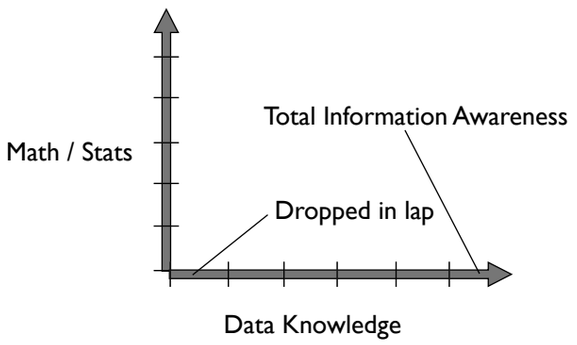
- DR in the Wild revealed broad set of users



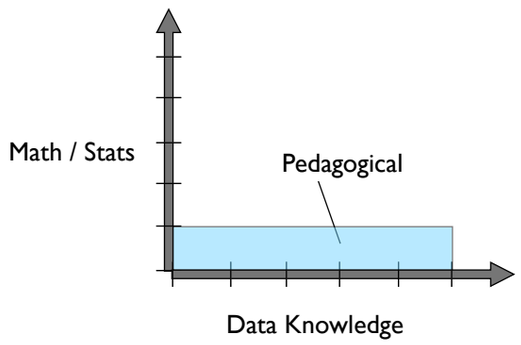
Who Might Use DR?



Who Might Use DR?



Who Might Use DR?



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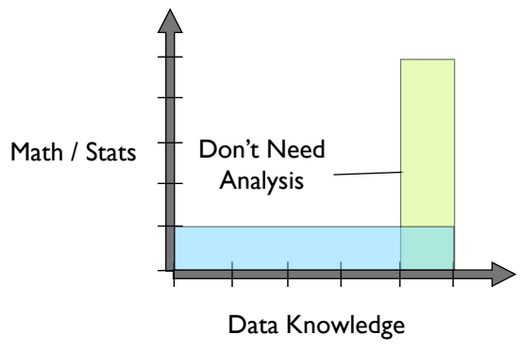

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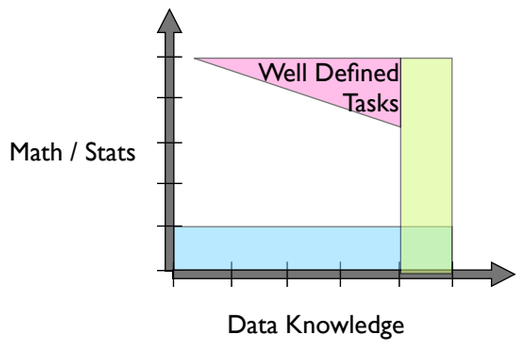
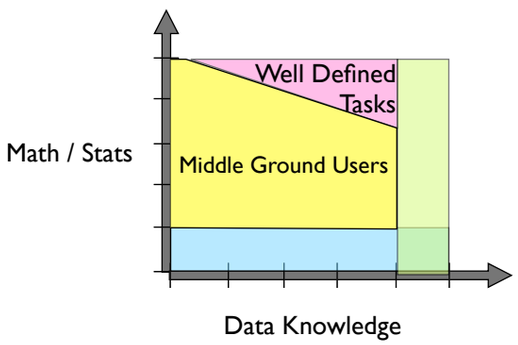
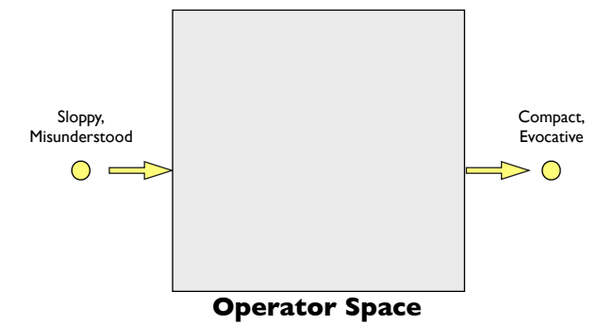


Who Might Use DR?

