

# Dimensionality Reduction From Several Angles

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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

# DR Example

Tumor  
Measurement  
Data

9 Dimensional  
Measured Space

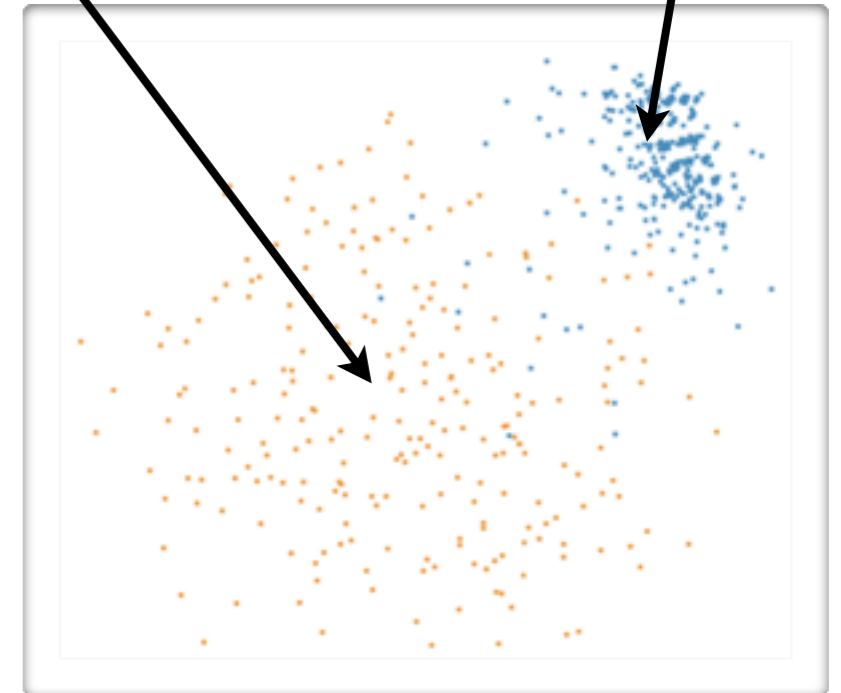


**DR**



Malignant

Benign



2 Dimensional  
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**

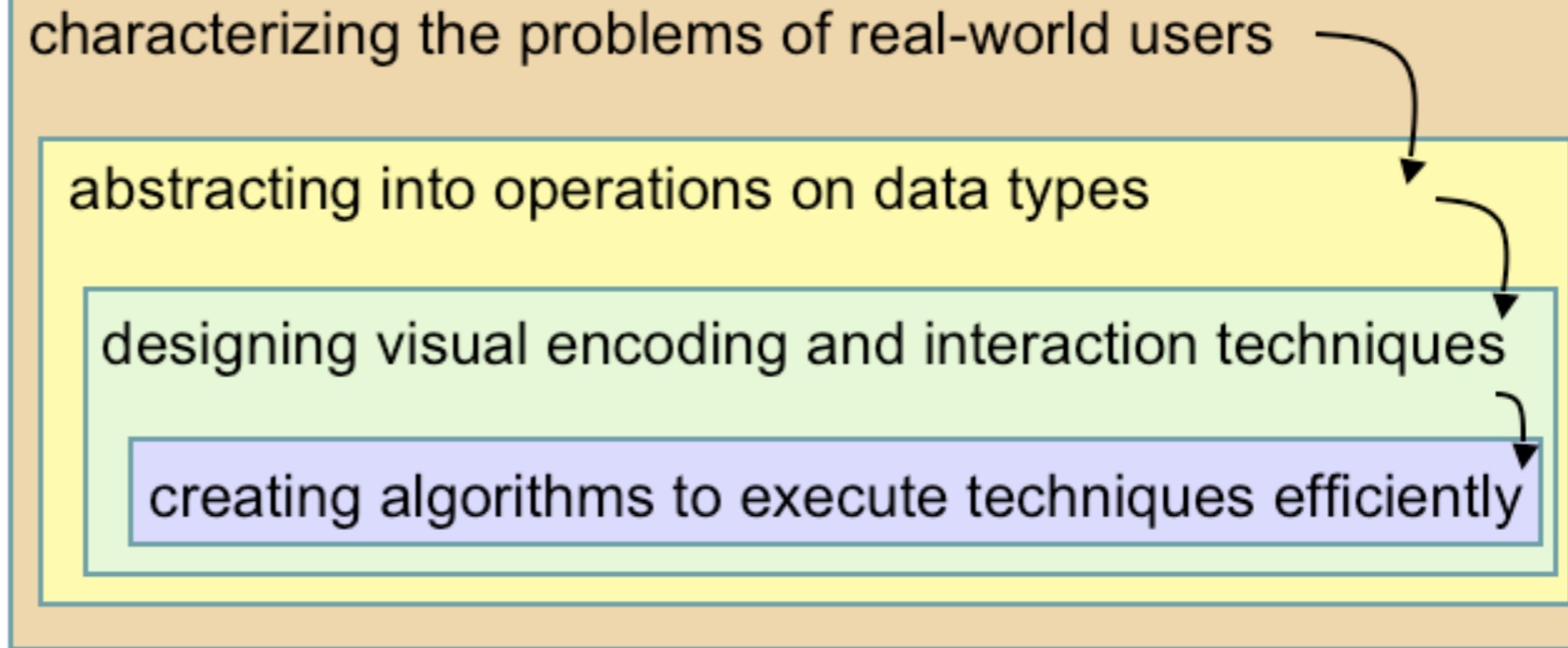


# Two-Year Cross-Domain Qualitative Study

- **in the wild**
  - 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!



# 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

# 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: measure system time/memory

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?



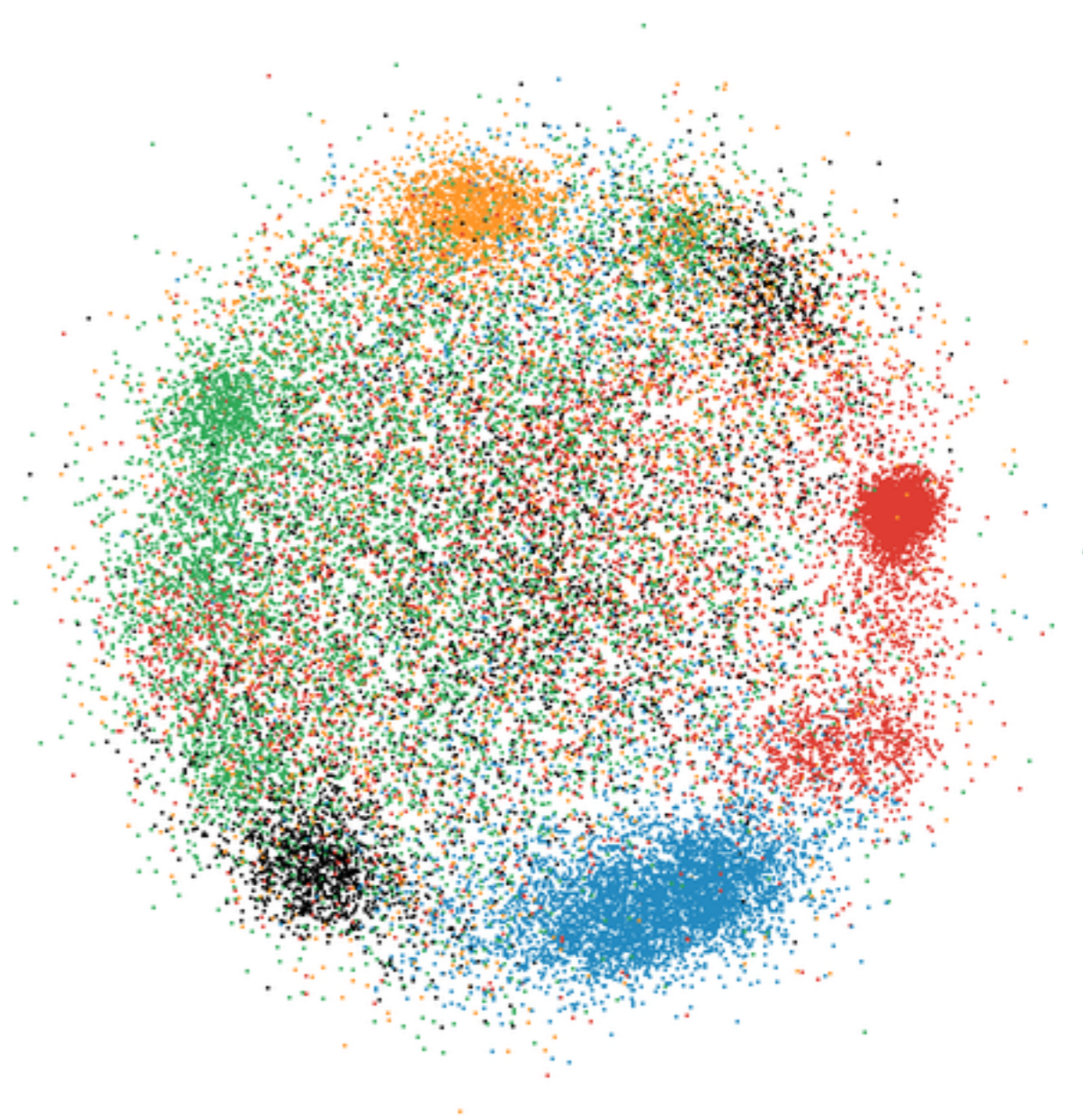
# Glimmer

## *Multilevel MDS on the GPU*

**joint work with:**

Stephen Ingram, Marc Olano

<http://www.cs.ubc.ca/labs/imager/tr/2008/glimmer/>



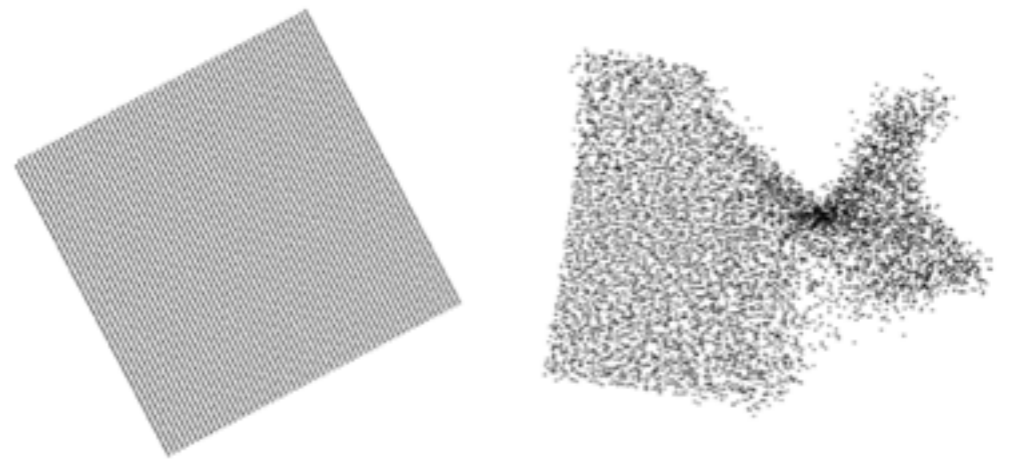
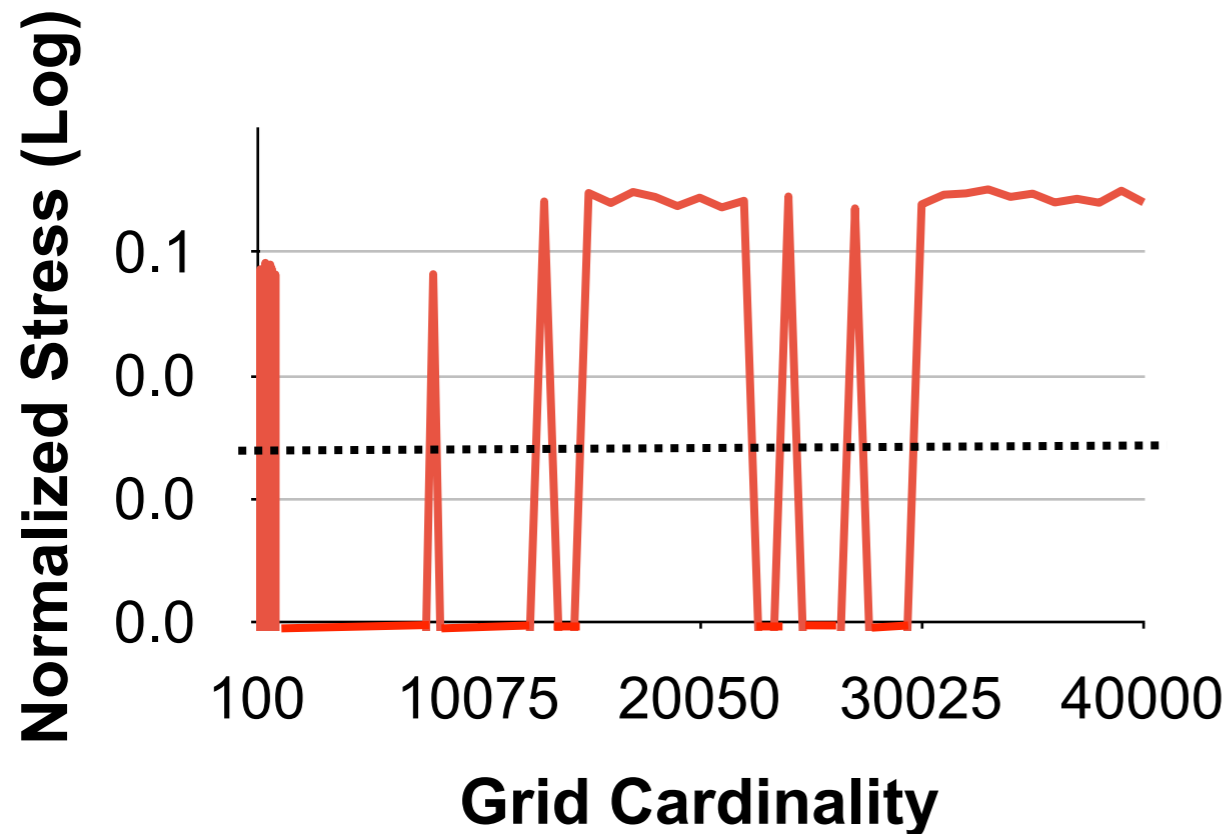
Glimmer: Multilevel MDS on the GPU.  
Ingram, Munzner, Olano. *IEEE TVCG* 15(2):249-261, 2009.

# 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

**Glimmer**

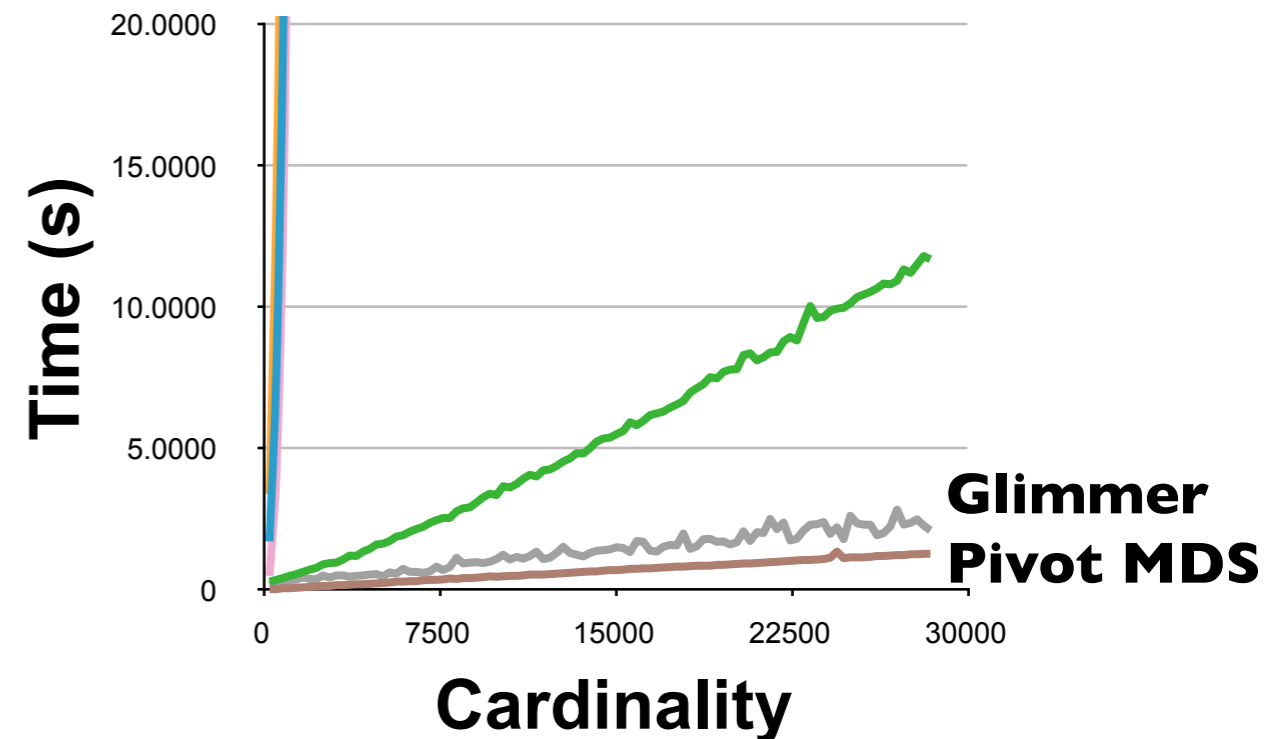
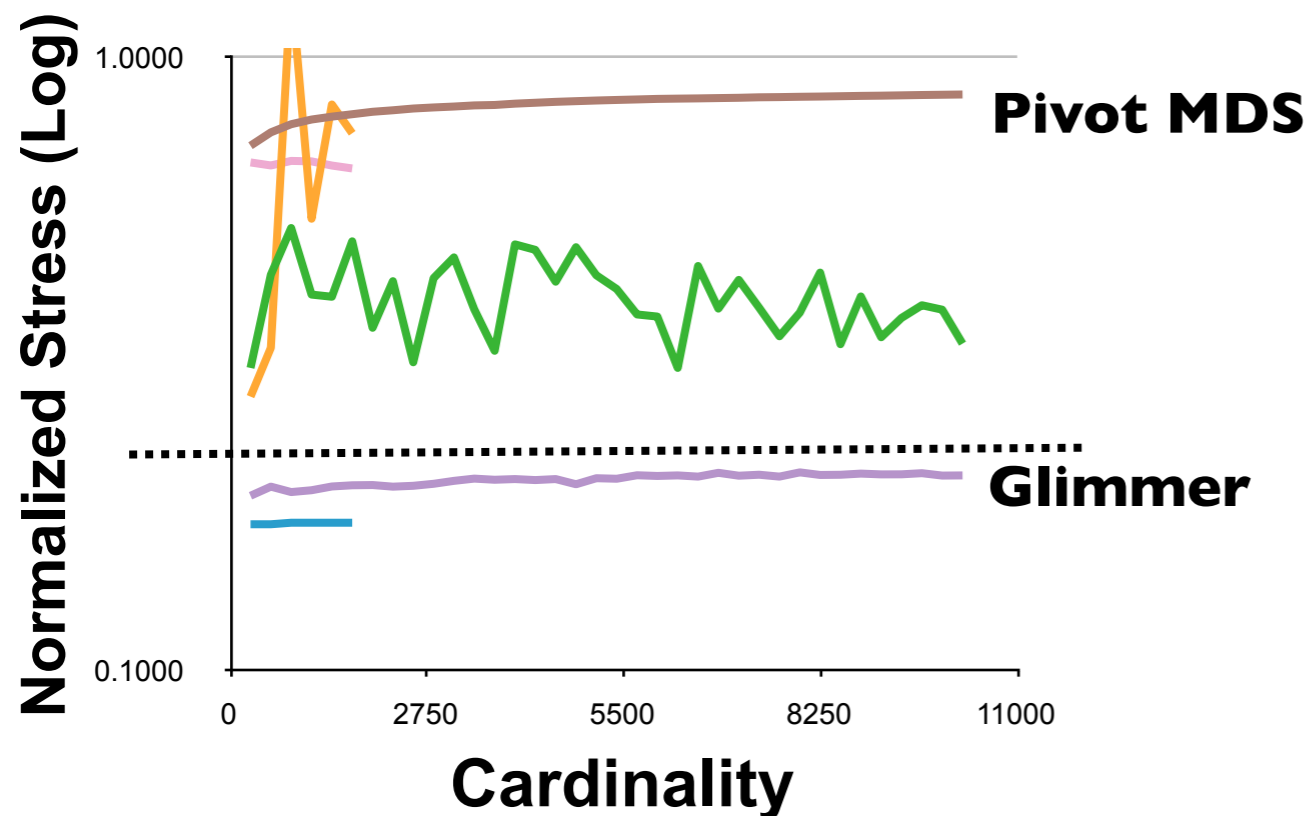


