

# Dimensionality Reduction From Several Angles

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SCI Distinguished Lecture  
University of Utah  
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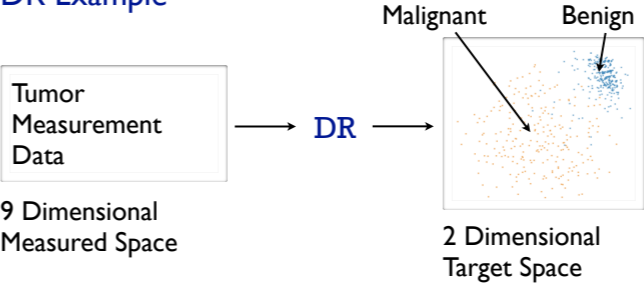
<http://www.cs.ubc.ca/~tmm/talks.html#utah13>

## 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

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## DR Example



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## 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

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## 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?

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## 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?

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# Dimensionality Reduction In the Wild

## Tasks and Challenges

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

work in progress

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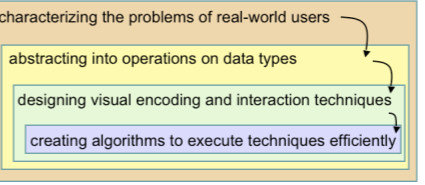
## Two-Year Cross-Domain Qualitative Study

- 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
- 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!

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## A Nested Model of Visualization Design and Validation

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

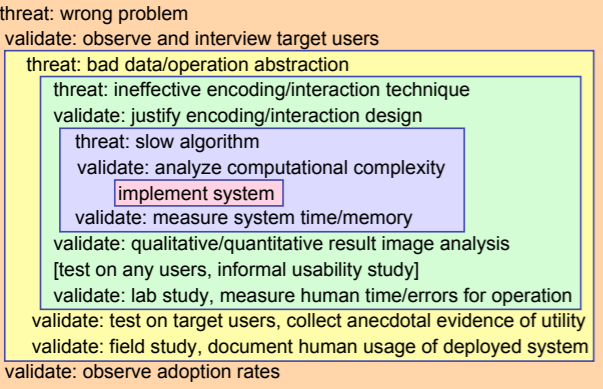
A Nested Model of Visualization Design and Validation.  
Munzner. IEEE TVCG 15(6):921-928, 2009 (Proc. InfoVis 2009).

## Four Levels of Design and Validation

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

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## Matching Validation With Design Level



## 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

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## 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?

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# 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.

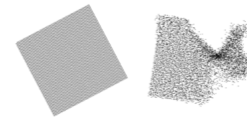
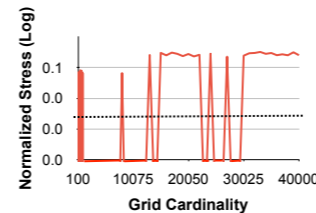


## MDS: Multidimensional Scaling

- 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

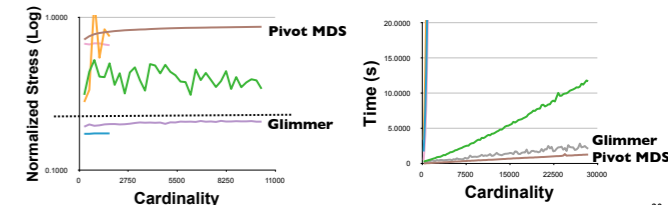
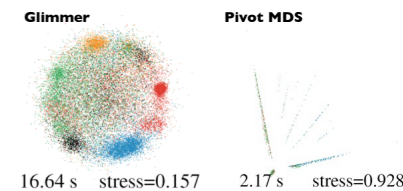
- Stochastic force alg suitable for fast GPU port
  - but systematic testing shows it often terminates too soon