- middle ground users benefit from guidance



Global Guidance



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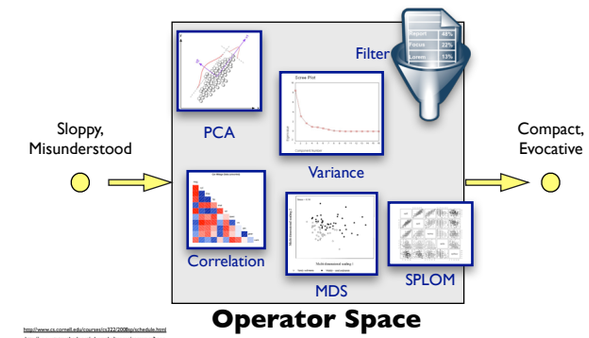
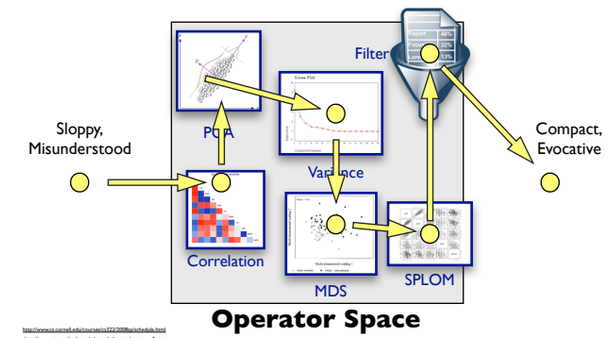


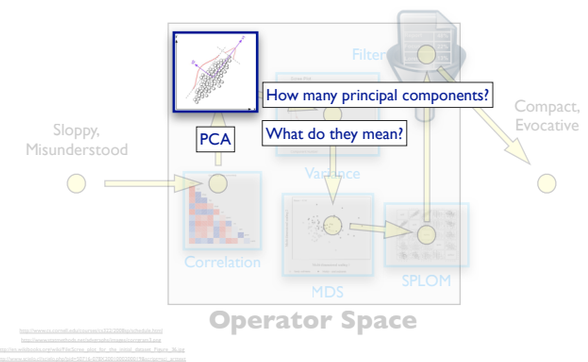
Global Guidance

- which operations and in which order?

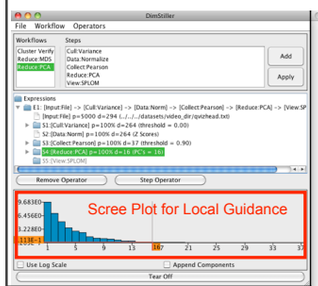


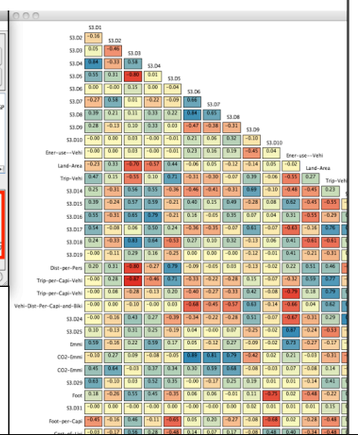
Local Guidance

- what to do with a given operator?



DimStiller





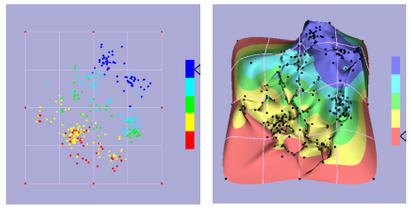
- pre-built workflows
- sequence of operators
- local guidance for each operator
  - – example: estimate true dimensionality with scree plot

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?



Spatialization Design

Comparing Points and Landscapes

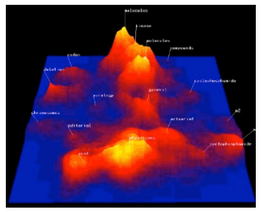
joint work with:
Melanie Tory, David W. Sprague, Fuqu Wu, Wing Yan So

http://webhome.cs.uvic.ca/~mtory/publications/infovis2007.pdf

Spatialization Design: Comparing Points and Landscapes.
Tory, Sprague, Wu, So, and Munzner.
IEEE TVCG 13(6):1262–1269, 2007 (Proc. InfoVis 07).