16.64 s stress=0.157

**Pivot MDS**



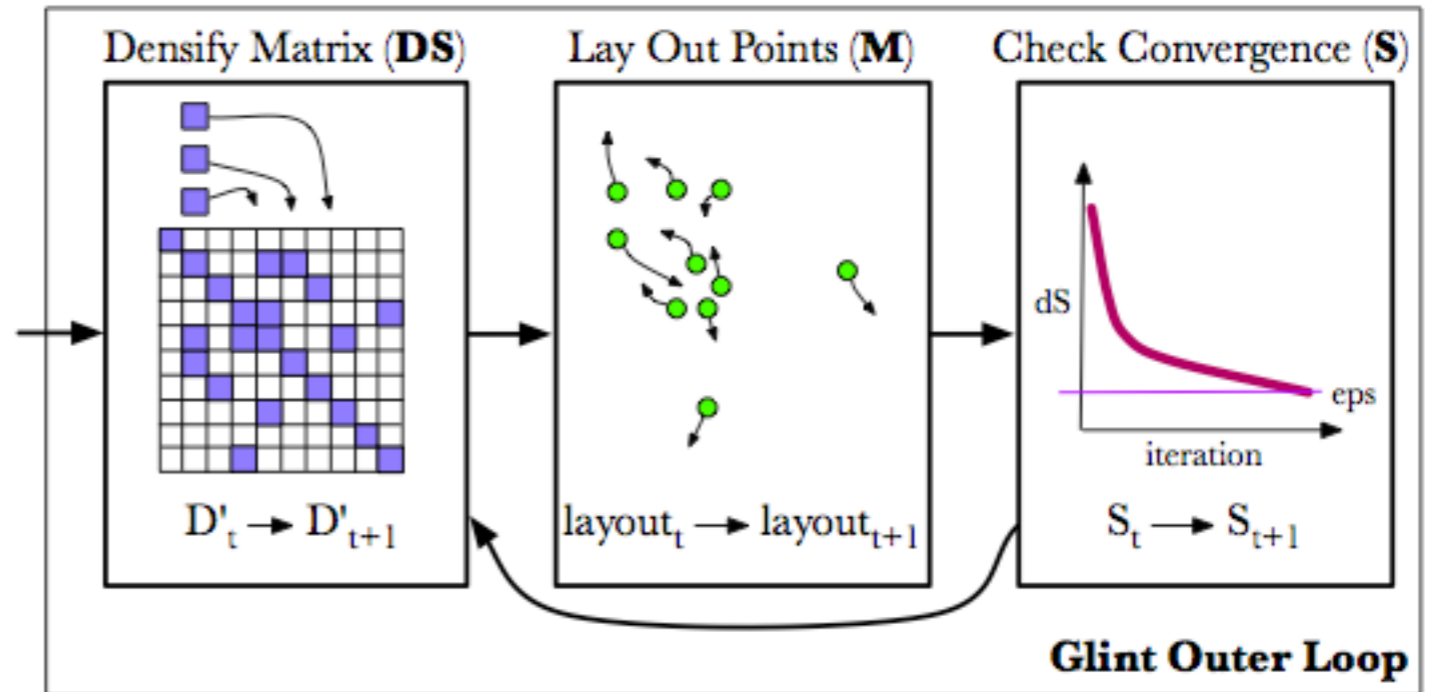
2.17 s stress=0.928



# 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

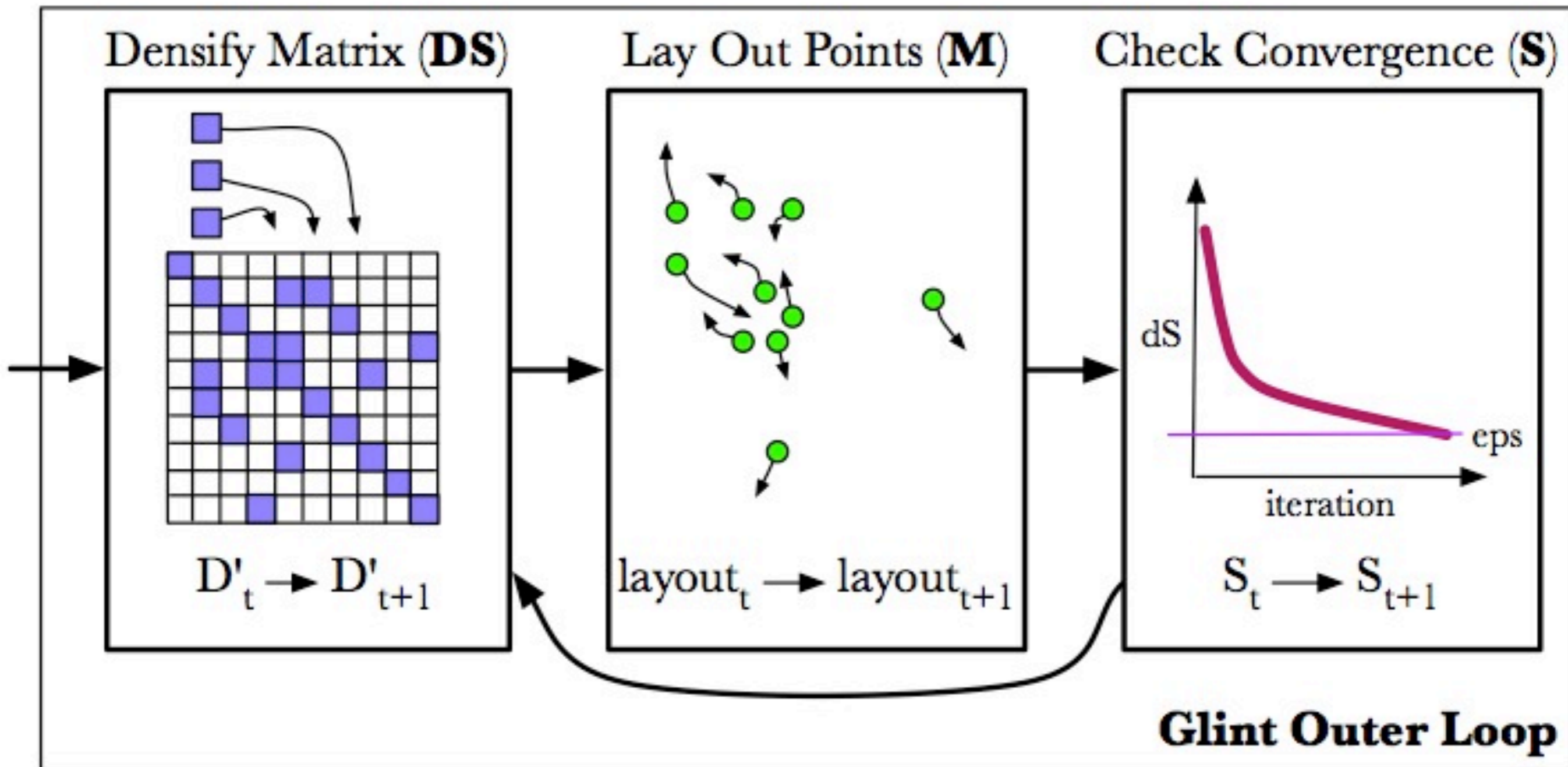
# Costly Distances

- DR in the Wild revealed many real-world examples

	<b>Distance function</b>	<b>Cost (seconds)</b>
<b>Cheap</b>	Euclidean on 9-D data	0.00001
	Database Query	0.001
<b>Costly</b>	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

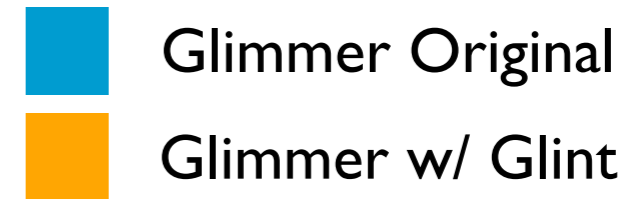
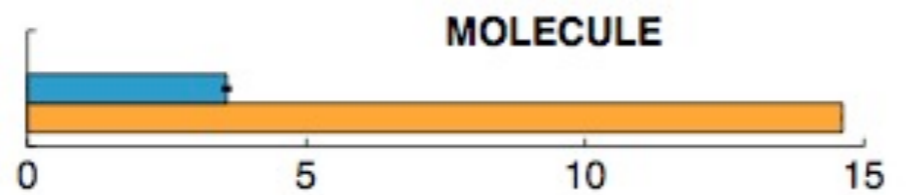
MDS Algorithm Type	Chosen Algorithm
Gradient-based Optimization	SMACOF
Spectral/Analytic	Pivot MDS
Force-Directed	Glimmer

# Force-Directed Instantiation Results

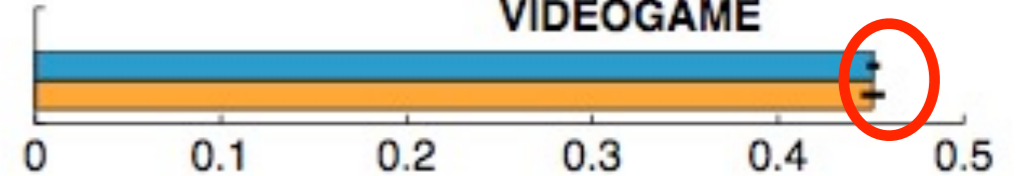
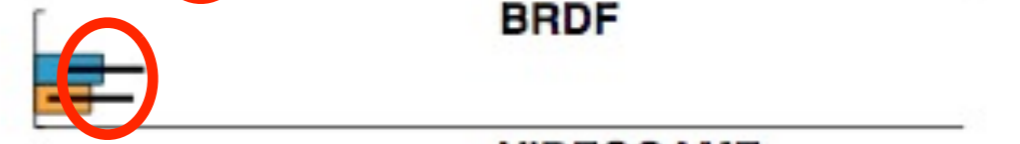
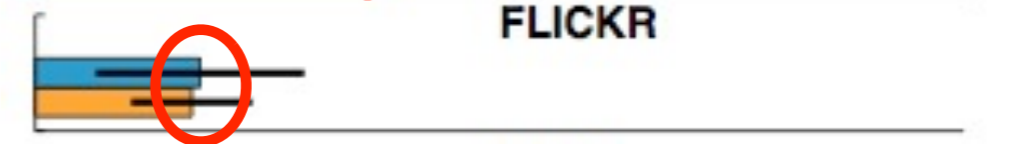
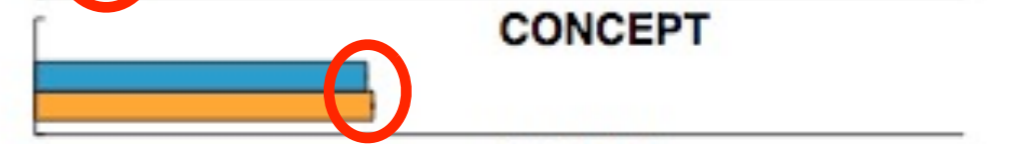
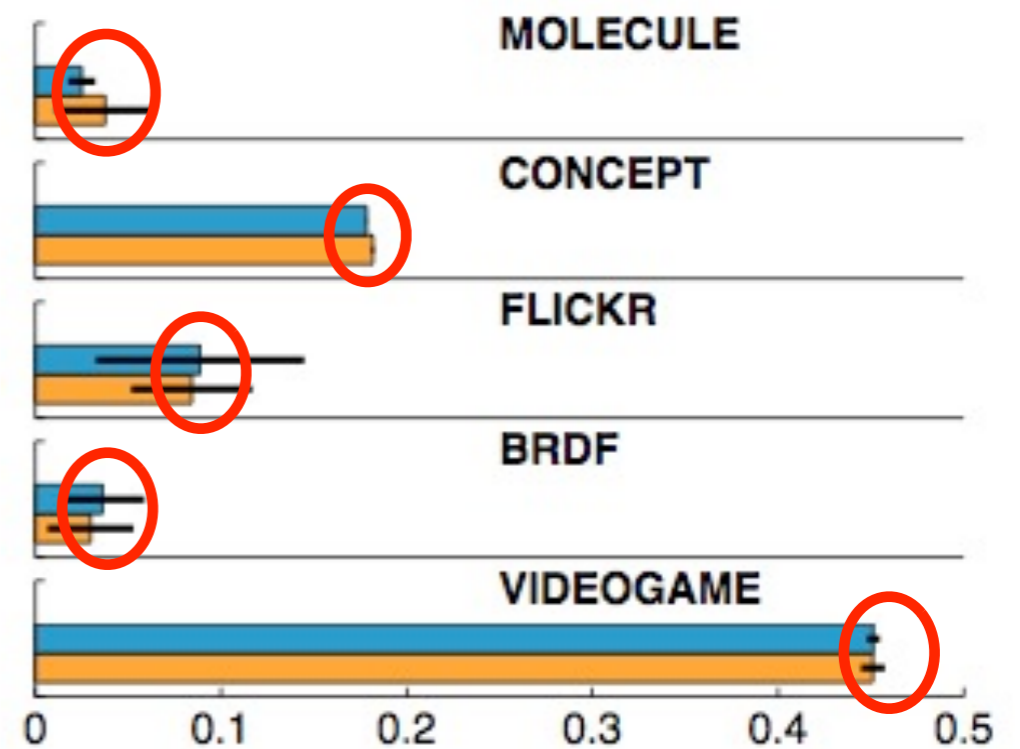
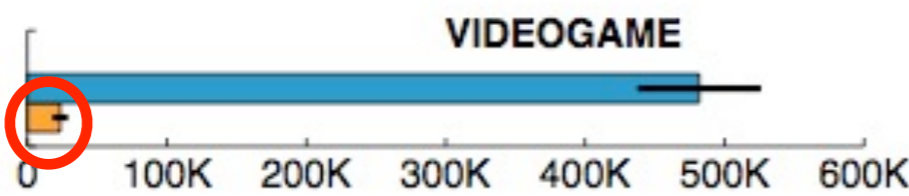
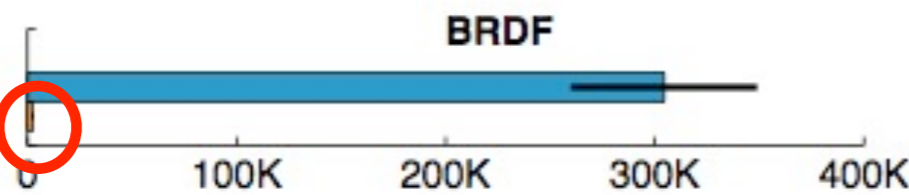
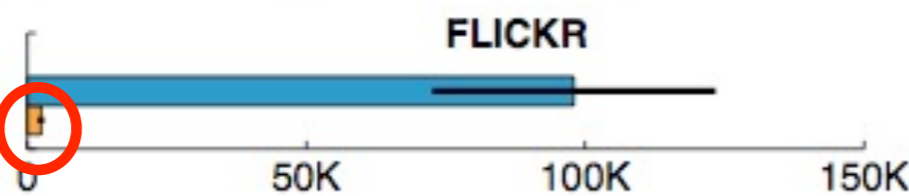
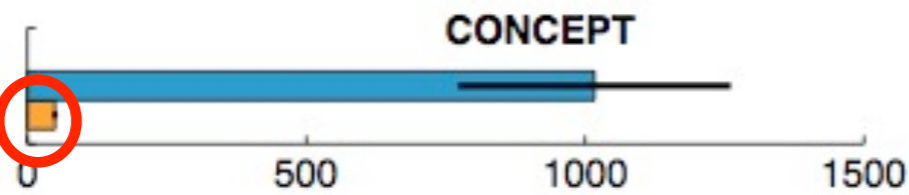
Speed

Quality

Cheap dist



Costly dists



major speed improvements while quality maintained

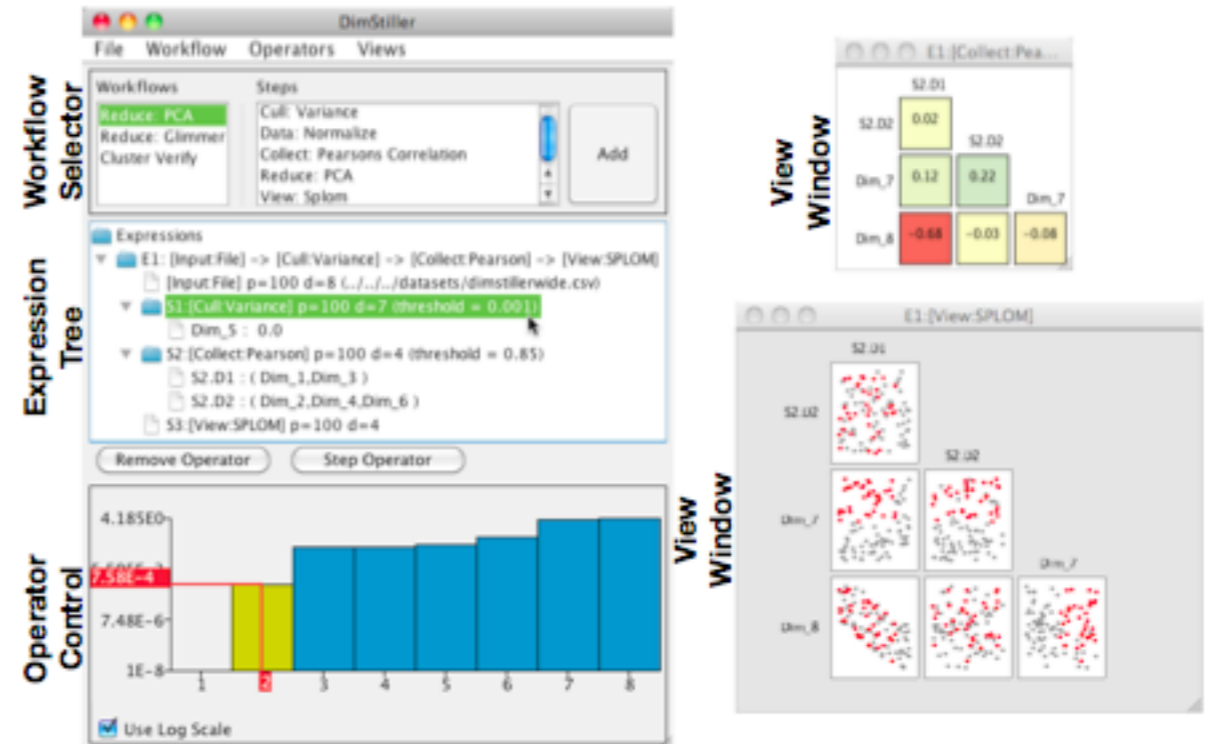
# Methods and Outcomes

- 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:**

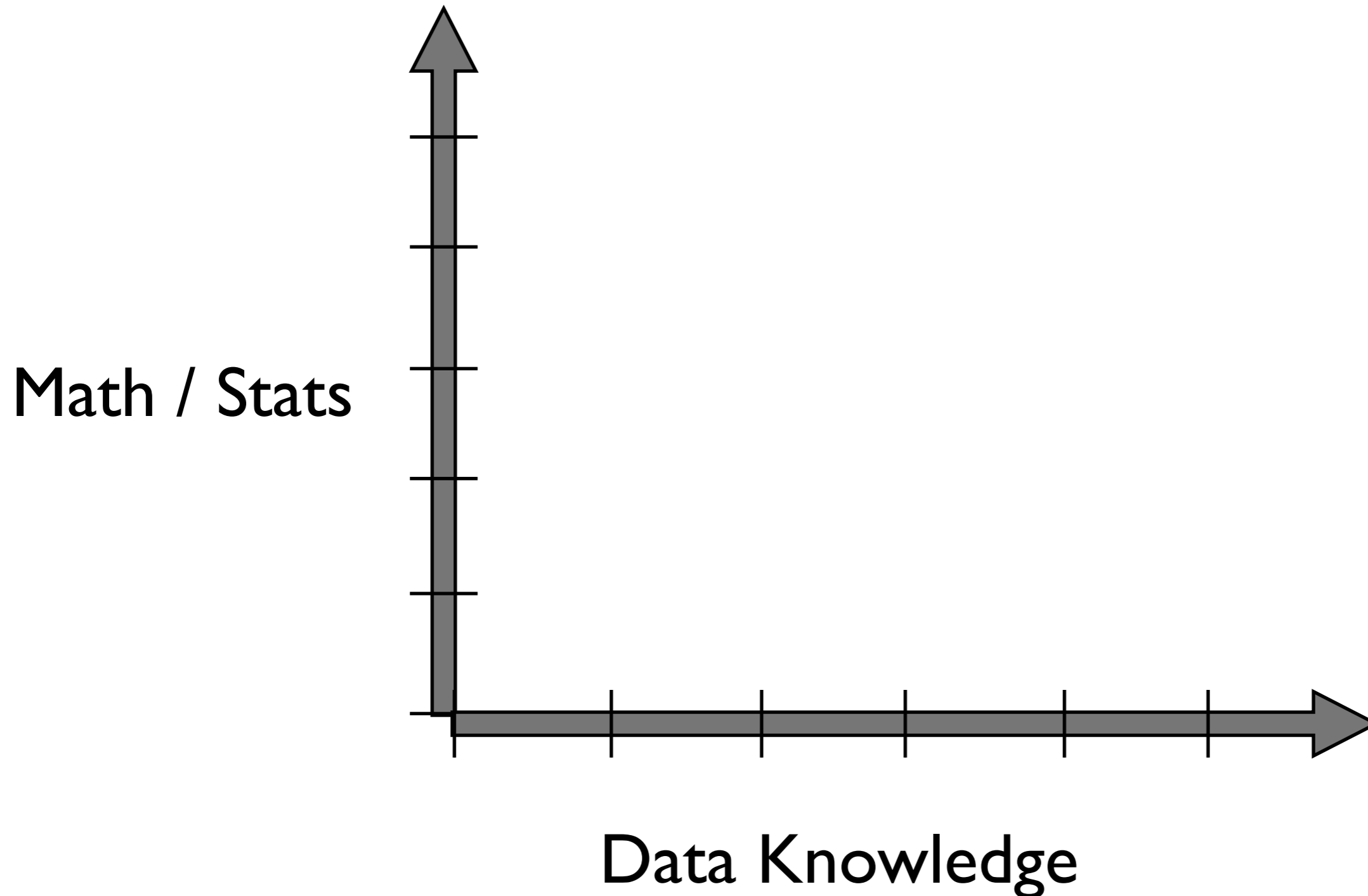
Stephen Ingram, Veronika Irvine, Melanie Tory, Steven Bergner, Torsten Möller