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

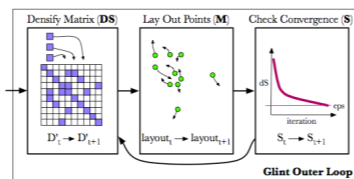
## Sparse Dataset (docs): N=D=28K

- 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

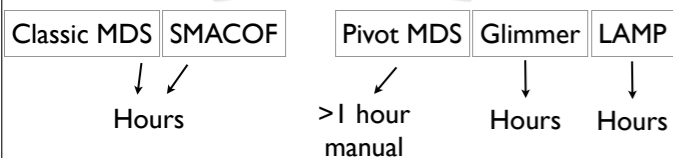
shuttle benchmark  
N = 43K  
D = 9



- time to calculate distance between two points
  - 0.00001 second

## MDS Speed on Distance Matrix Data

flickr benchmark  
N = 1925  
d = EMD



- 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

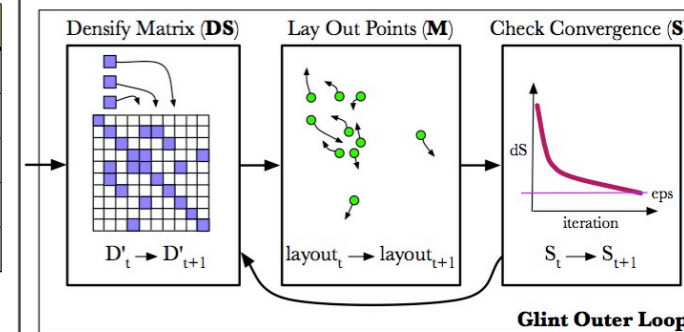
## Costly Distances

- 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

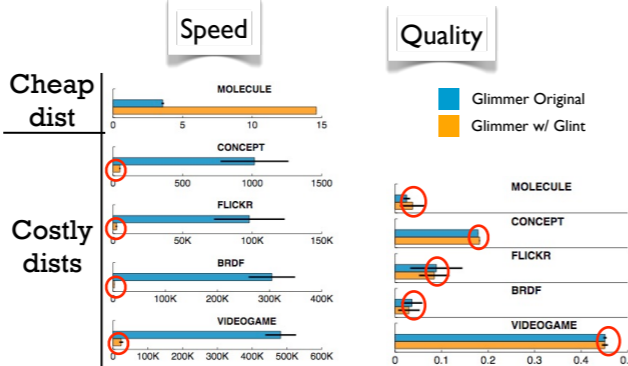


## Glint Instantiations

- 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?

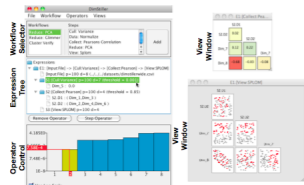
# DimStiller

Workflows for Dimensional Analysis and Reduction

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

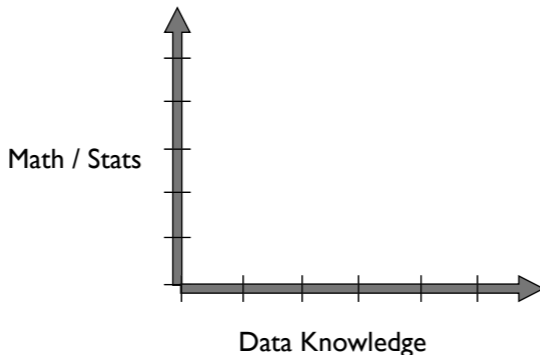
<http://www.cs.ubc.ca/labs/imager/tr/2010/DimStiller/>

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



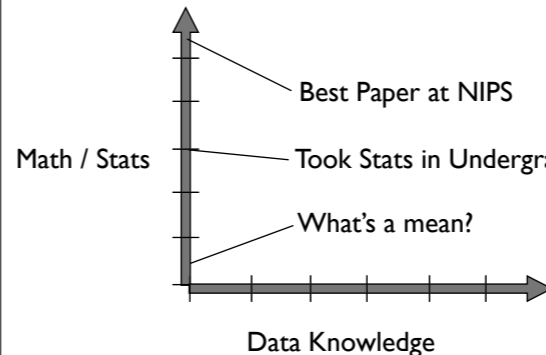
## Who Might Use DR?