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



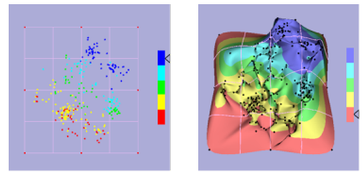
Themescape:
[http://www.k-n-o-r-z.de/publ/example/retriev1.htm]

[Guide to MicroPatent Aureka 9 ThemeScape]

Understanding User Task

- abstract: search involving spatial areas and estimation

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

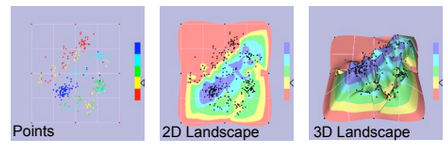


- domain-specific examples

"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

Lab Study: Test Human Response Time and Error



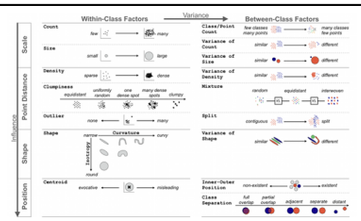
- hypotheses
  - points are better than landscapes
    - result: yes!
    - much better: 2-4 × faster, 5-14 × more accurate
  - 2D landscapes (color only) better than 3D landscapes (color + height redundantly encoded)
    - result: yes
    - significantly faster, no significant difference in accuracy

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...

A Taxonomy of

Visual Cluster Separation Factors



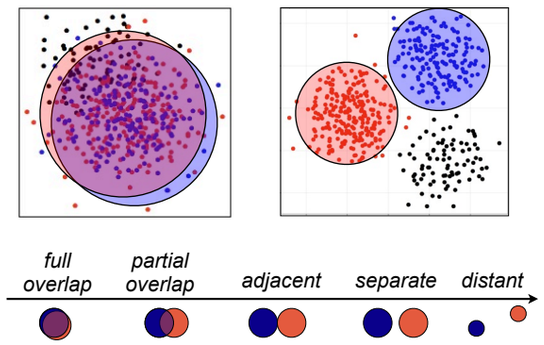
joint work with:
Michael Sedlmair, Andrada Tatu, Melanie Tory

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

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

Cluster Separation

- simple idea

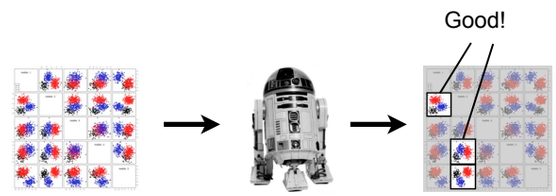


Visual Cluster Separation Measures

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

Sips et al.: Selecting good views of high-dimensional data using class consistency [EuroVis 2009]

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



Visual Cluster Separation Measures

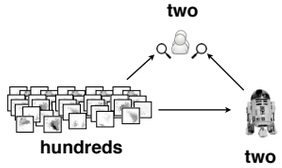
- goal: number captures whether human looking at layout sees something interesting
  - after computation is done, not to refine clustering
- measures checked with user studies

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

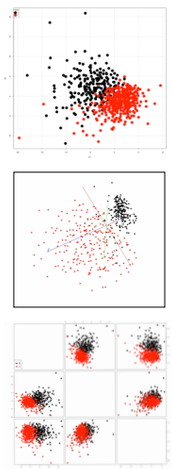
User vs. Data Study

- user study
  - previous work on validating cluster measures
  - many users, few datasets
  - missing: dataset variety
- data study
  - few users, many datasets

