Dimensionality Reduction From Three Angles

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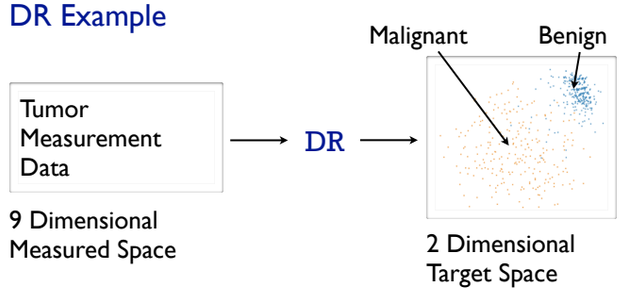
http://www.cs.ubc.ca/~tmm/talks.html#eda14

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
- what's the goal?
  - improve performance of downstream algorithm
    - avoid curse of dimensionality
  - data analysis
    - if look at the output: **visual data analysis**

DR Example



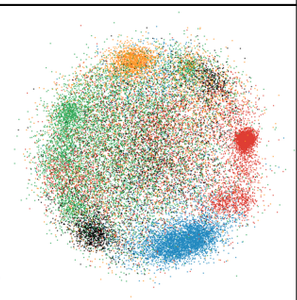
Angles of Attack

- invent algorithms
- build 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?
  - 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?



Glimmer

Multilevel MDS on the GPU

joint work with:
Stephen Ingram, Marc Olano

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

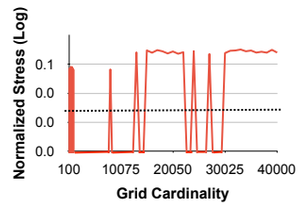
Glimmer: Multilevel MDS on the GPU.
Ingram, Munzner, Olano. IEEE TVCG 15(2):249-261, 2009.

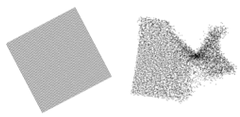
MDS: Multidimensional Scaling

- 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

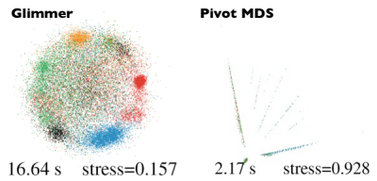


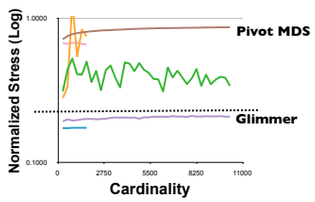


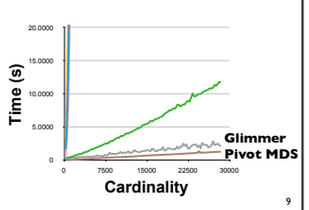
- Use as subsystem within new multilevel GPU alg with much better convergence properties

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

- quality higher
- speed equivalent

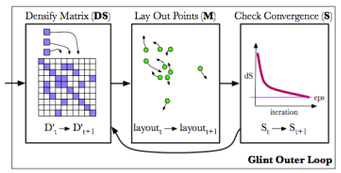






Methods and Outcomes

- 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.

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
- how should we show people DR results?

DimStiller

Workflows for Dimensional Analysis and Reduction

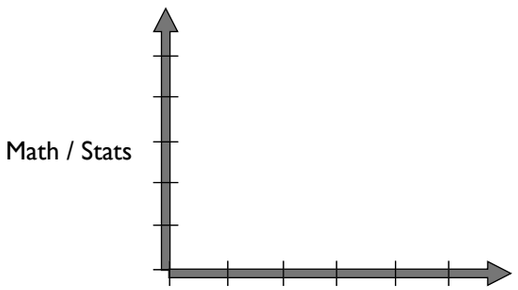
joint work with:
Stephen Ingram, Veronika Irvine, Melanie Tory, Steven Bergner, Torsten Möller

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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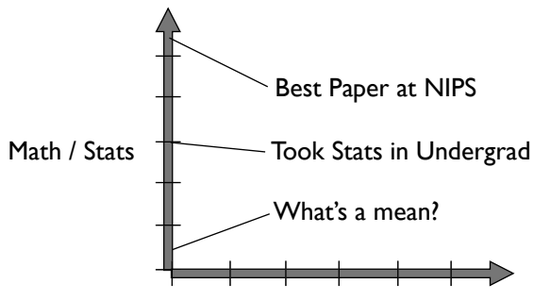