- DR in the Wild revealed broad set of users



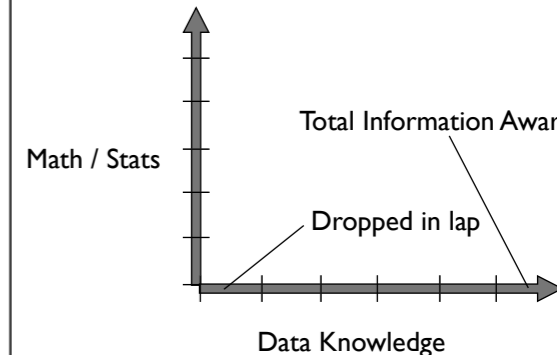
## Who Might Use DR?

- Best Paper at NIPS
- Took Stats in Undergrad
- What's a mean?

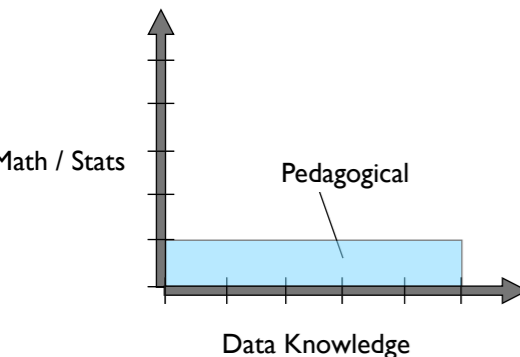


## Who Might Use DR?

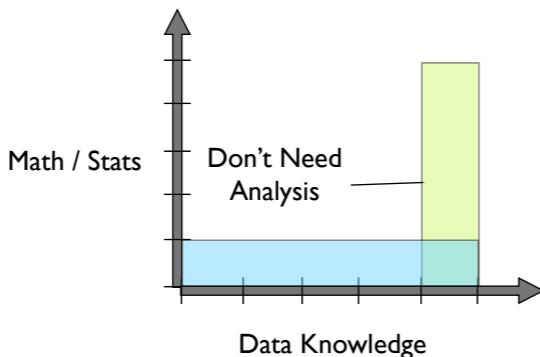
- Total Information Awareness
- Dropped in lap



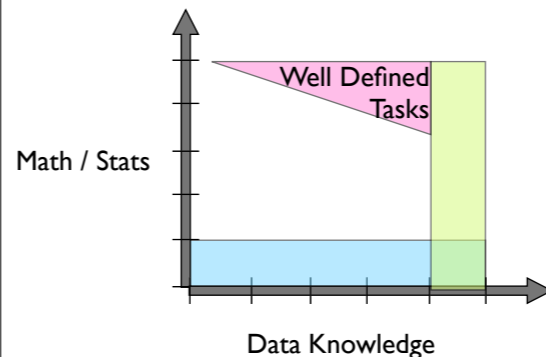
## Who Might Use DR?