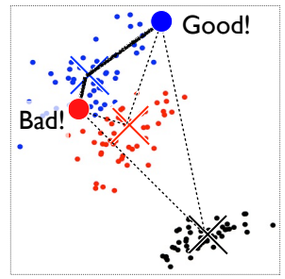


816 Dataset Instances

- 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



Centroid: 93

Analysis Approach

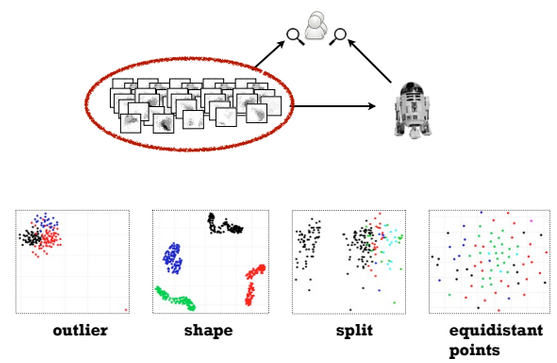
- qualitative method out of social science: coding
  - open coding: gradually build/refine code set
  - axial coding: relationships between categories

Charmaz, K. Constructing Grounded Theory: A Practical Guide through Qualitative Analysis. 2006.

Furniss, D., Blandford, A., Curzon, P. and Mary, Q. (2011). Confessions 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?

Qualitative Analysis I: Cluster Separation Factors



Analysis Approach

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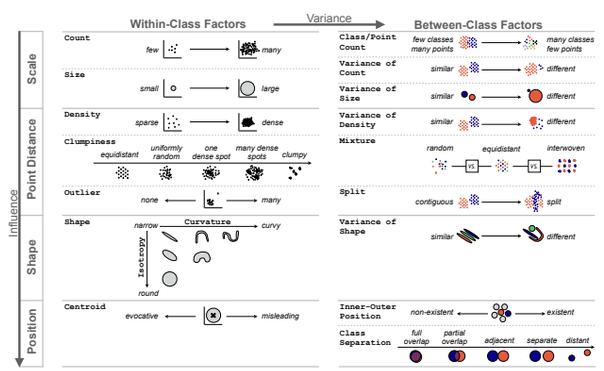
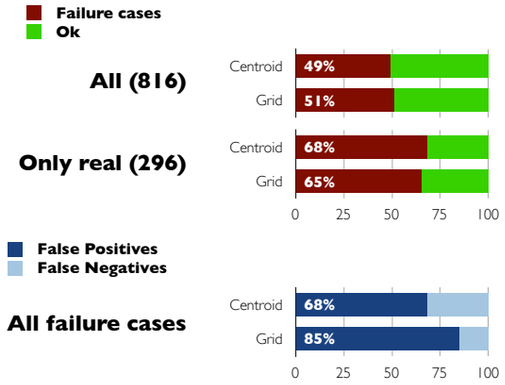
- evaluating the measures
  - metric aligns with human judgement?
  - if not: what are the reasons?
- building taxonomy of factors from reasons
- mapping measure failures onto taxonomy