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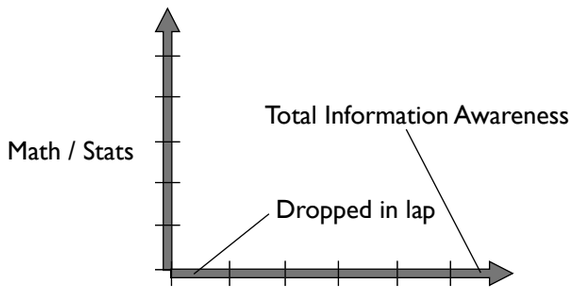

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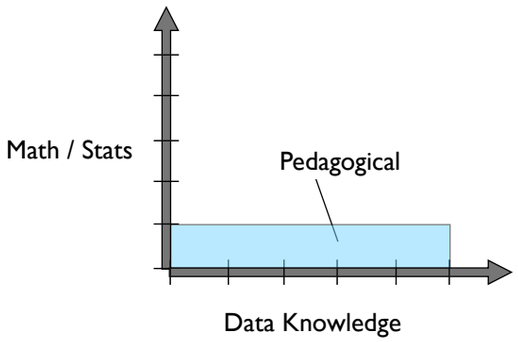

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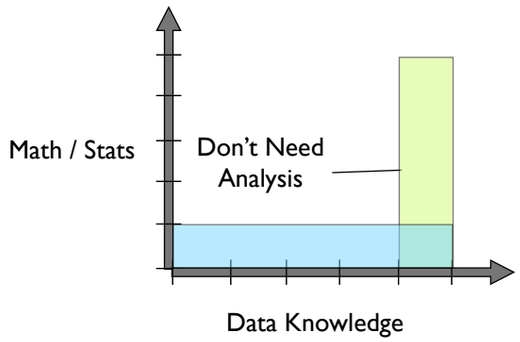

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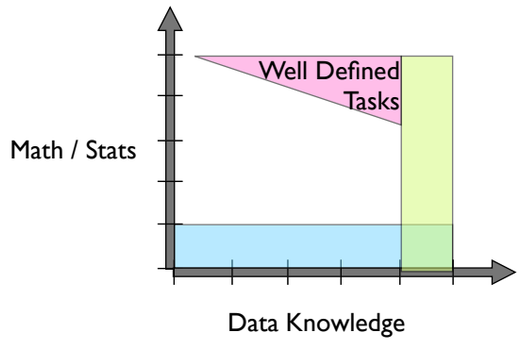
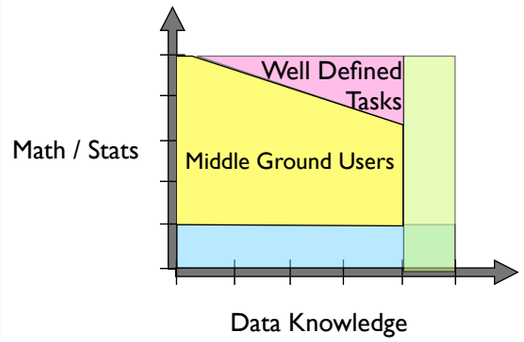
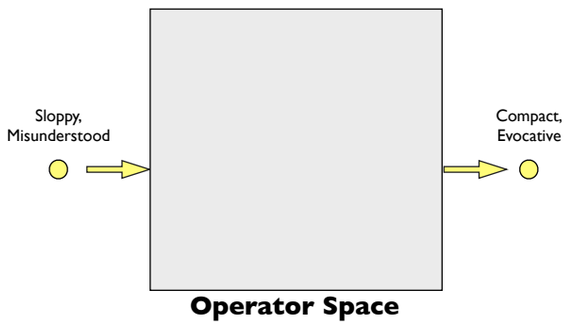


Who Might Use DR?