## Who Might Use DR?

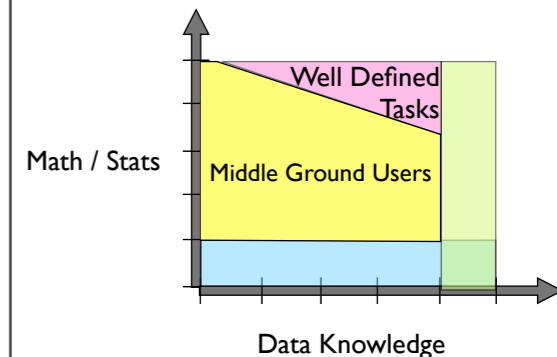


## Who Might Use DR?

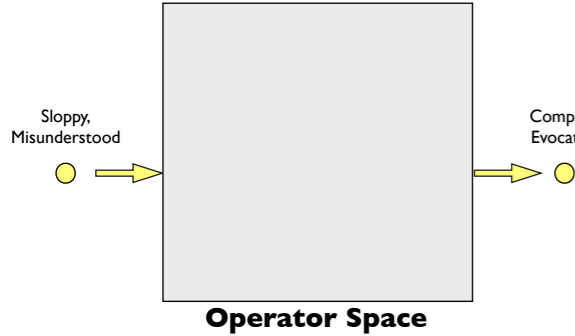


## Who Might Use DR?

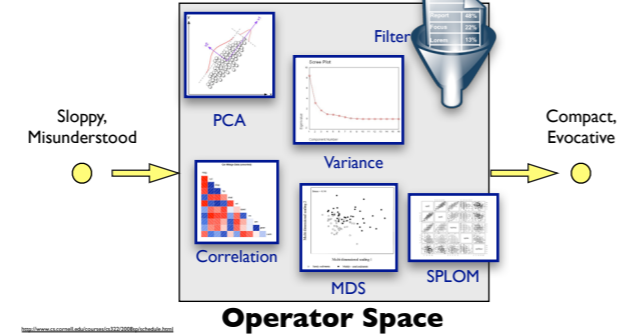
- middle ground users benefit from guidance



## Global Guidance

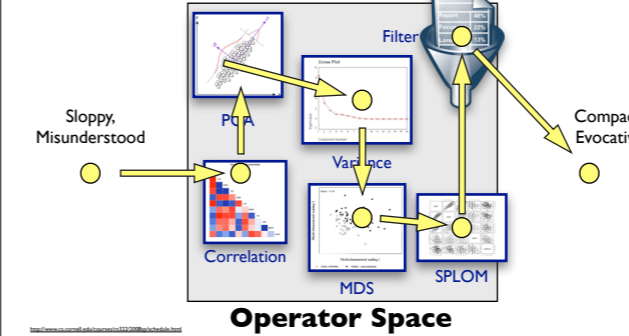


## Global Guidance



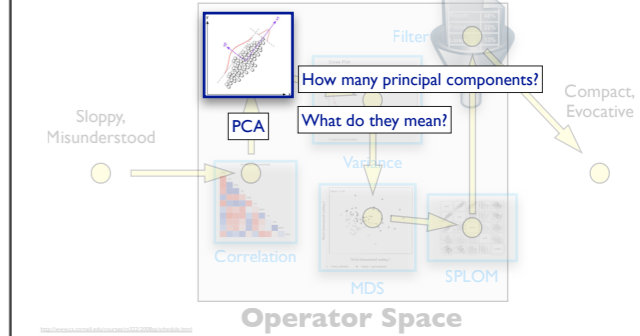
## Global Guidance

- which operations and in which order?

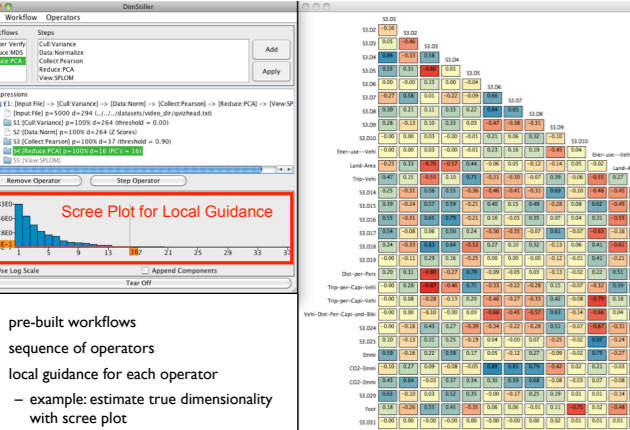


## Local Guidance

- 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

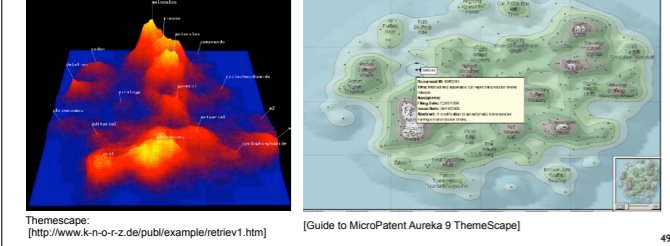
<http://webhome.cs.uvic.ca/~mtory/publications/infovis2007.pdf>