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

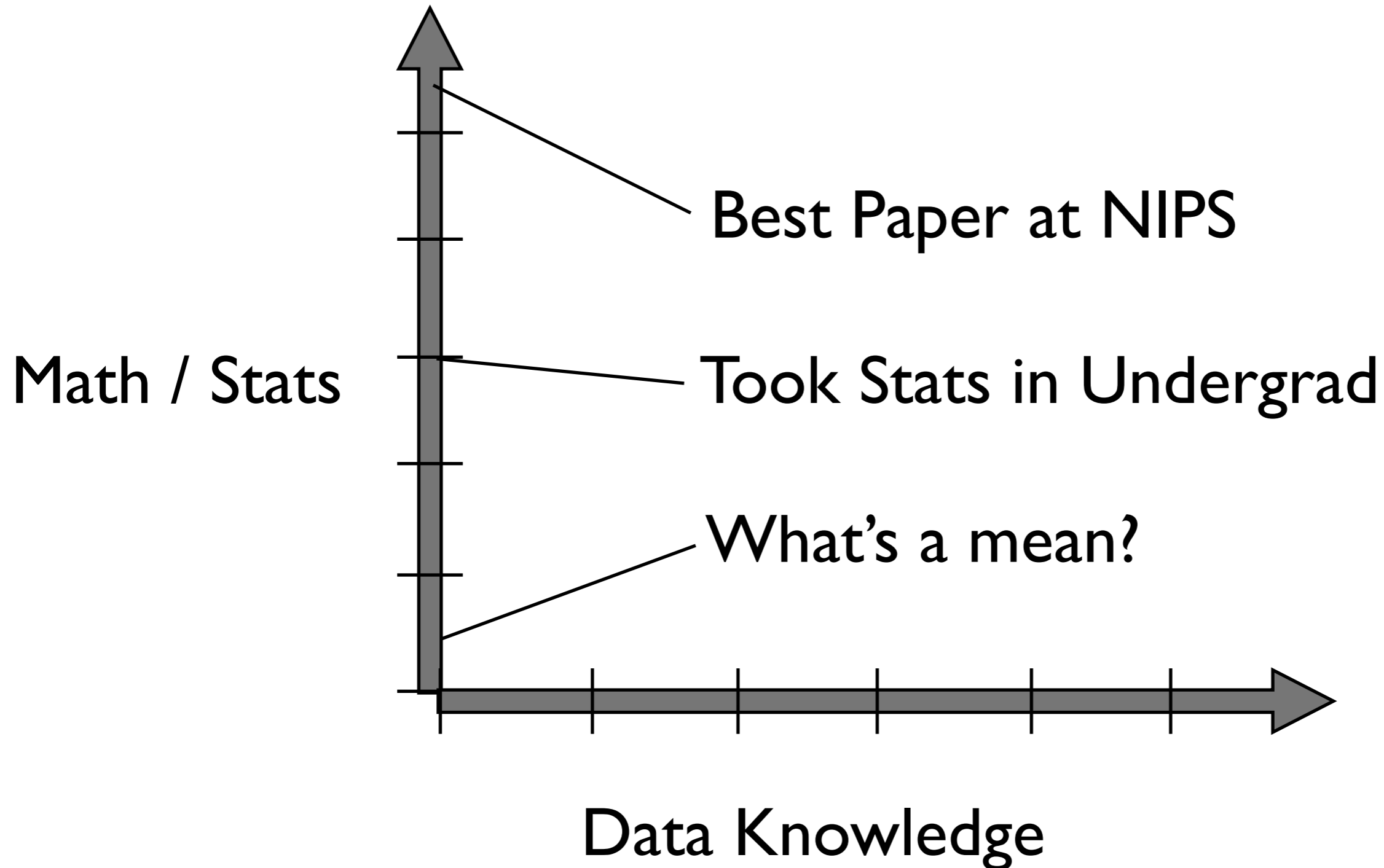
DimStiller: Workflows for dimensional analysis and reduction.  
 Ingram, Munzner, Irvine, Tory, Bergner, Moeller. Proc. VAST 2010, p 3-10.

# Who Might Use DR?

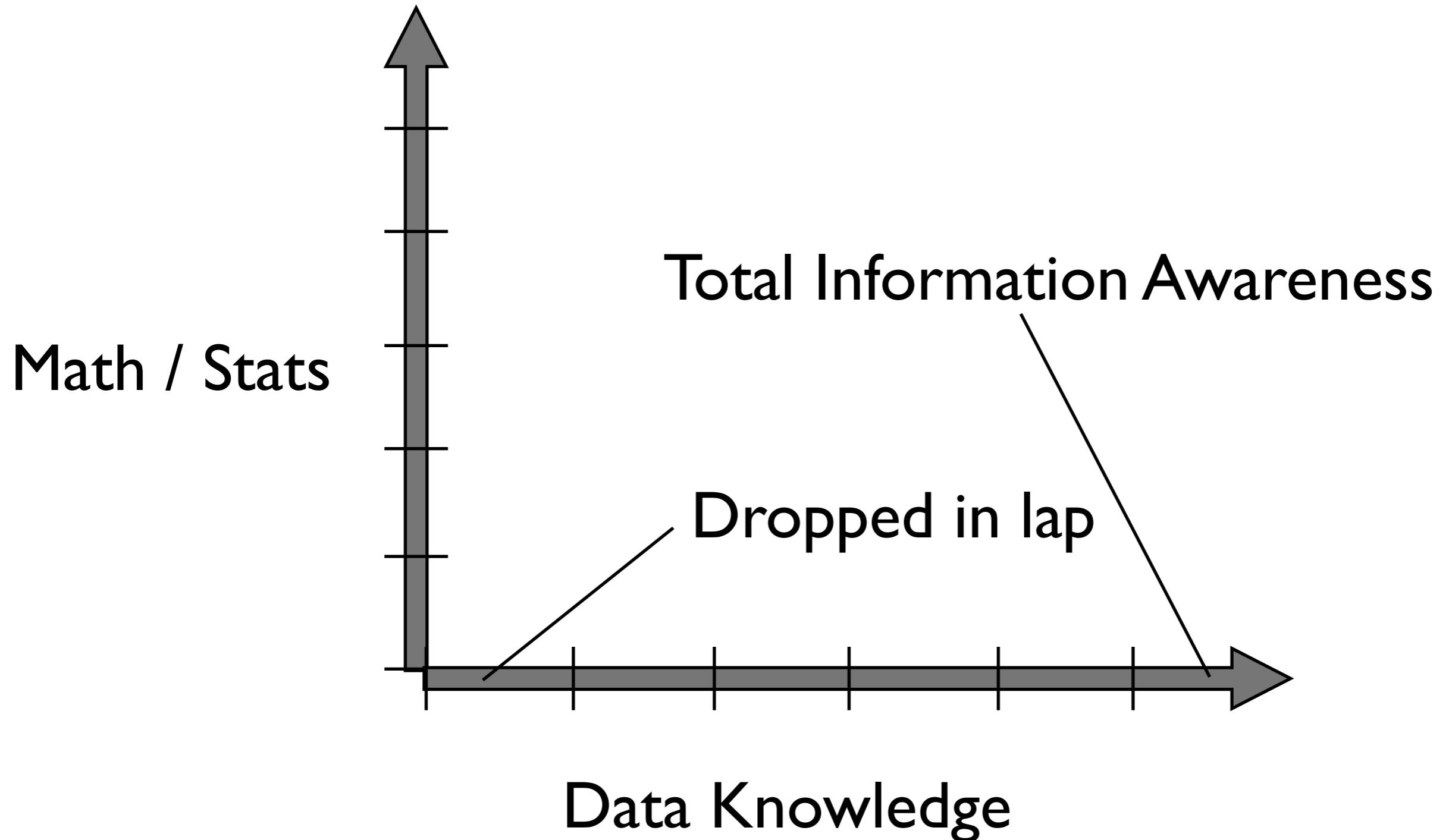
- DR in the Wild revealed broad set of users



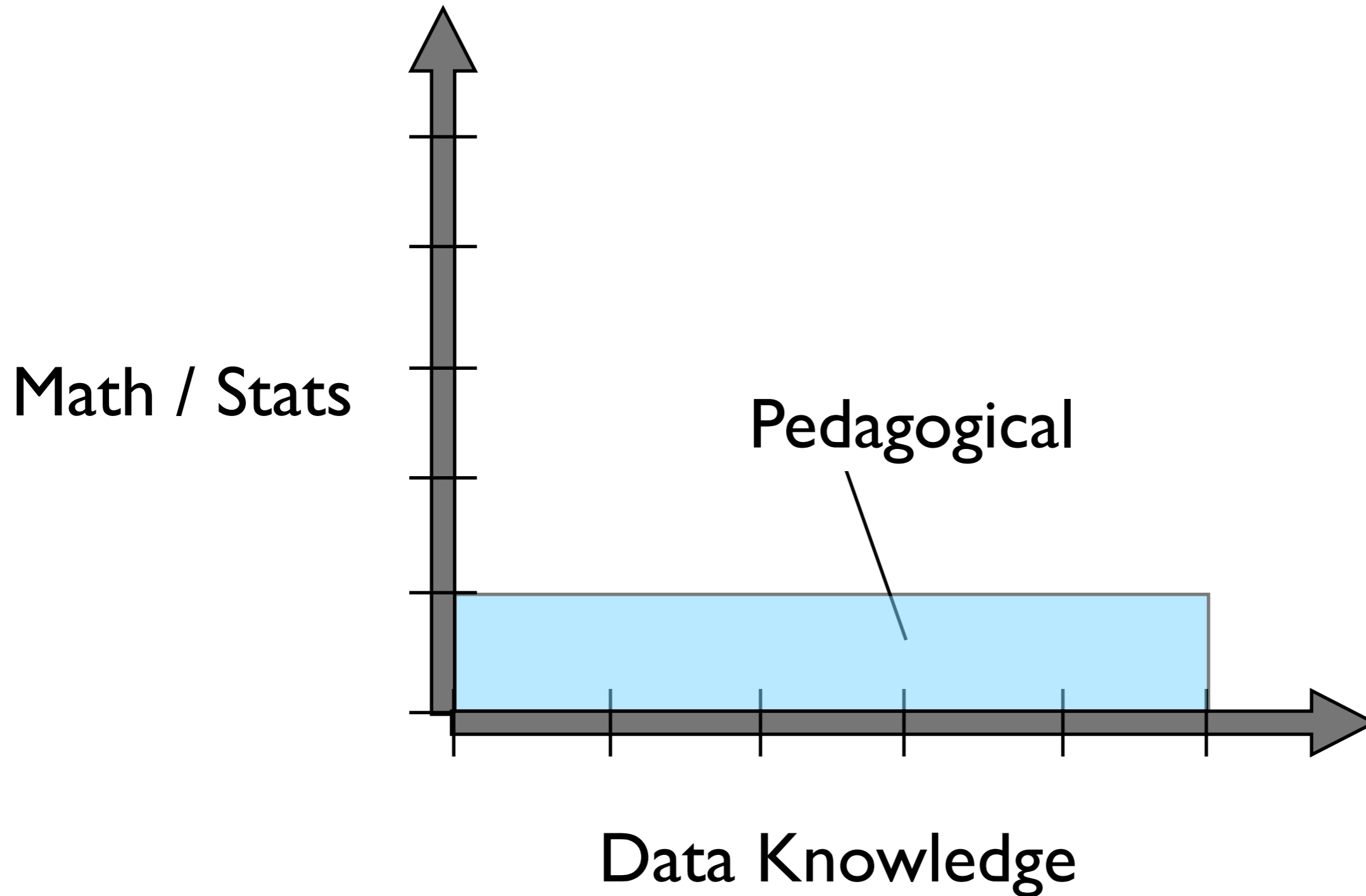
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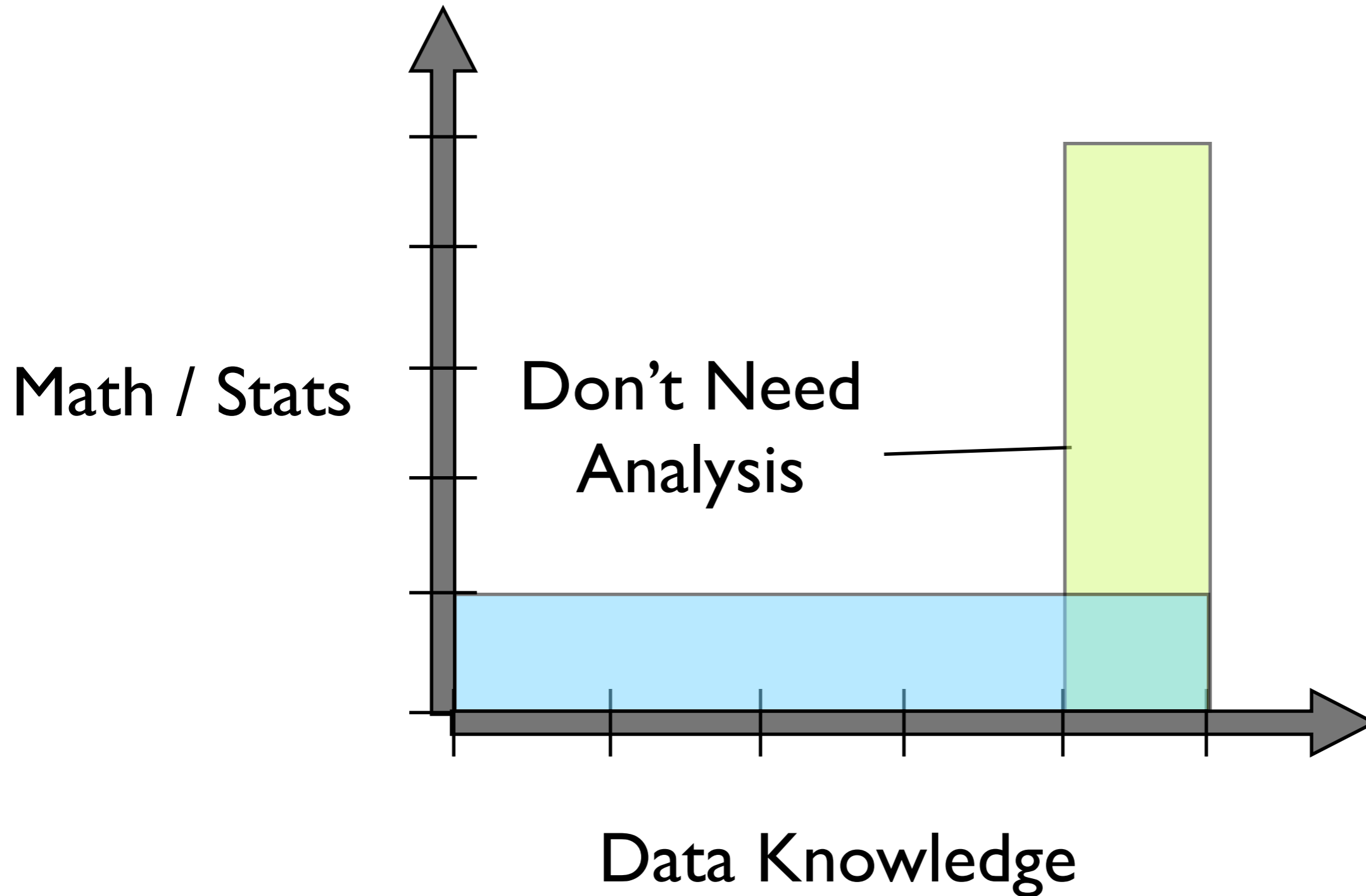
# Who Might Use DR?



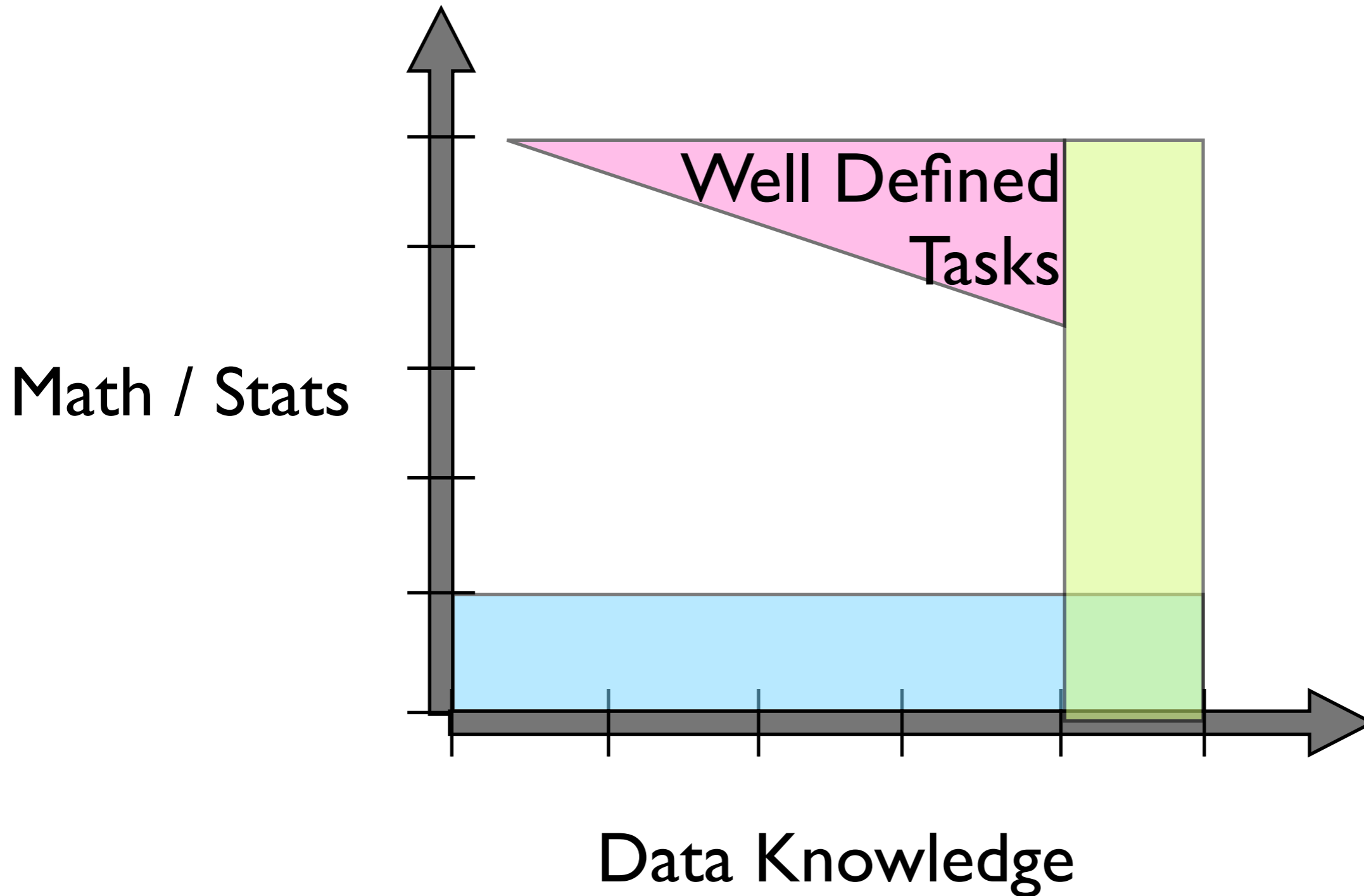
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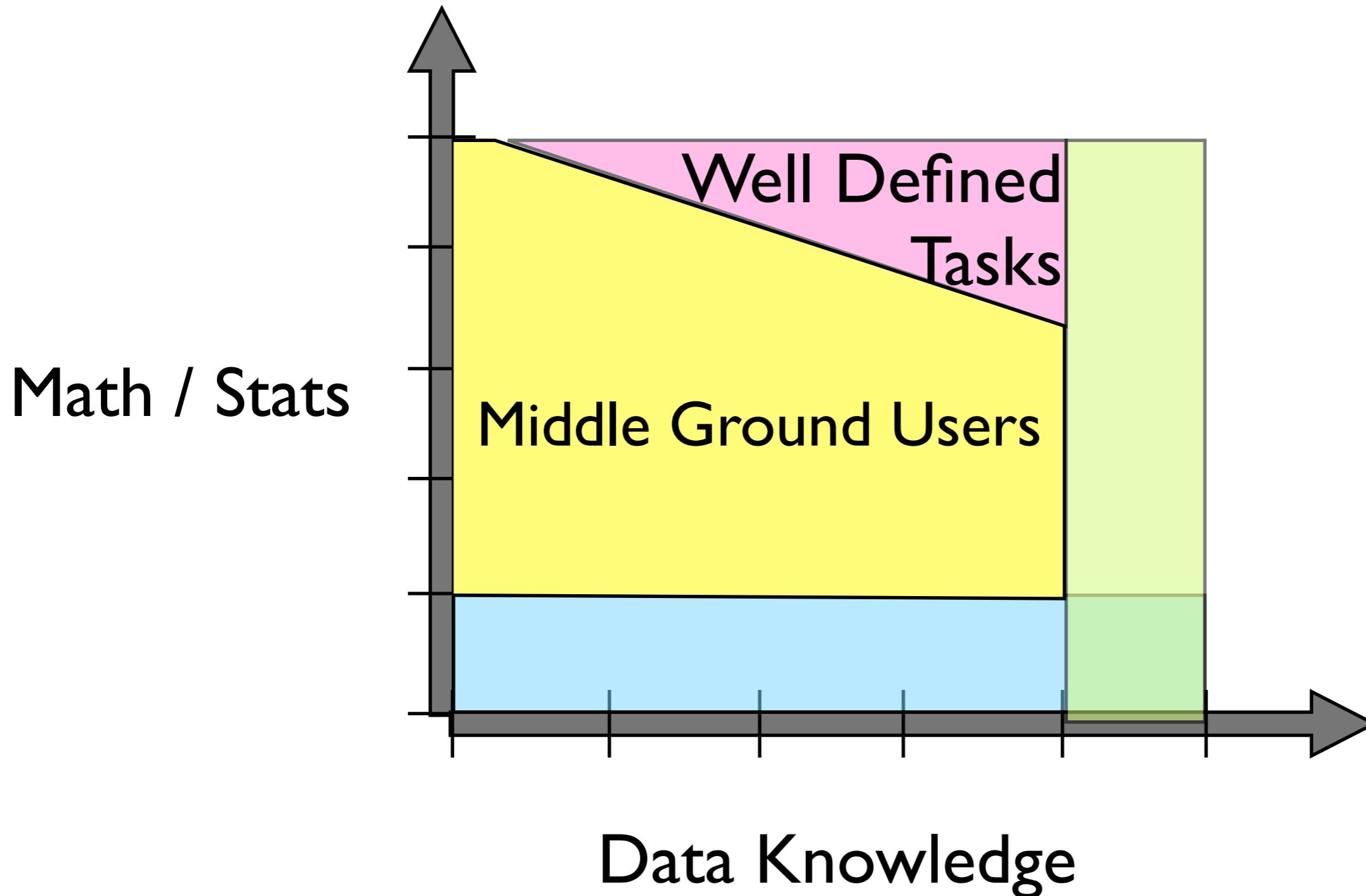