A Taxonomy of Cluster Separation Factors

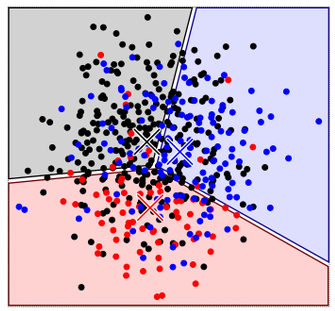


High-Level Results



Centroid Failure Example

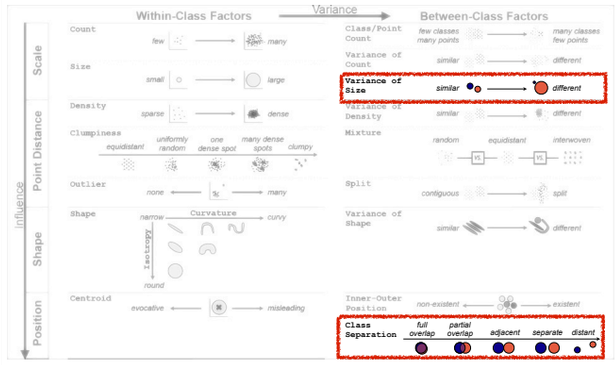
- big classes overspread small ones



Red: **77 (Good)**
Problem: **FP**

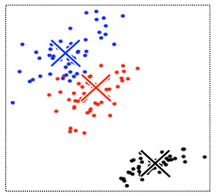
Data: Gaussian, synthetic
DR: MDS

Relevant Taxonomy Factors



Centroid: Mapping Assumptions Into Taxonomy

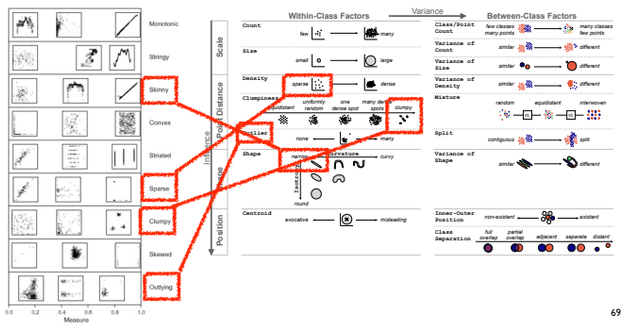
- centroid only reliable if
  - round-ish clusters
  - not more than one dense spot
  - no outliers
  - similar sizes & number of points



- 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

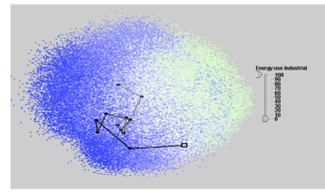
Outline

- 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

Reflections on

QuestVis

A Visualization System for an Environmental Sustainability Model



joint work with:
Aaron Barsky, Matt Williams

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

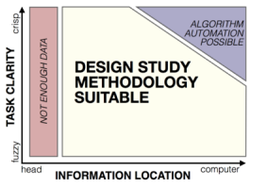
Reflections on QuestVis: A Visualization System for an Environmental Sustainability Model
Munzner, Barsky, Williams. Scientific Visualization: Interactions, Features, Metaphors. Dagstuhl Follow-Ups 2, 2011, Chapter 17, p 240–259.

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

Reflections from the Trenches and from the Stacks

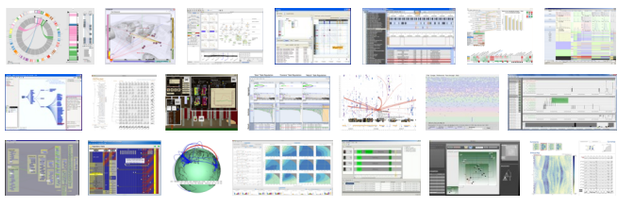
joint work with:
Michael Sedlmair, Miriah Meyer

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).

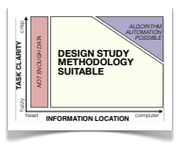
Design Studies

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

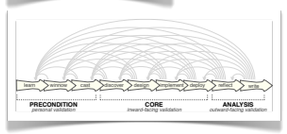


How To Do Design Studies

- definitions



- 9-stage framework



- 32 pitfalls and how to avoid them

PF-1	premature advance: jumping forward over stages	general
PF-2	premature start: insufficient knowledge of vis literature	learn
PF-3	premature commitment: collaboration with wrong people	winnow
PF-4	no real data available (yet)	winnow
PF-5	insufficient time available from potential collaborators	winnow
PF-6	no need for visualization: problem can be automated	winnow
PF-7	researcher expertise does not match domain problem	winnow
PF-8	no need for research: engineering vs. research project	winnow
PF-9	no need for change: existing tools are good enough	winnow

Pitfall Example: Premature Publishing

technique-driven

Must be first!

http://www.prlog.org/10480334-wolverhampton-horse-racing-live-streaming-wolverhampton-handicap-8-jan-2010.html

problem-driven

Am I ready?

http://www.alaineknipes.com/interests/violin_concert.jpg

Methods and Outcomes

- methods
  - 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!

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#sydney15
  - http://www.cs.ubc.ca/group/infovis
- acknowledgements
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  - joint work: all collaborators
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  - feedback on this talk
    - Matthew Brehmer, Joel Ferstay, Stephen Ingram, Torsten Möller, Michael Sedlmair, Jessica Dawson