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



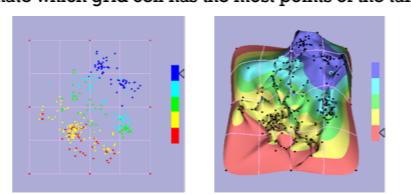
# Information Landscapes

- 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



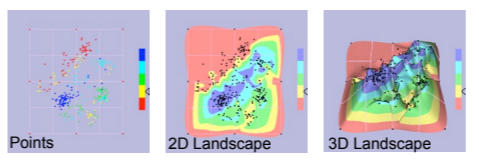
# Understanding User Task

- 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

full overlap partial overlap adjacent separate distant

## 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
  - Good!
  - No!

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

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

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

## Qualitative Analysis I: Cluster Separation Factors

## Analysis Approach

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

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

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

## A Taxonomy of Cluster Separation Factors

## High-Level Results

■ Failure cases ■ Ok

**All (816)**

Centroid: 49% Failure cases, 51% Ok

Grid: 51% Failure cases, 49% Ok

**Only real (296)**

Centroid: 68% Failure cases, 32% Ok

Grid: 65% Failure cases, 35% Ok

**All failure cases**

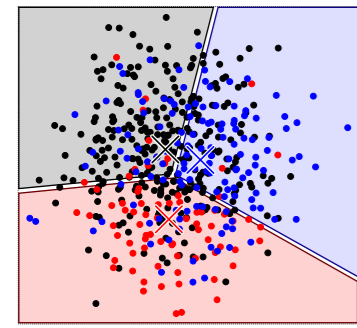
Centroid: 68% False Positives, 32% False Negatives

Grid: 85% False Positives, 15% False Negatives

# Centroid Failure Example

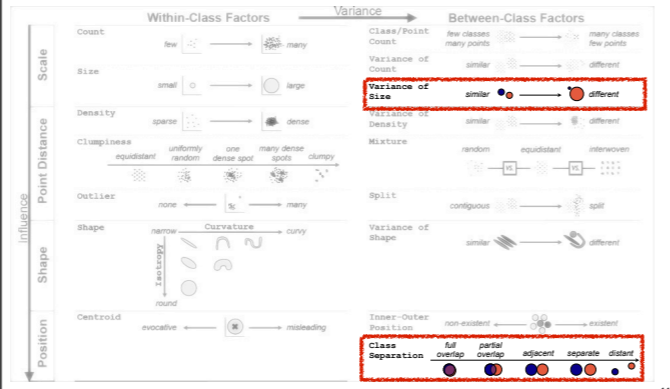


- big classes overspread small ones



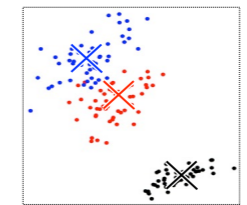
Red: **77 (Good)**  
 Problem: **FP**  
 Data: Gaussian, synthetic  
 DR: MDS

# Relevant Taxonomy Factors



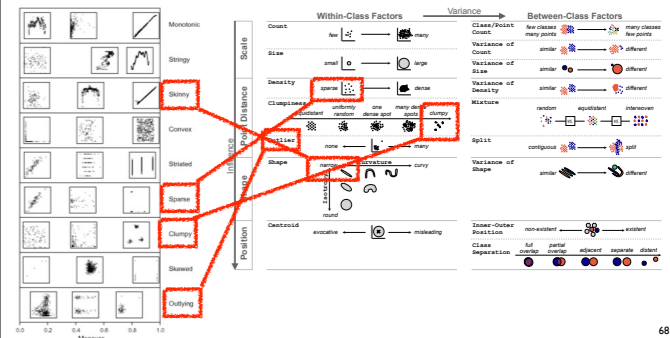
# Centroid: Mapping Assumptions Into Taxonomy

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

# Pitfall Example: Premature Publishing

technique-driven vs. problem-driven

**Must be first!** (with image of a horse race)

**Am I ready?** (with image of a concert)

# 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!

# 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 Stray@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#utah13>
  - <http://www.cs.ubc.ca/~tmm/papers>
- acknowledgements
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  - 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