# Who Might Use DR?



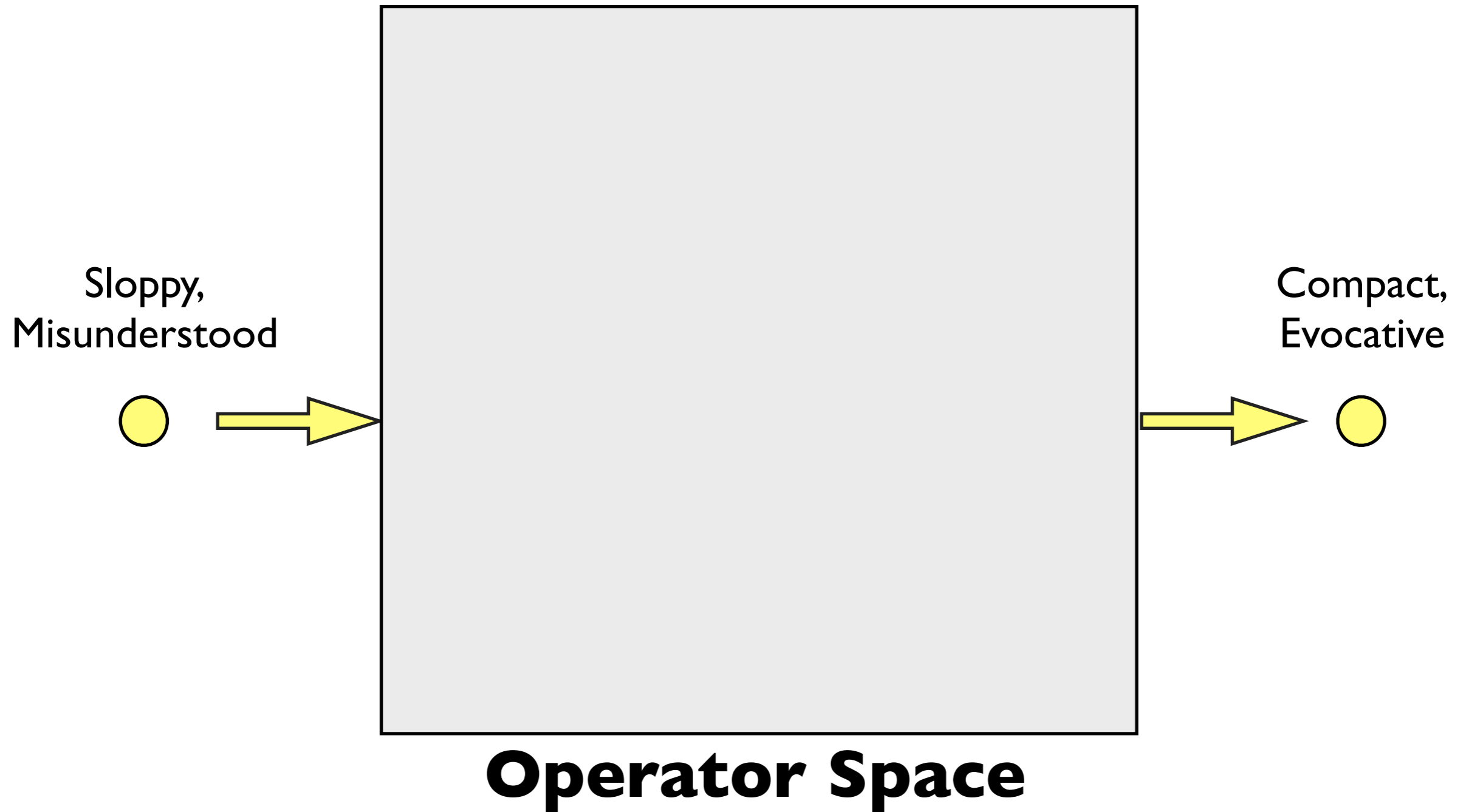
# Who Might Use DR?

- middle ground users benefit from guidance

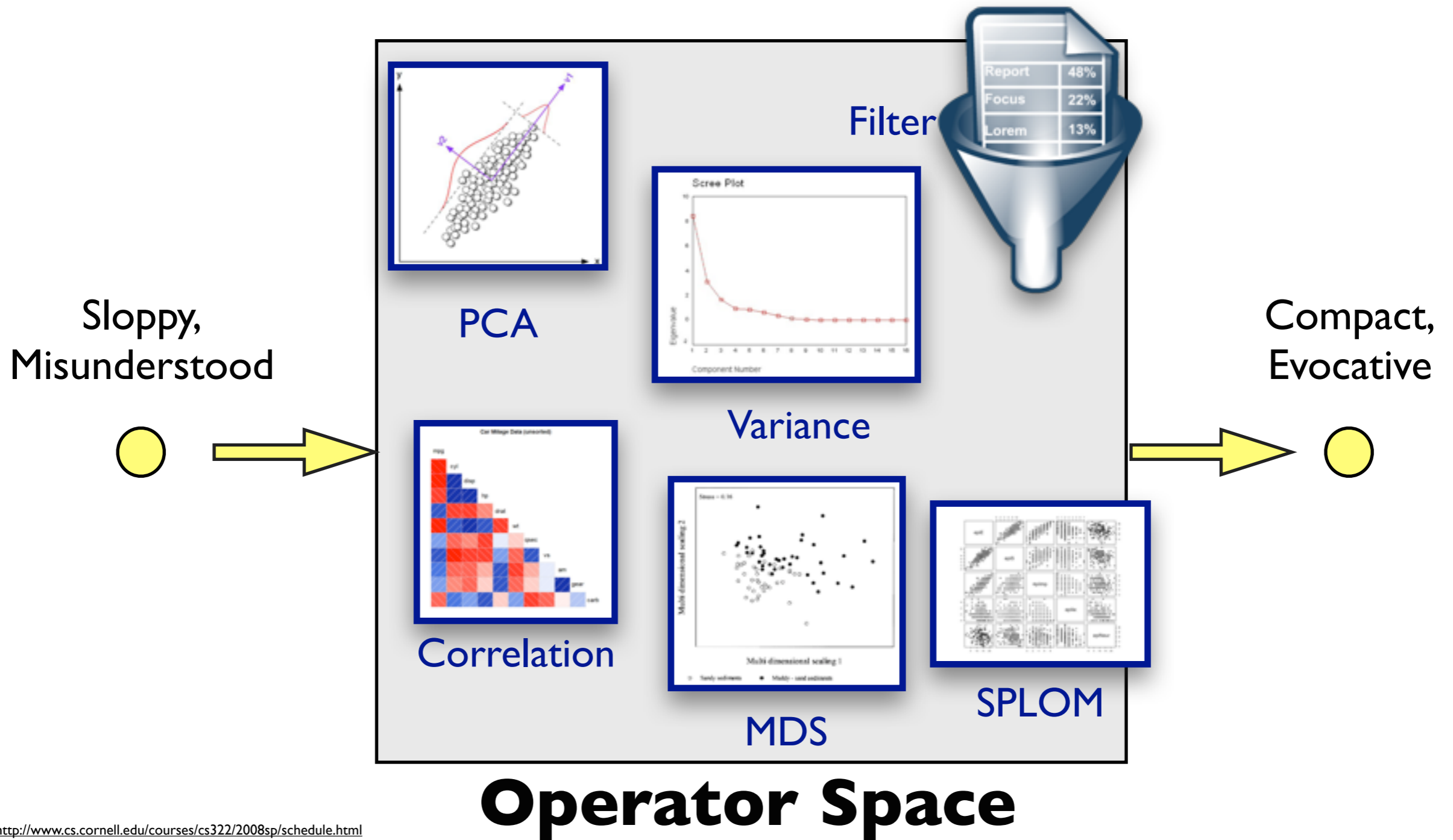




# Global Guidance



# Global Guidance



## Operator Space

<http://www.cs.cornell.edu/courses/cs322/2008sp/schedule.html>

<http://www.statmethods.net/advgraphs/images/corrgram3.png>

[http://en.wikibooks.org/wiki/File:Scree\\_plot\\_for\\_the\\_initial\\_dataset\\_Figure\\_36.jpg](http://en.wikibooks.org/wiki/File:Scree_plot_for_the_initial_dataset_Figure_36.jpg)

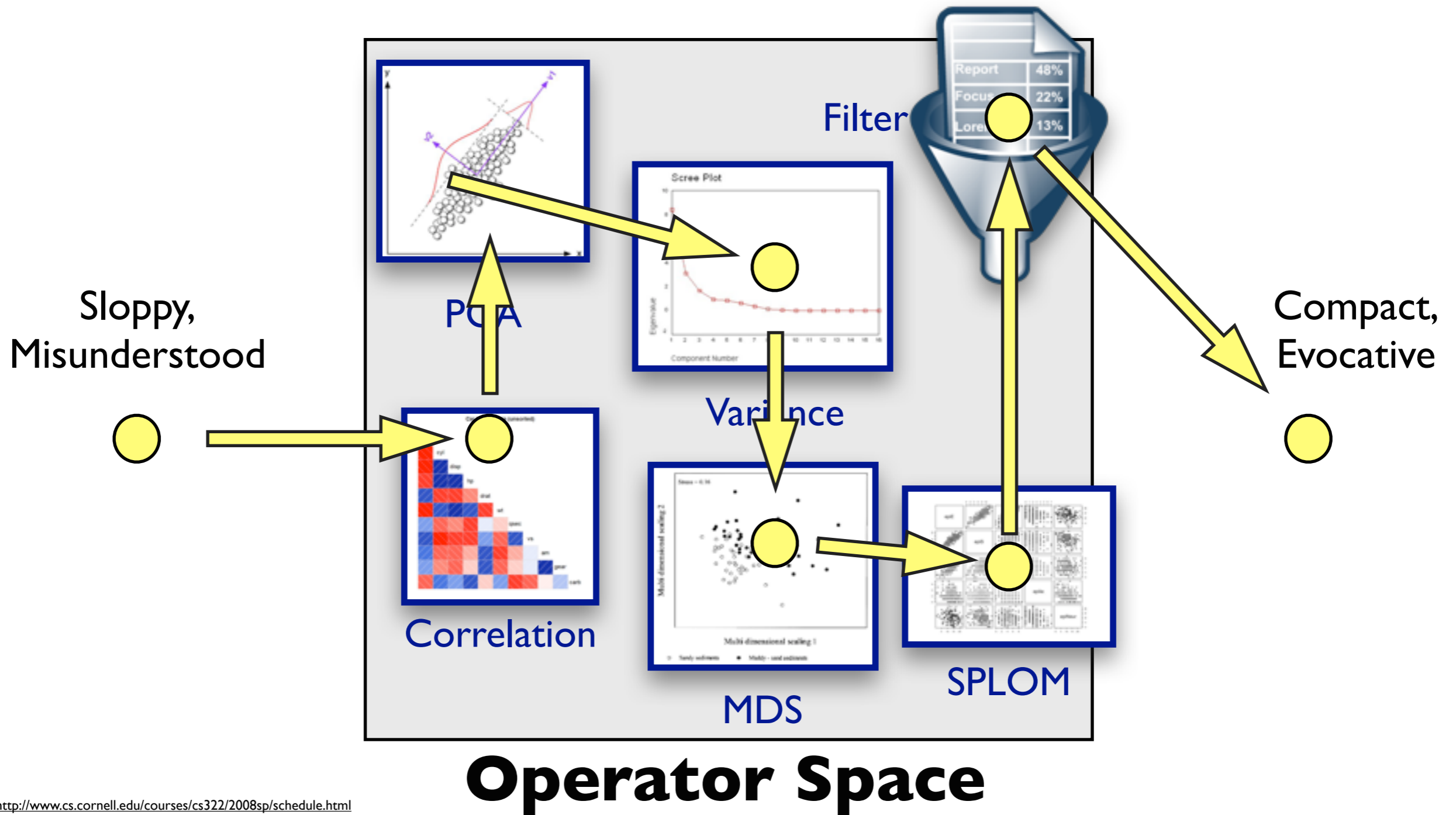
[http://www.scielo.cl/scielo.php?pid=S0716-078X2001000200019&script=sci\\_arttext](http://www.scielo.cl/scielo.php?pid=S0716-078X2001000200019&script=sci_arttext)

[http://www.iconfinder.com/icondetails/44818/400/data\\_filter\\_icon?r=1](http://www.iconfinder.com/icondetails/44818/400/data_filter_icon?r=1)

<http://www.personality-project.org/R/>

# Global Guidance

- which operations and in which order?



## Operator Space

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<http://www.statmethods.net/advgraphs/images/corrgram3.png>

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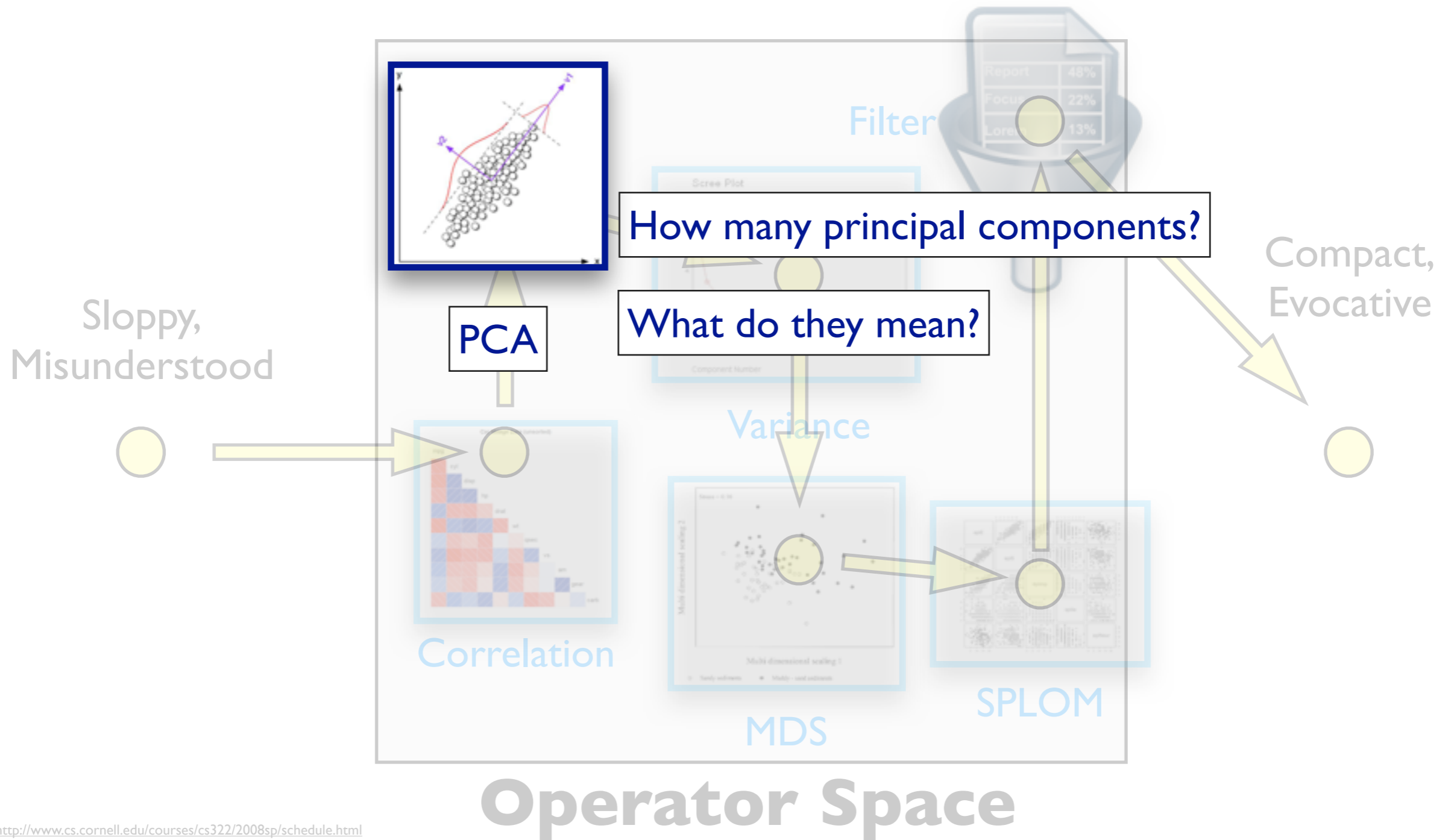
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<http://www.personality-project.org/R/>

# Local Guidance

- what to do with a given operator?