- middle ground users benefit from guidance



Global Guidance



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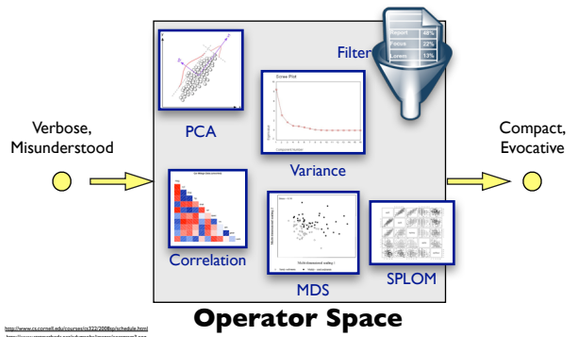
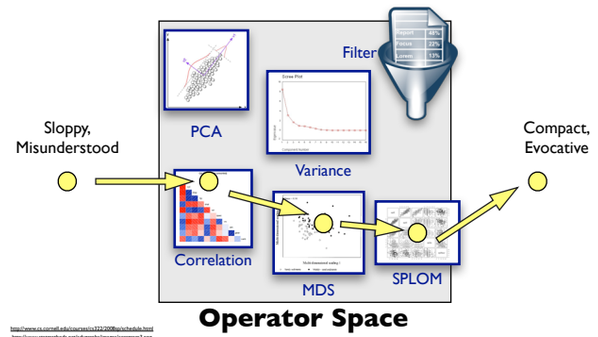
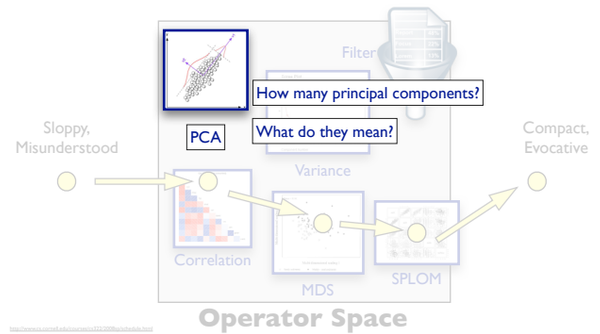


Global Guidance

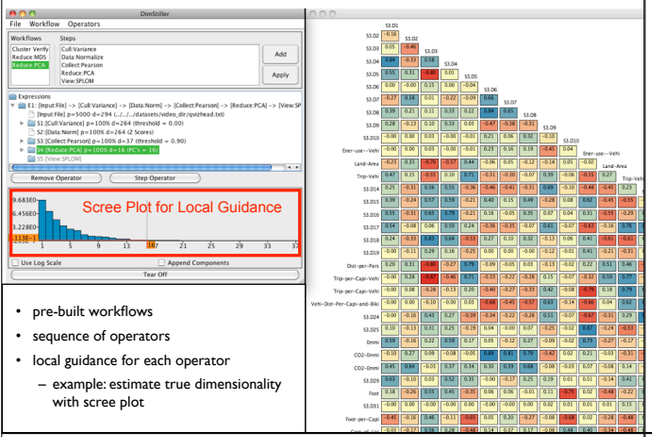
- which operations and in which order?



Local Guidance



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 field study 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 metric developers wrt human perception: Visual Cluster Separation Factors
  - (for system developers: Scatterplot and DR Technique Choices)
  - (visual encoding guidance for system developers: Points vs Landscapes)

A Taxonomy of

Visual Cluster Separation Factors

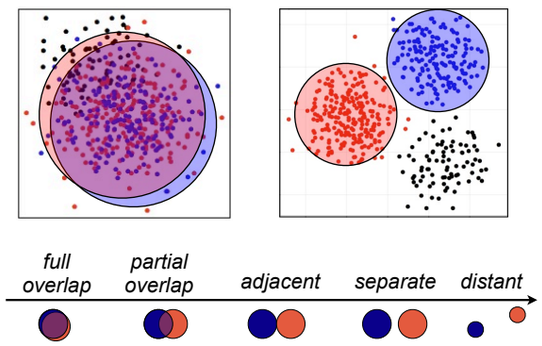
joint work with:
Michael Sedlmair, Andrada Tatu, Melanie Tory

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

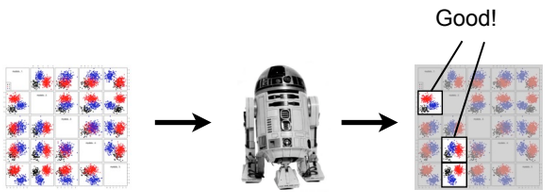


Visual Cluster Separation Measures

- 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]