**Operator Space**

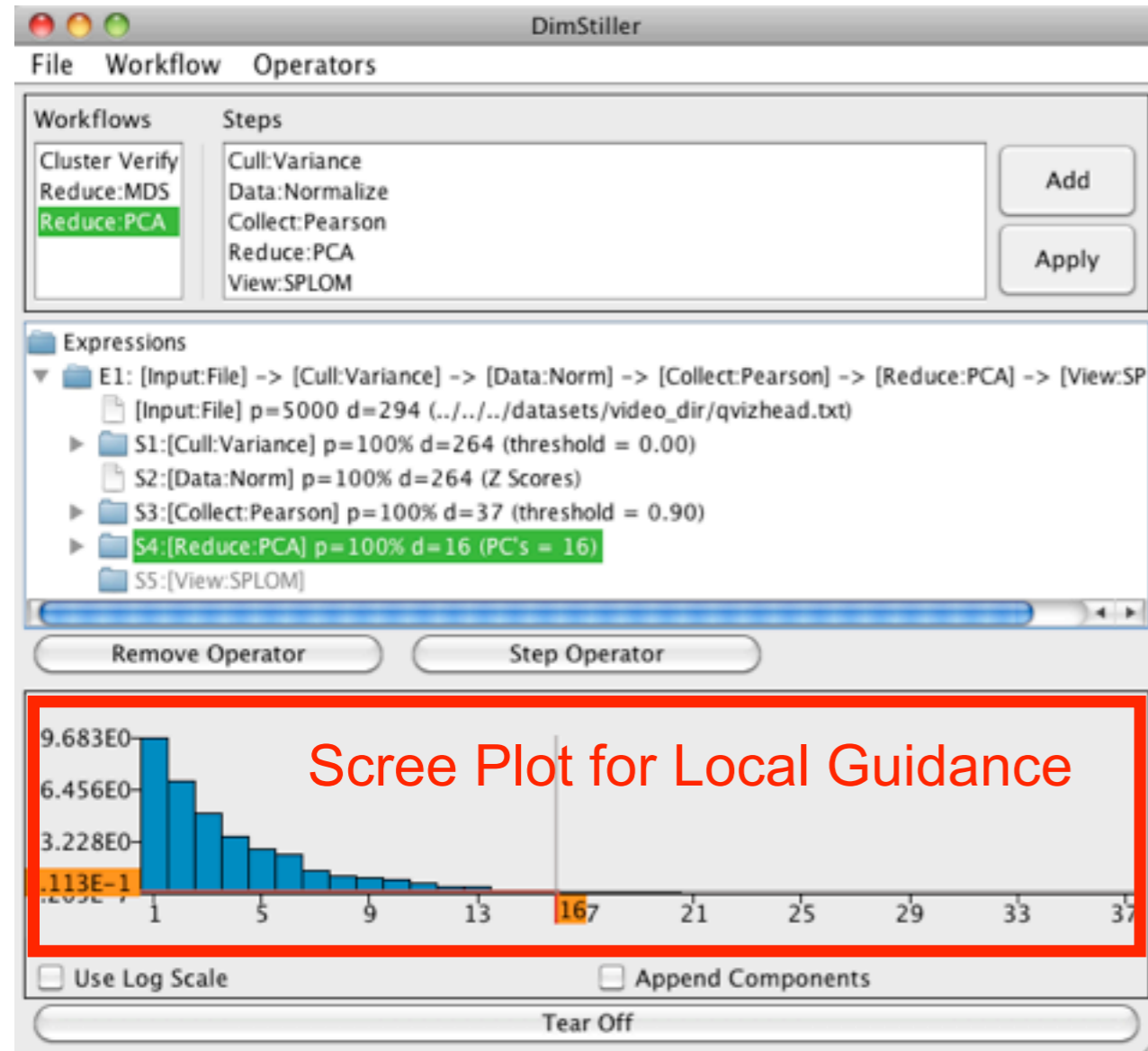
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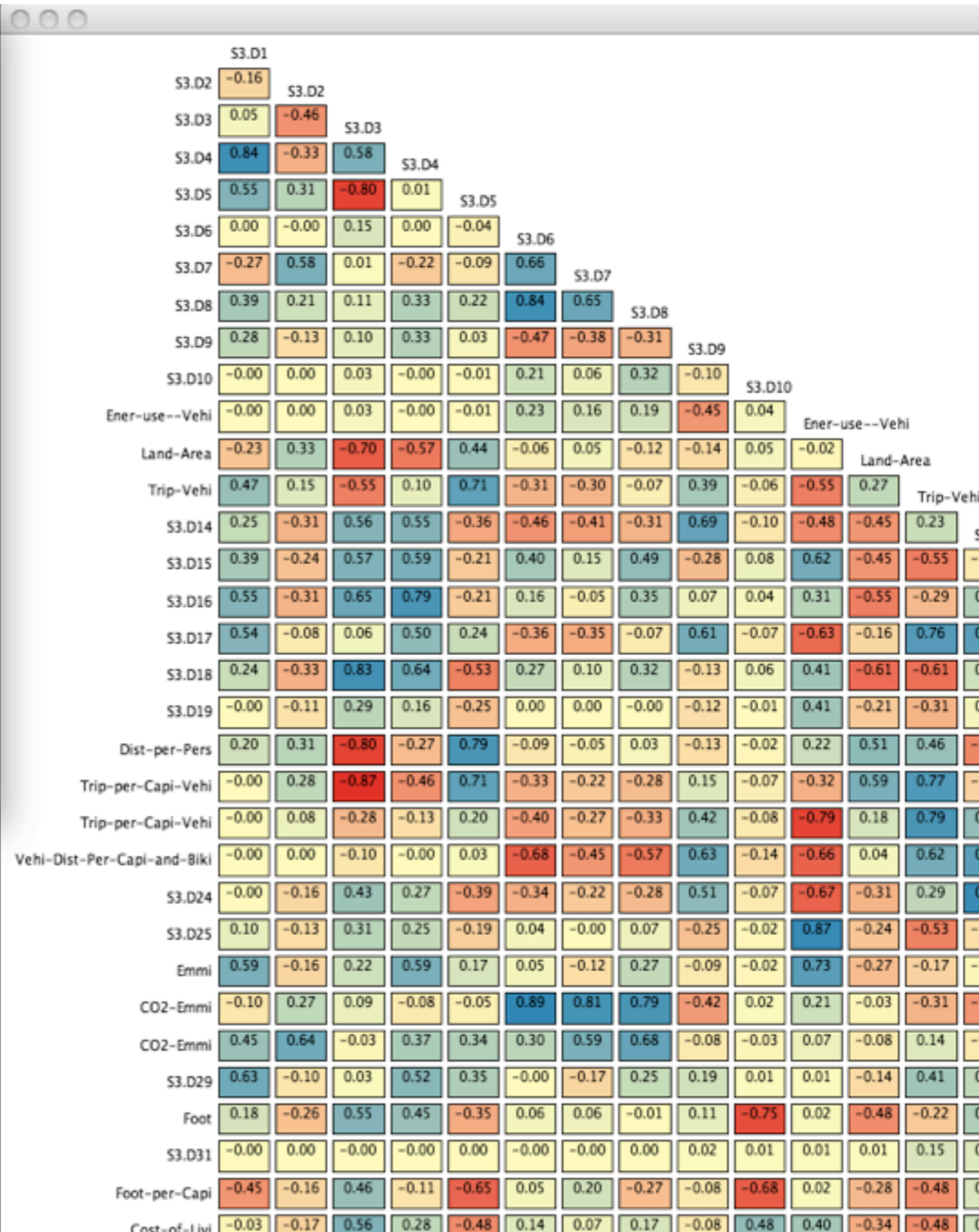
[http://en.wikibooks.org/wiki/File:Scree\\_plot\\_for\\_the\\_initial\\_dataset\\_Figure\\_36.jpg](http://en.wikibooks.org/wiki/File:Scree_plot_for_the_initial_dataset_Figure_36.jpg)

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# DimStiller



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



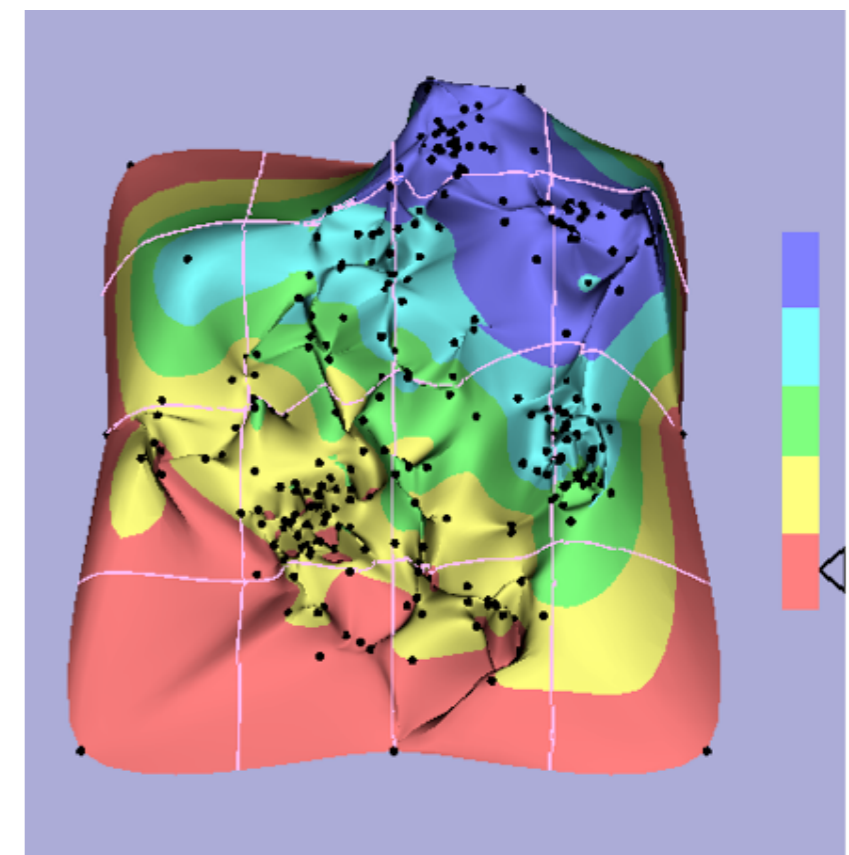
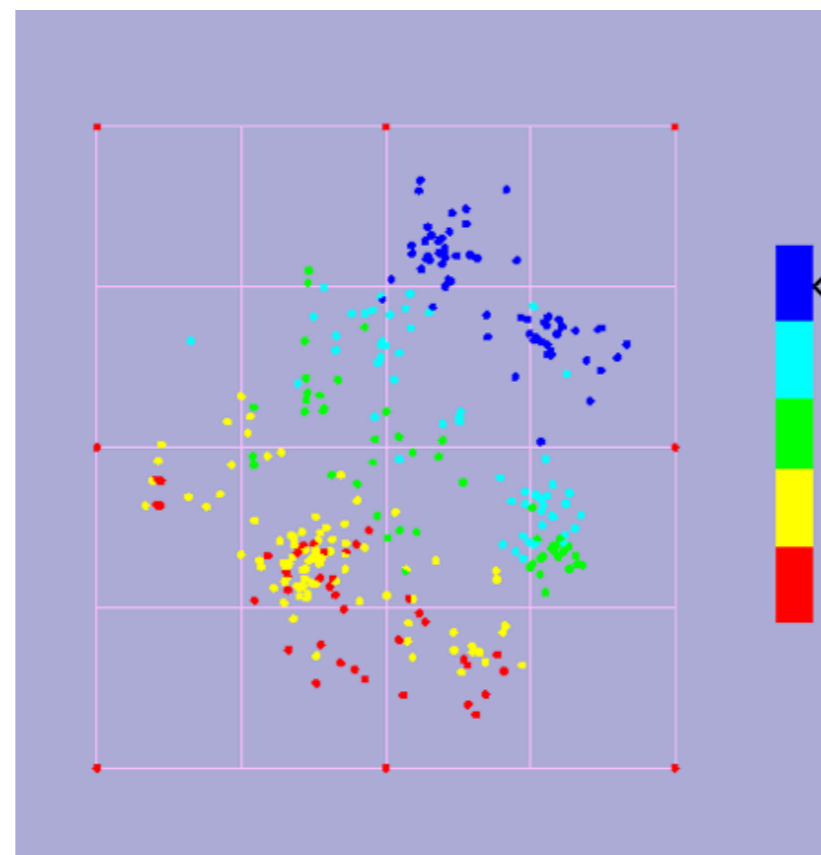
# Methods and Outcomes

- 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

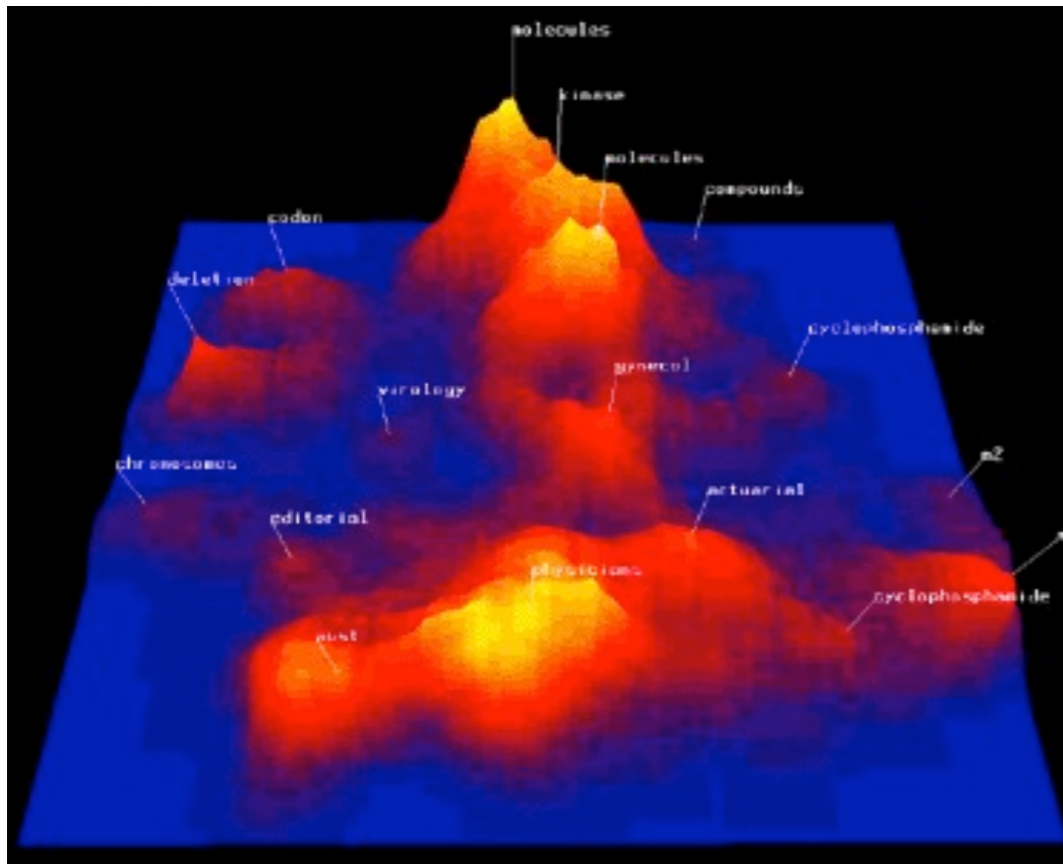
<http://webhome.cs.uvic.ca/~mtory/publications/infovis2007.pdf>

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>]

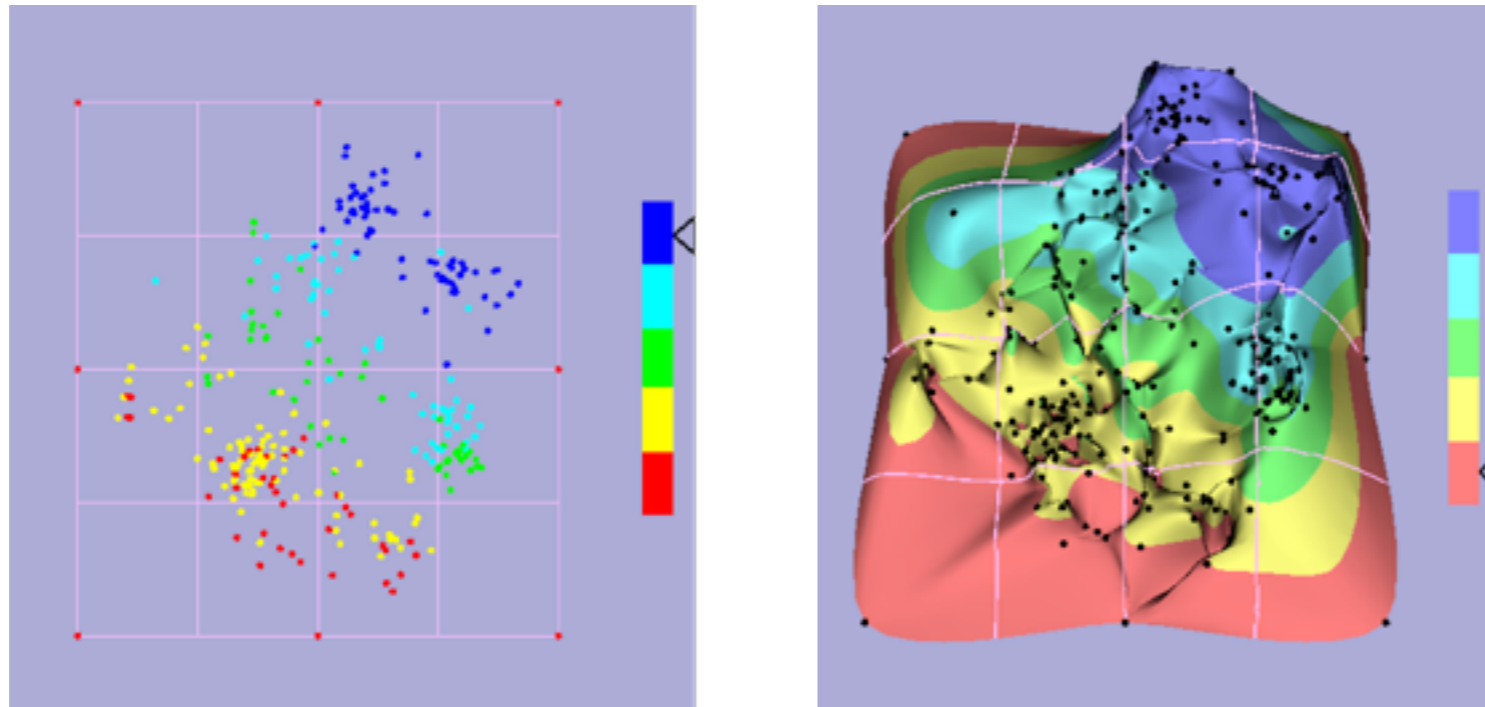


[Guide to MicroPatent Aureka 9 ThemeScape]

# 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

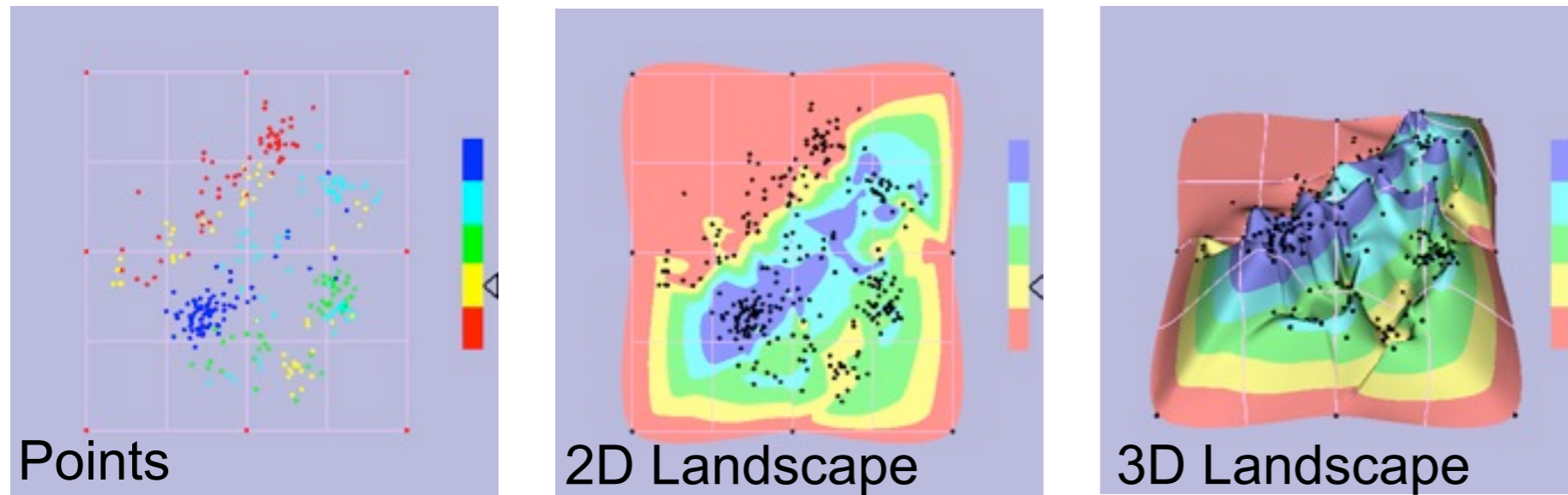
“Where in the display are people with high incomes?”

“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

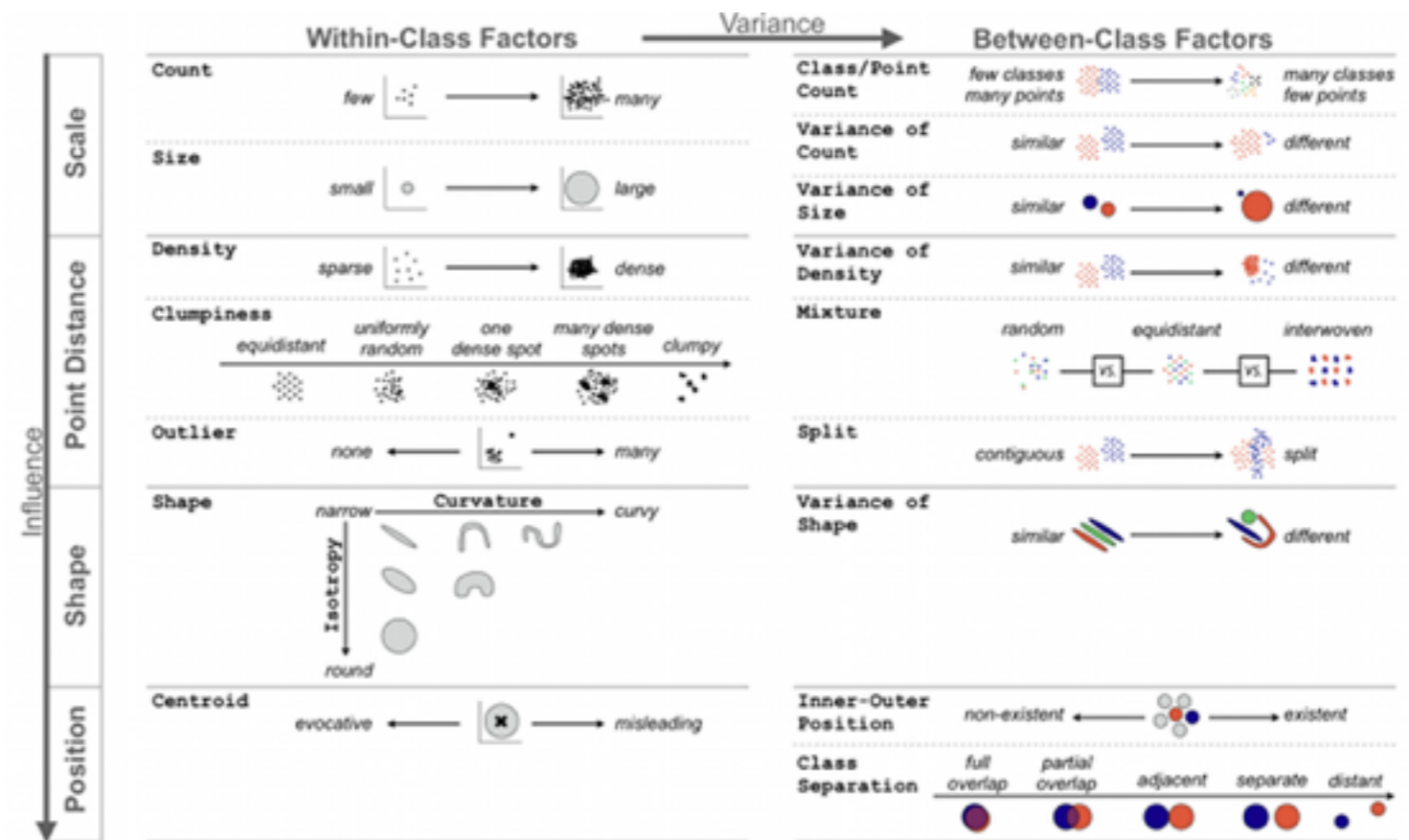
- 2D landscapes (color only) better than 3D landscapes (color + height redundantly encoded)

- 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

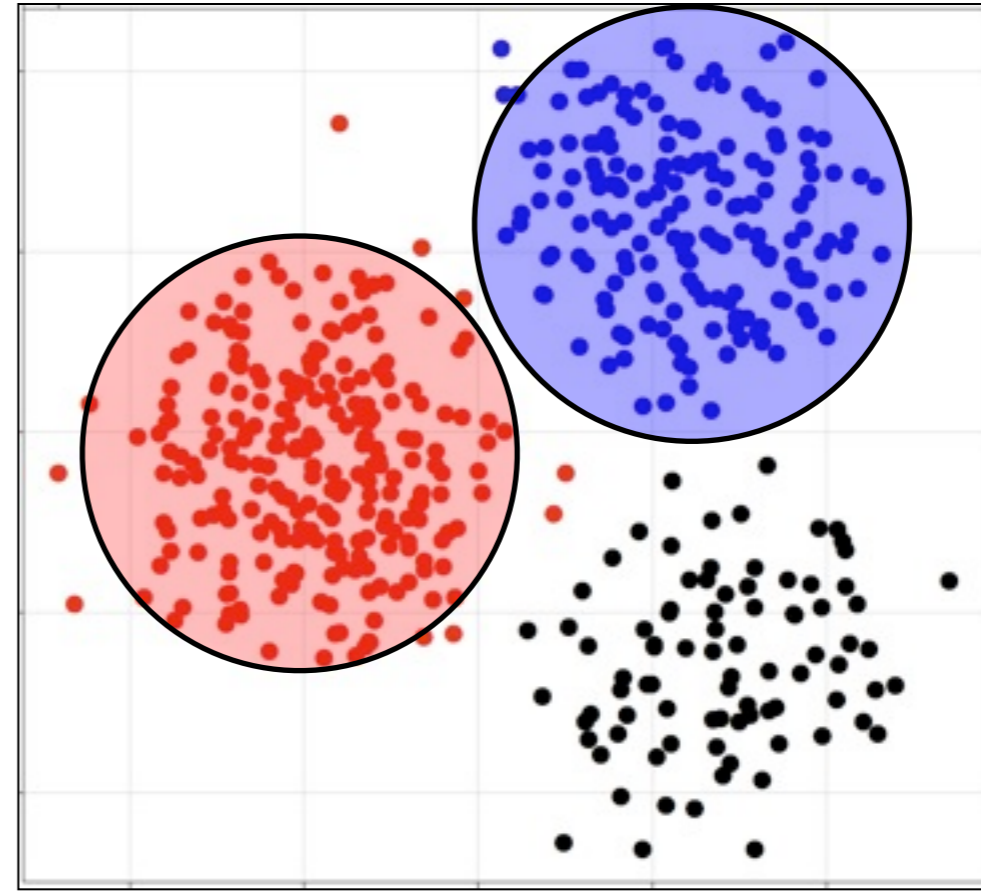
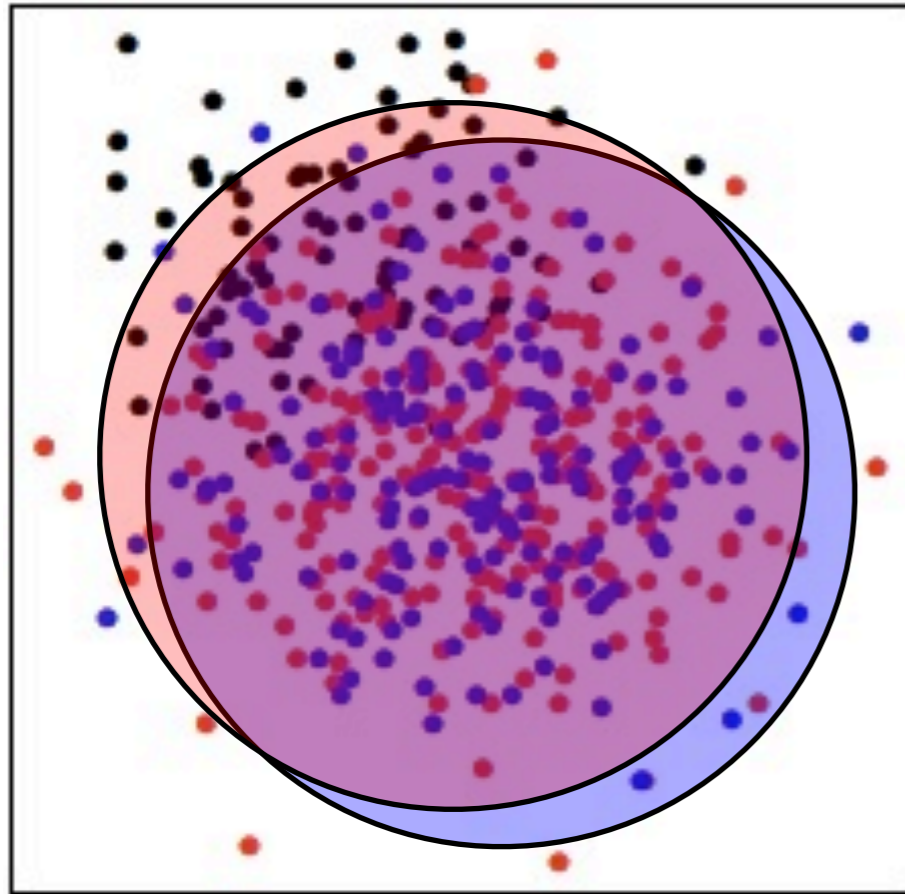
<http://www.cs.ubc.ca/labs/imager/tr/2012/VisClusterSep/>

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



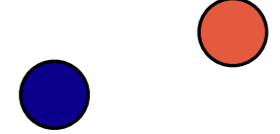
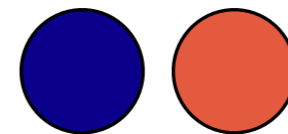
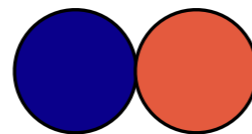
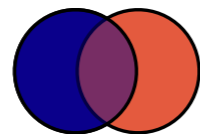
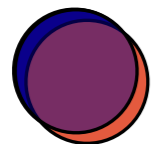
*full  
overlap*

*partial  
overlap*

*adjacent*

*separate*

*distant*

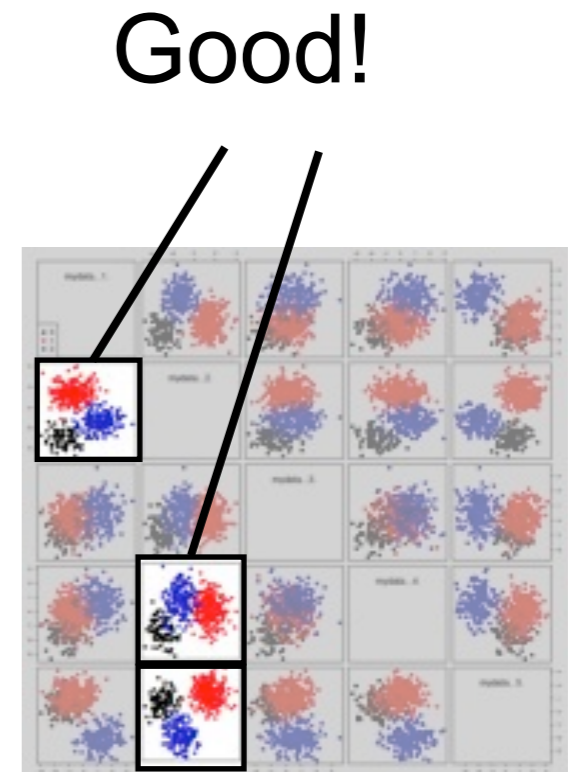
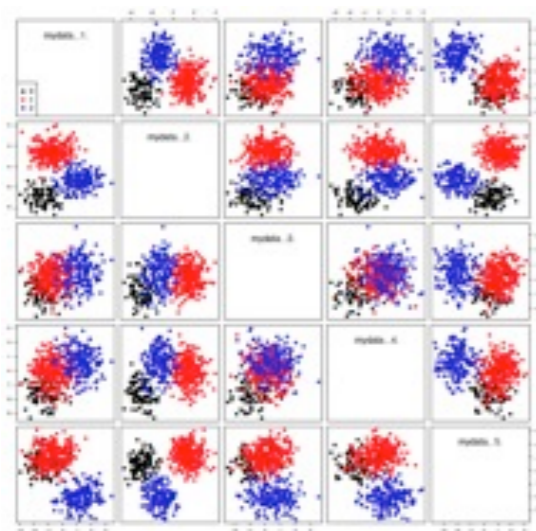


# Visual Cluster Separation Measures

- 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]

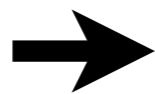
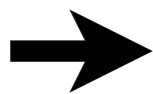
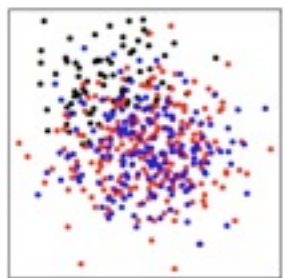


# Visual Cluster Separation Measures

- 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!



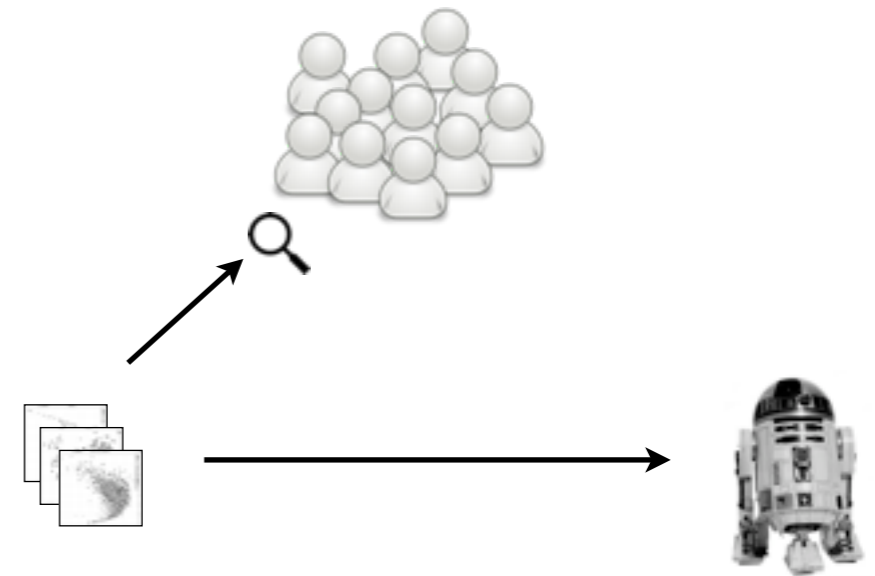
**No!**



# User vs. Data Study

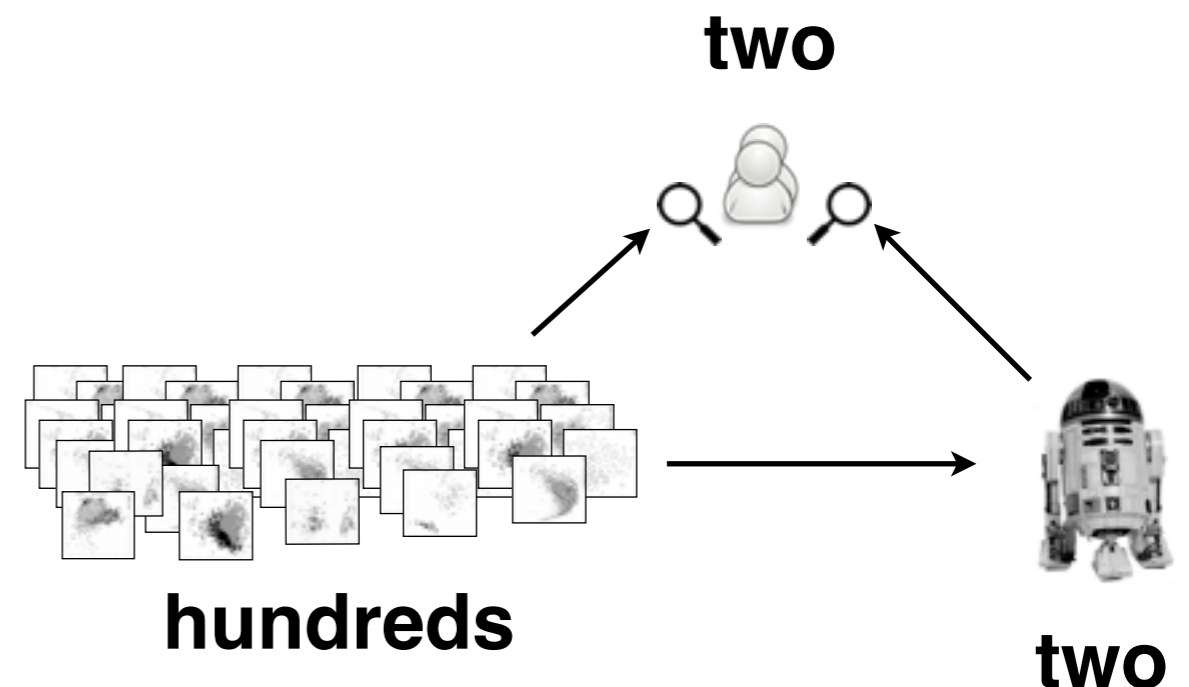
- user study

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



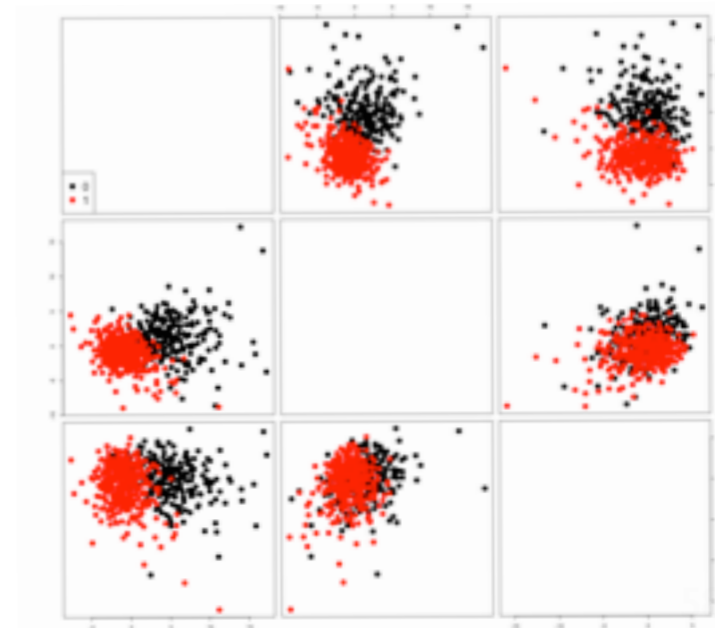
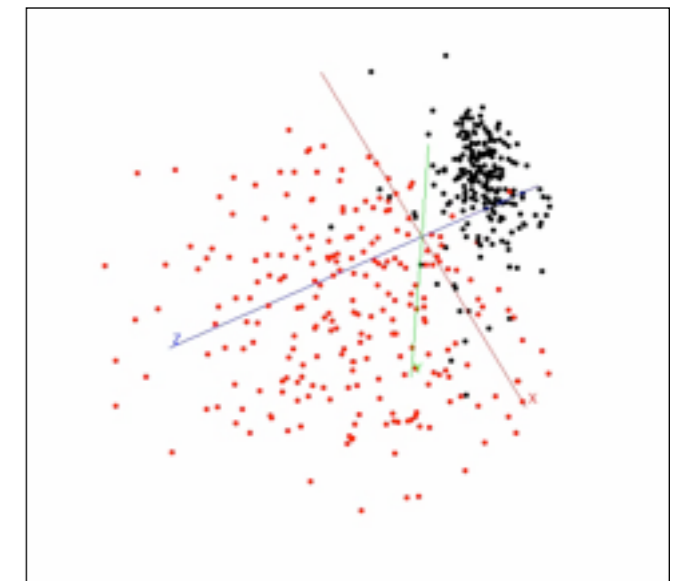
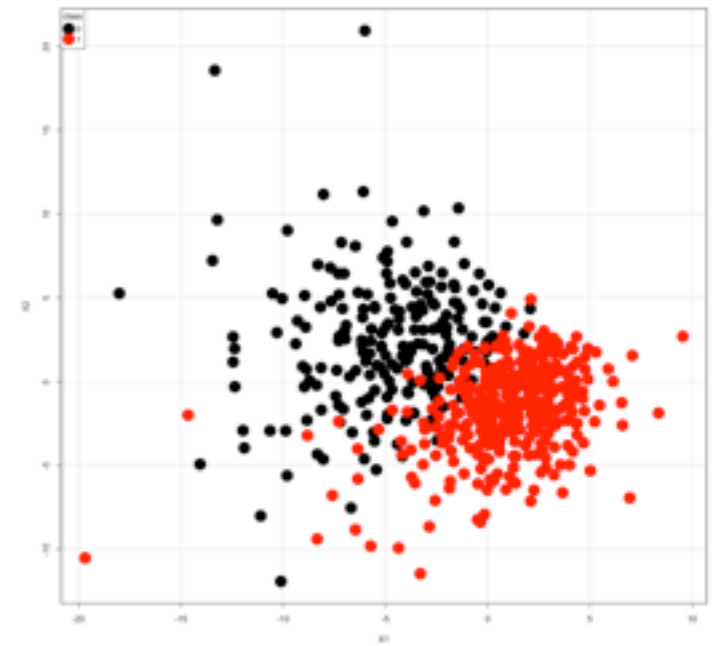
- data study

- few users, many datasets

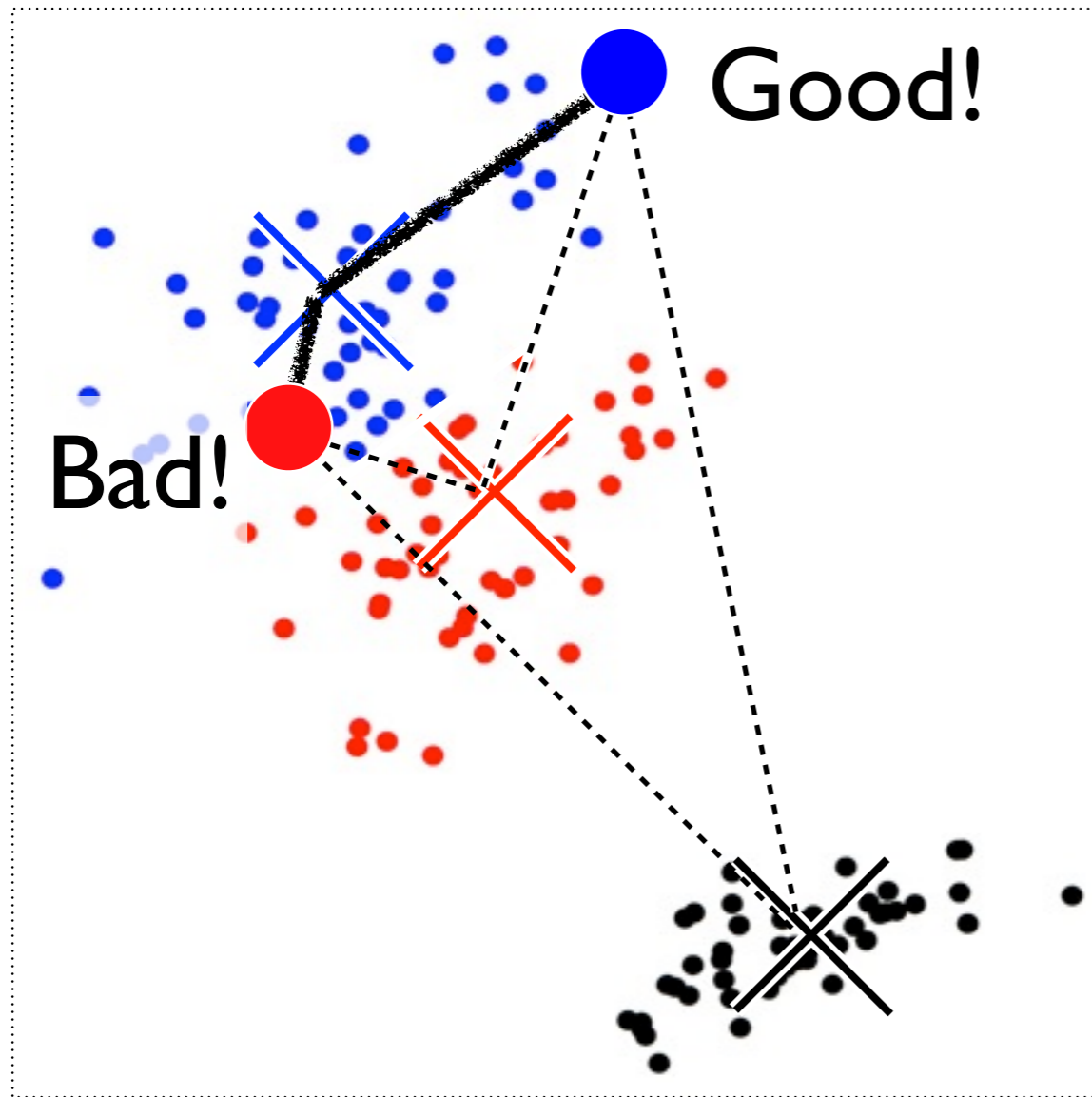


# 816 Dataset Instances

- 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

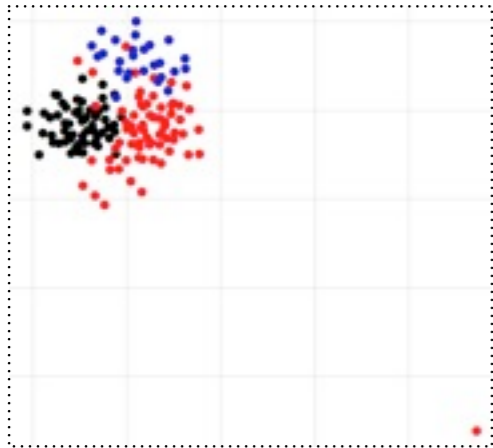
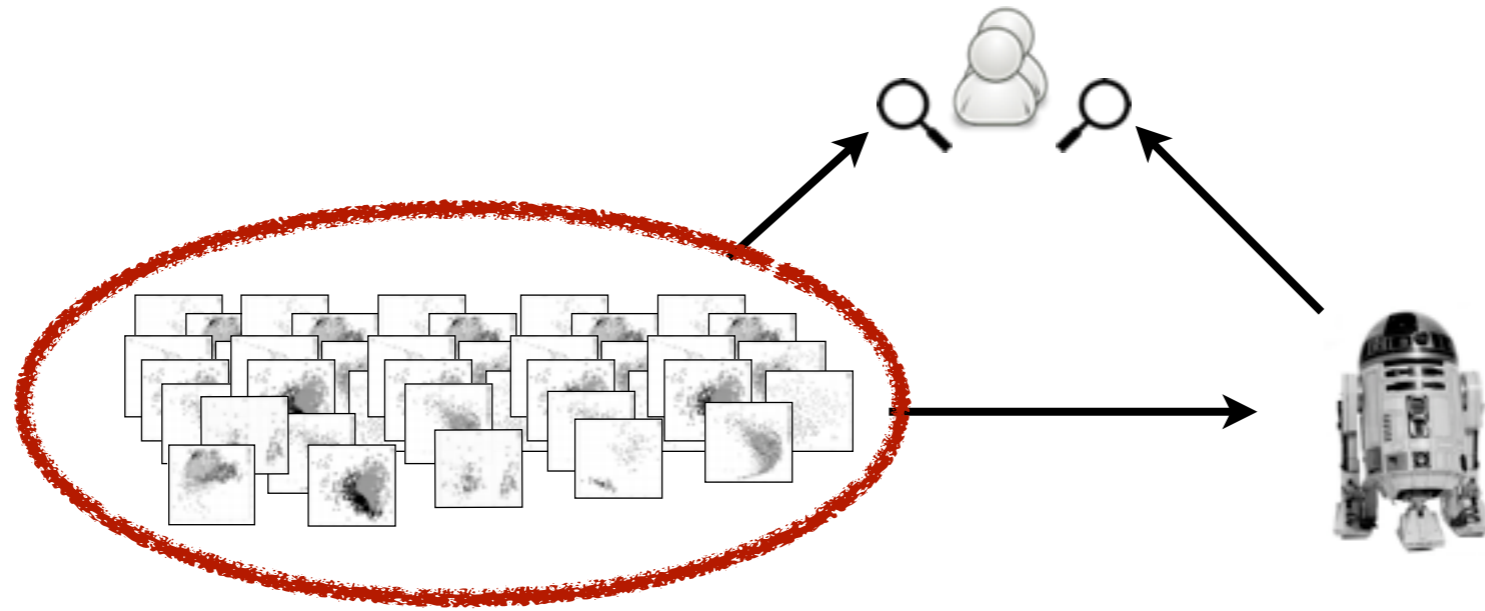
- qualitative method out of social science: coding
  - open coding: gradually build/refine code set
  - axial coding: relationships between categories

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

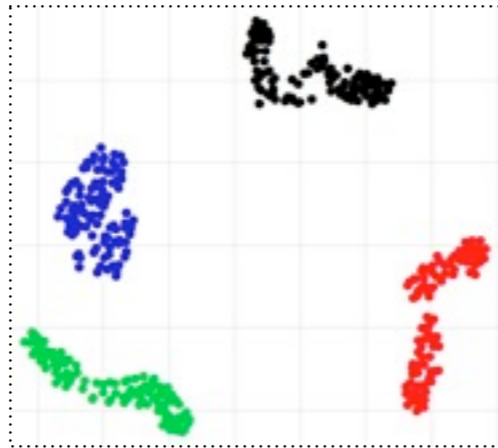
Furniss, D., Blandford, A., Curzon, P. and Mary, Q. (2011). Confessions from a grounded theory PhD: experiences and lessons learnt. *Proc. ACM CHI 2011*, p 113-122.

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

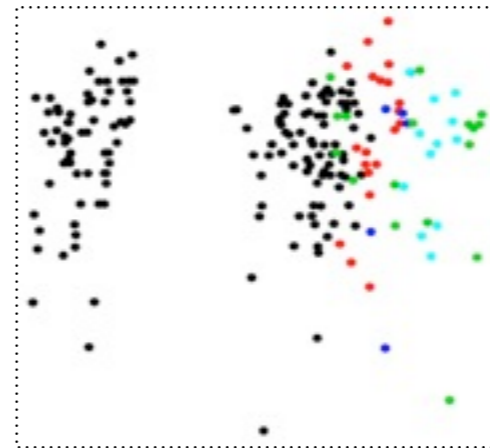
# Qualitative Analysis I: Cluster Separation Factors



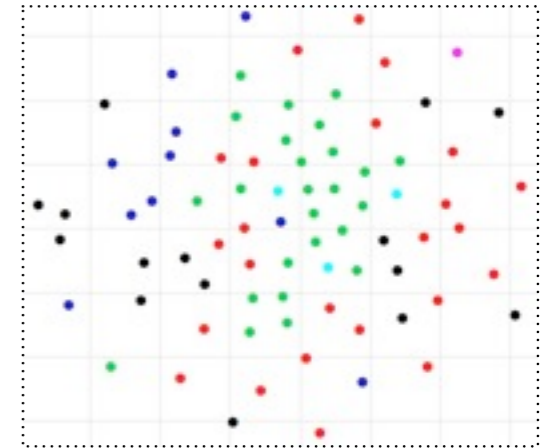
**outlier**



**shape**



**split**



**equidistant  
points**

# Analysis Approach

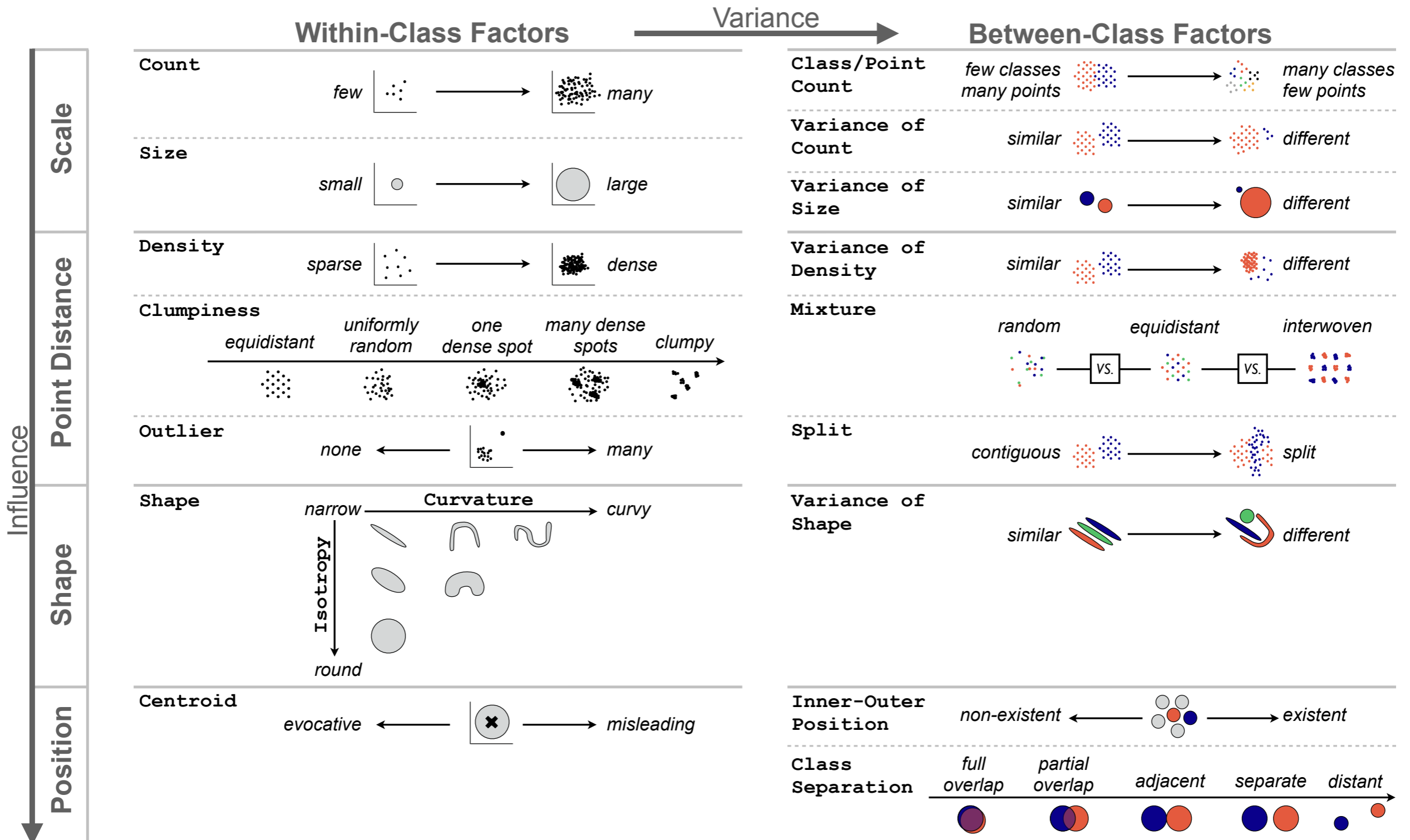
- qualitative method out of social science: coding
  - open coding: gradually build/refine code set
  - axial coding: relationships between categories

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?
- building taxonomy of factors from reasons
- mapping measure failures onto taxonomy

# A Taxonomy of Cluster Separation Factors



# High-Level Results

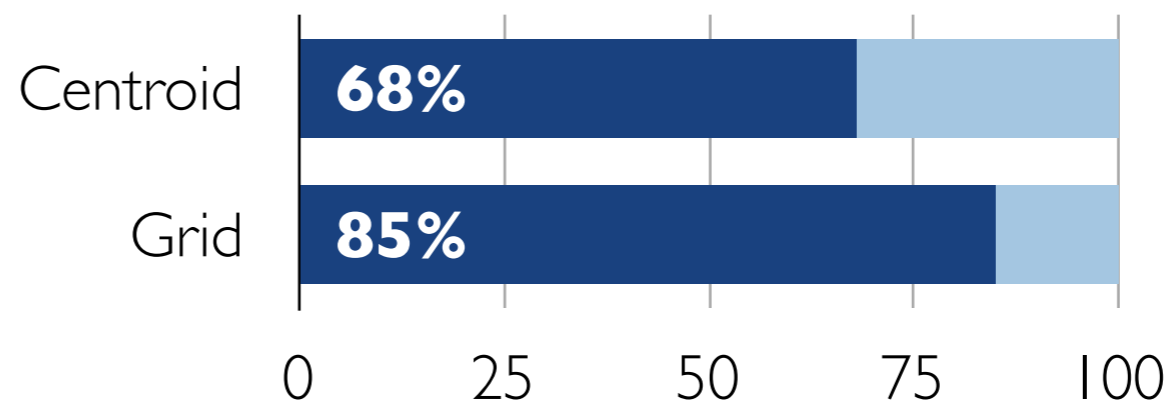
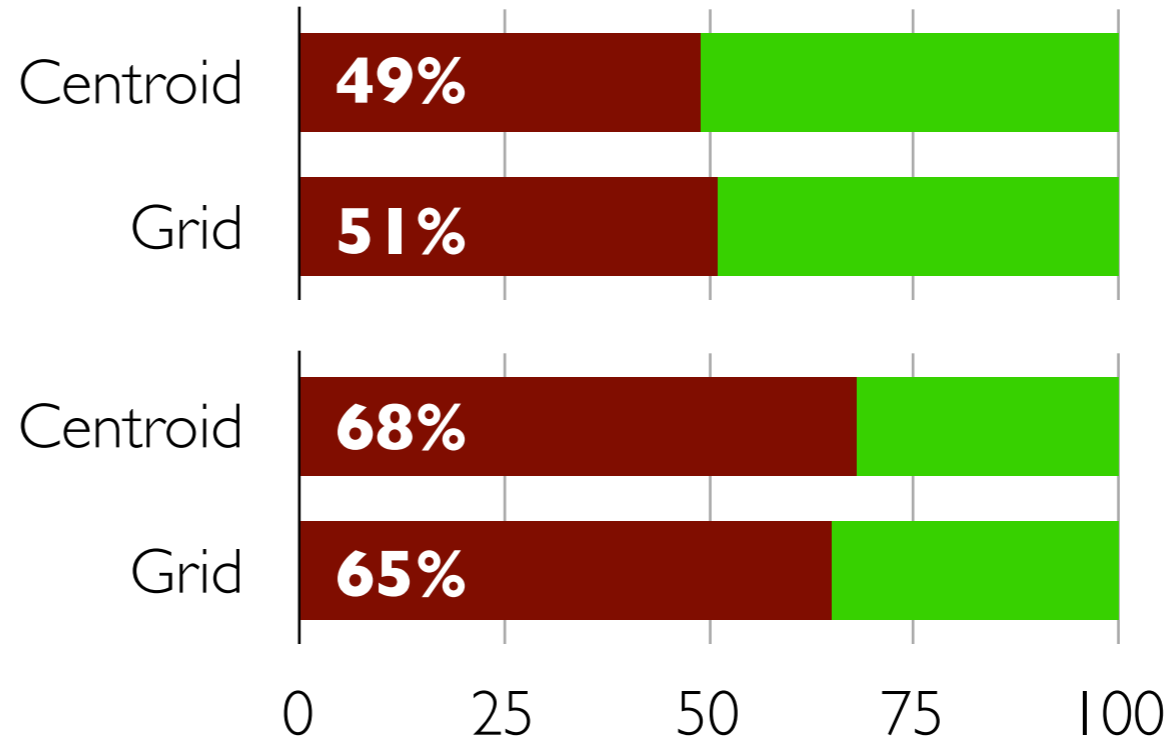


**All (816)**

**Only real (296)**



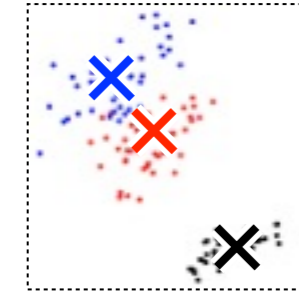
**All failure cases**





# Centroid Failure Example

- big classes overspread small ones

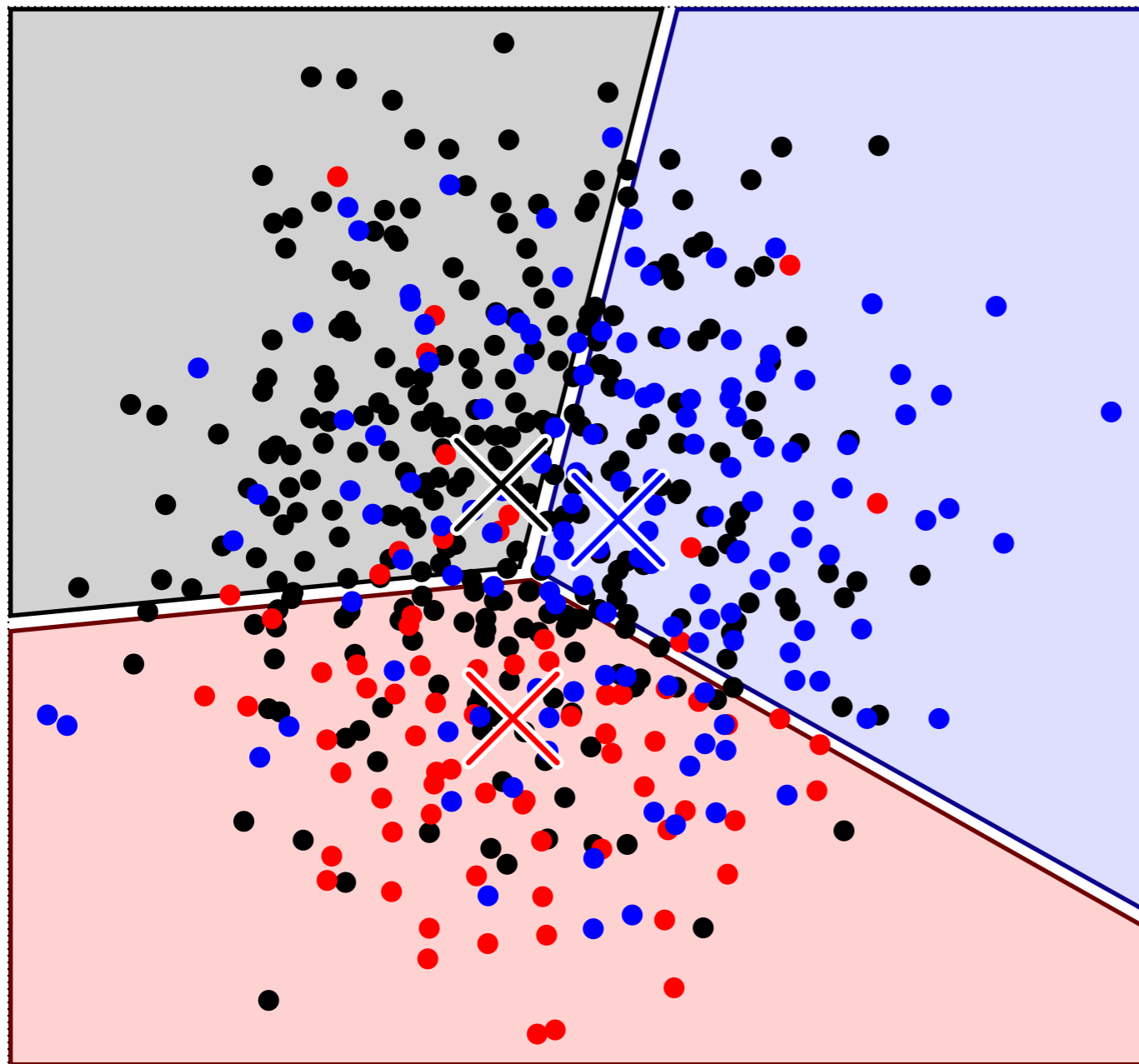


Red: **77 (Good)**

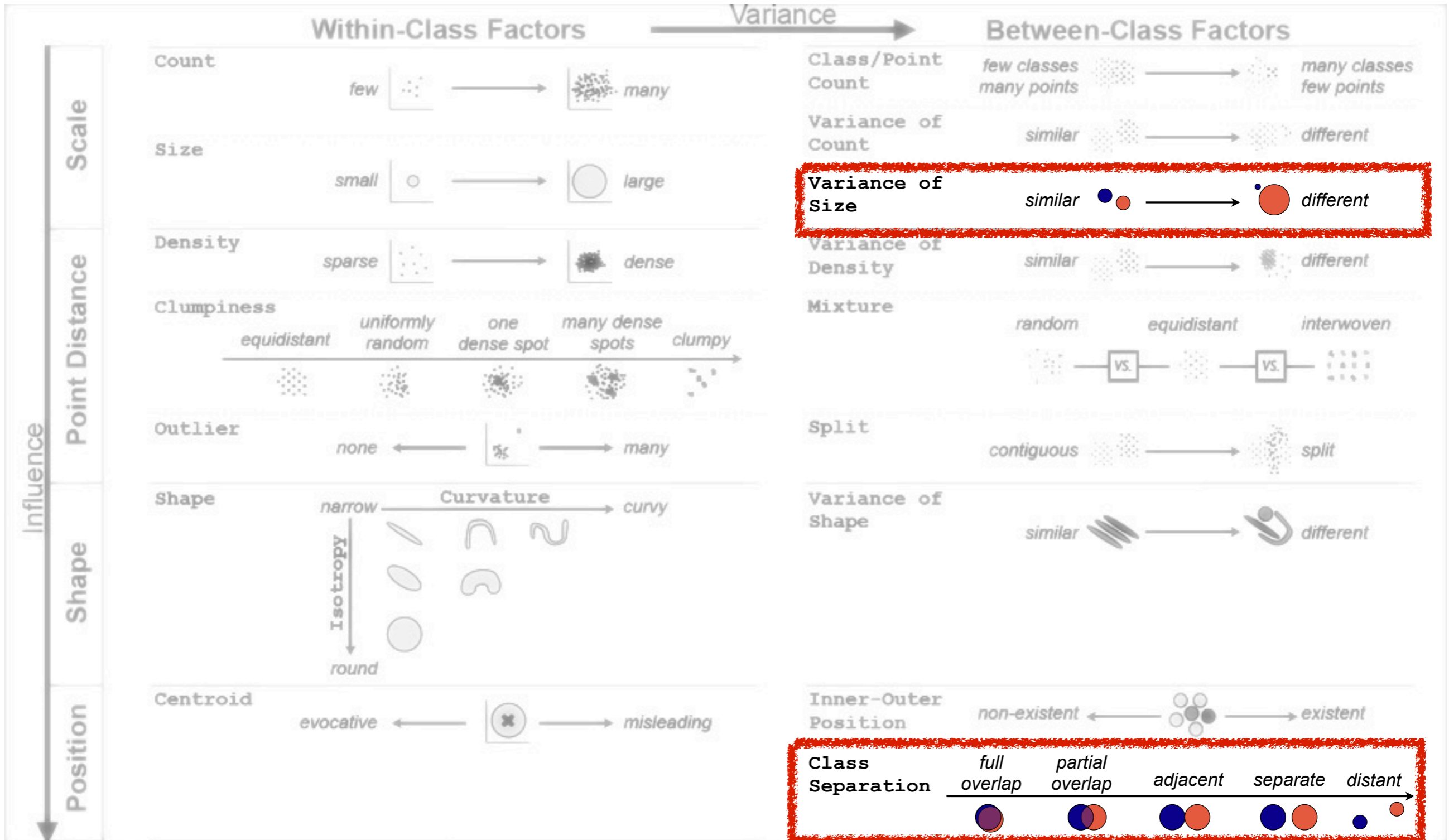
Problem: **FP**

Data: Gaussian, synthetic

DR: MDS

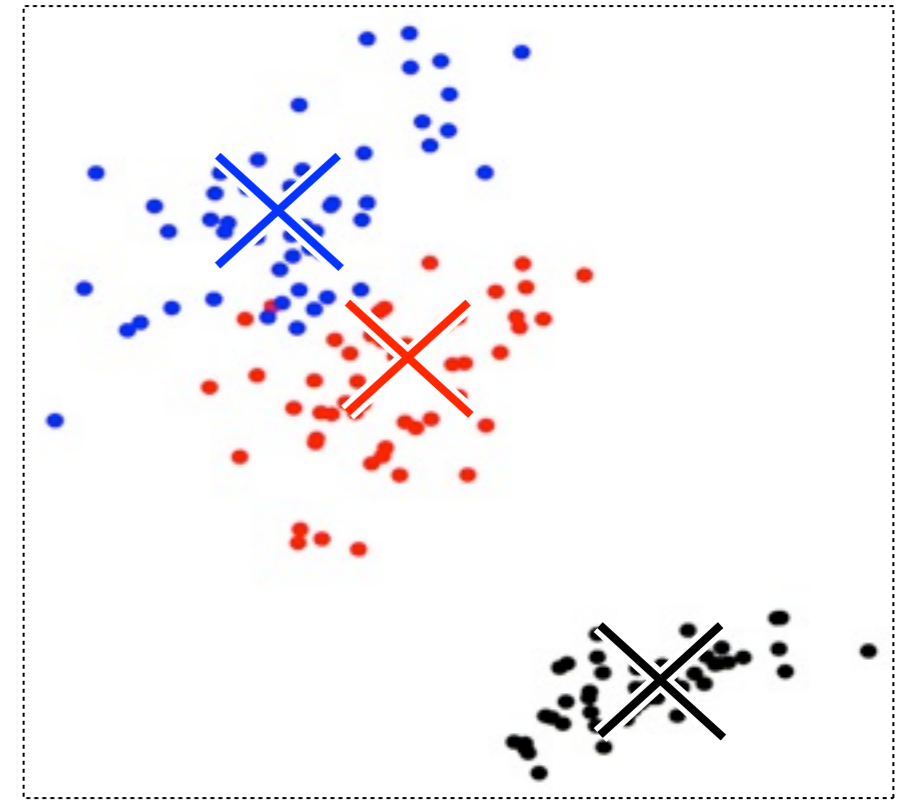


# Relevant Taxonomy Factors



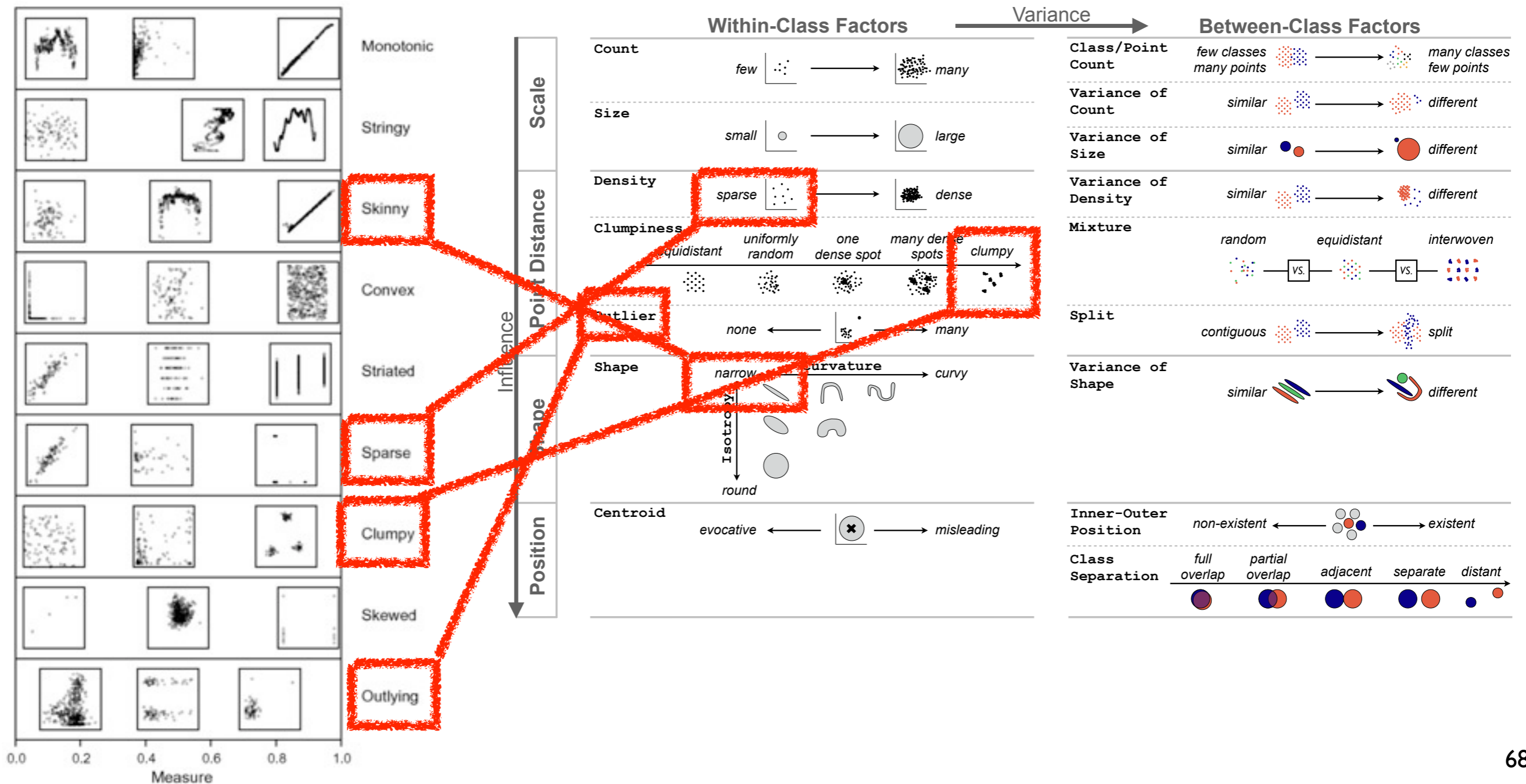
# Centroid: Mapping Assumptions Into Taxonomy

- 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*

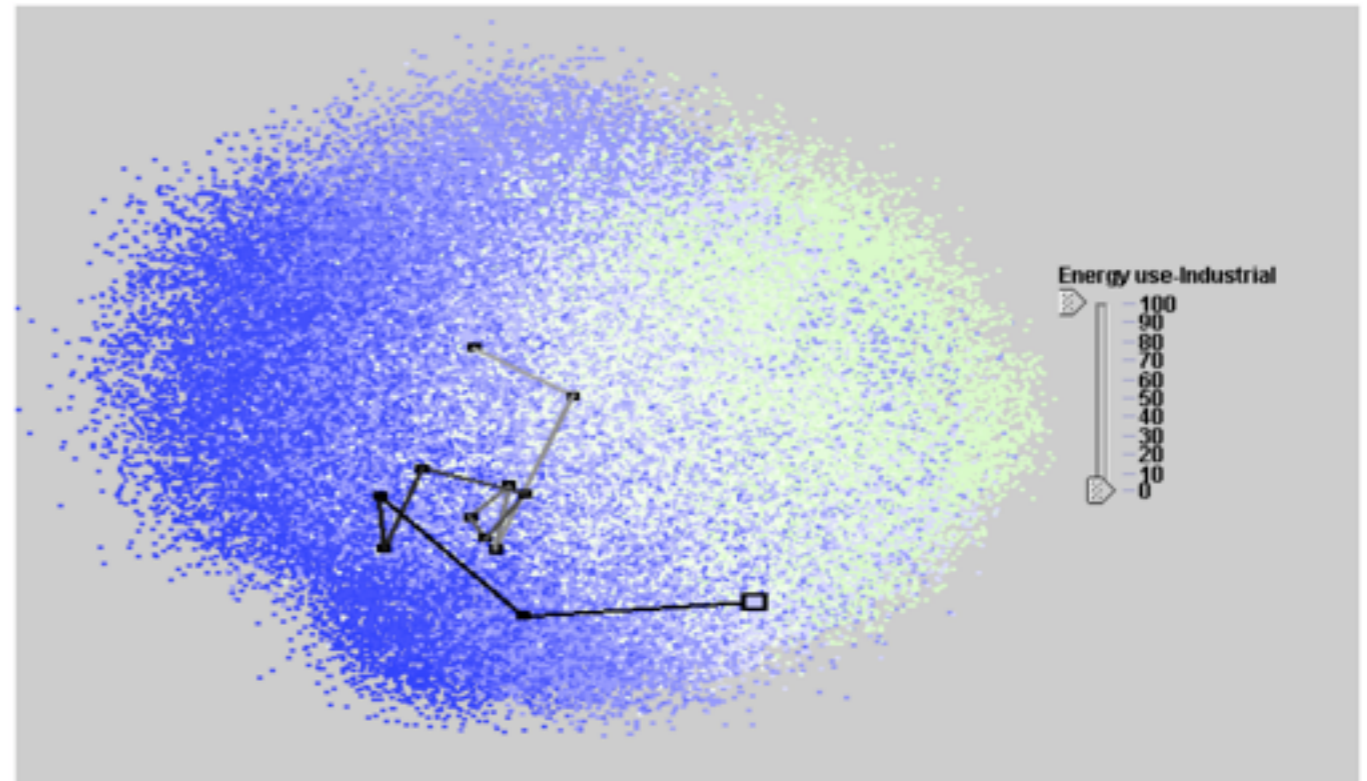
# QuestVis

*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

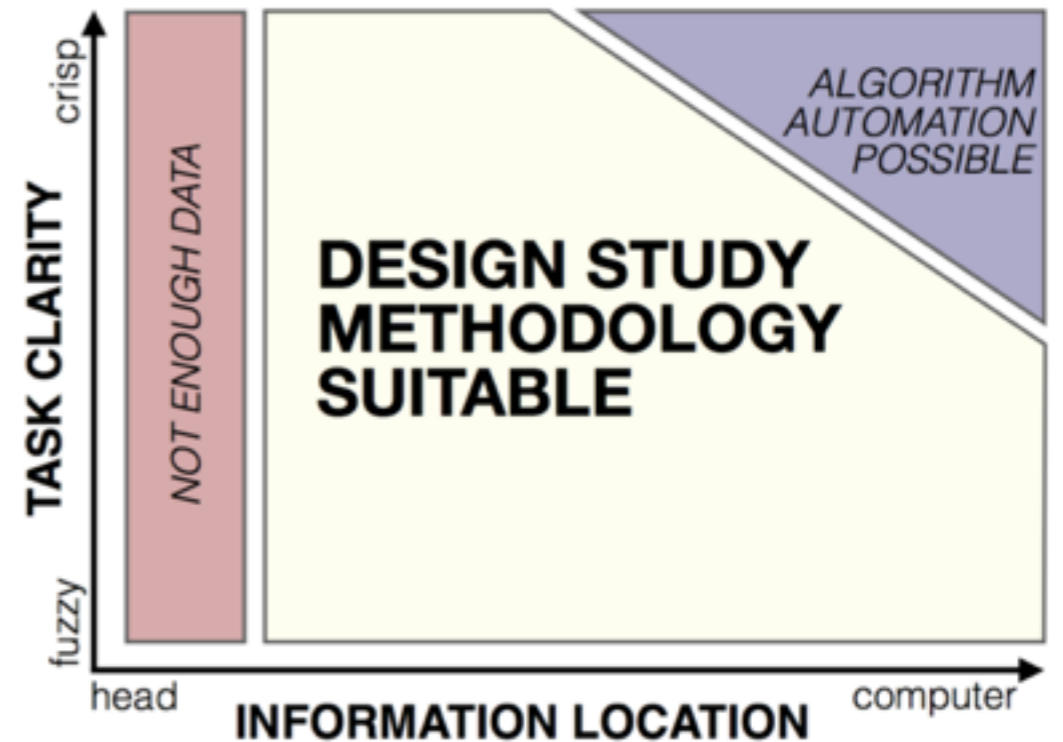
# Design Study Methodology

*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).

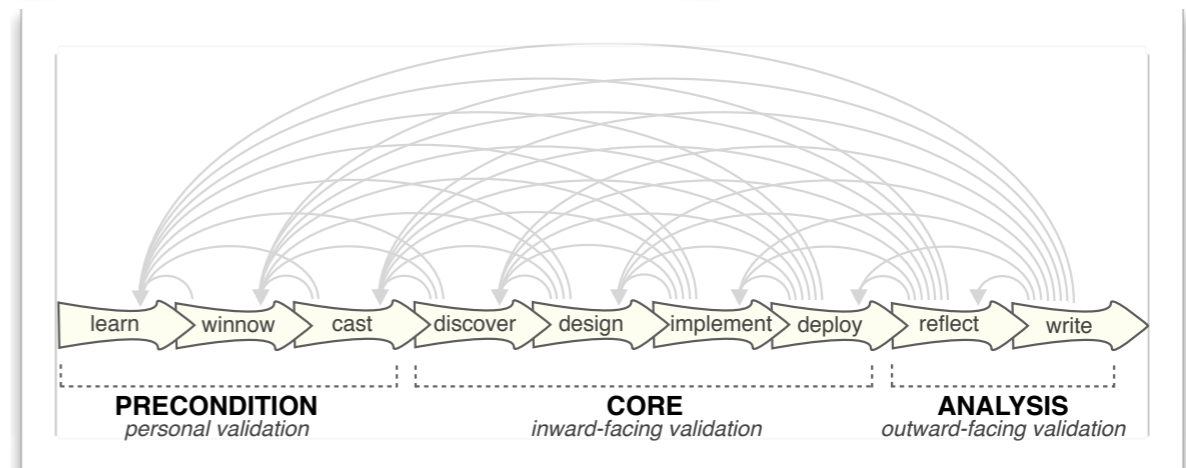
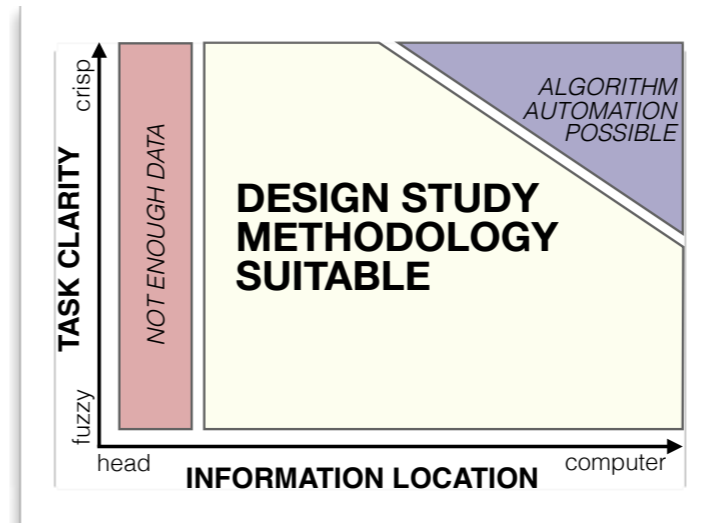
# Design Studies

- 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

problem-driven

**Must be first!**

**Am I ready?**



# 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
  - 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