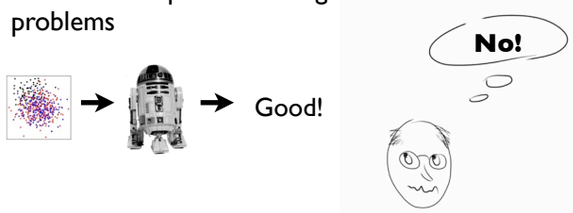


Visual Cluster Separation Measures

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

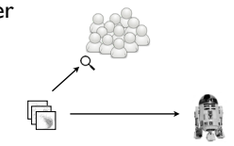
Tatu et al.: Visual quality metrics and human perception: an initial study on 2D projections of large multidimensional data [AVI 2010]

- but our attempt to use for guidance showed problems

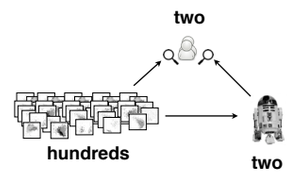


User vs. Data Study

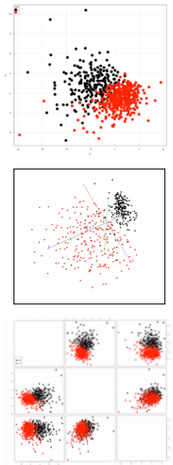
- user study
  - previous work on validating cluster measures
  - many users, few datasets
  - missing: dataset variety



- 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

Analysis Approach

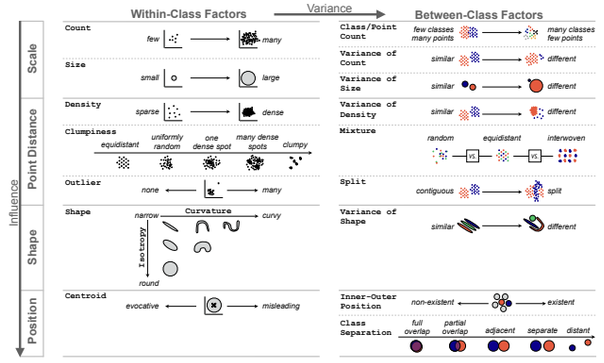
- qualitative method out of social science: coding
  - open coding: gradually build/refine code set
  - axial coding: relationships between categories

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

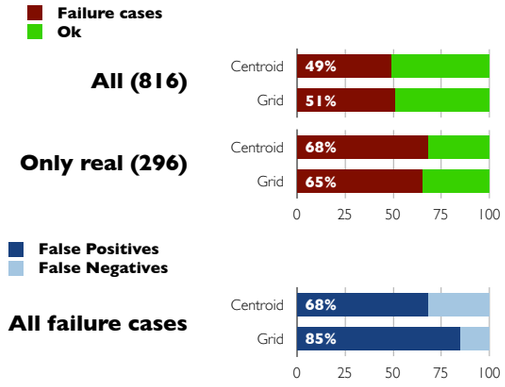
Furniss, D., Blandford, A., Curzon, P. and Mary, Q. (2011). Confessions from a grounded theory PhD: experiences and lessons learnt. Proc. ACM CHI 2011, p 113-122.

- 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

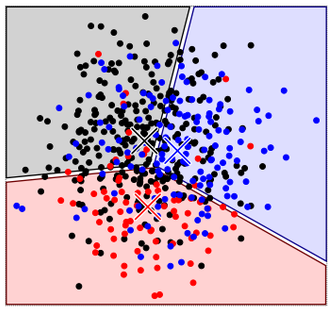


High-Level Results



Centroid Failure Example

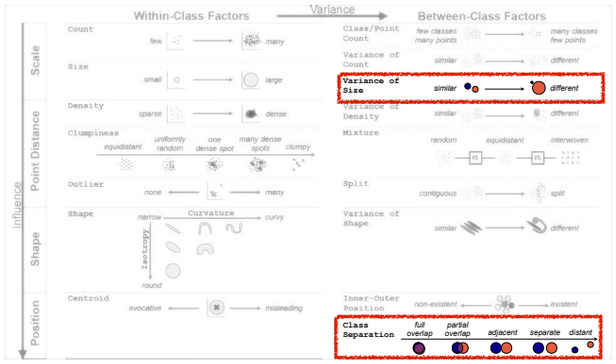
- big classes overspread small ones



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

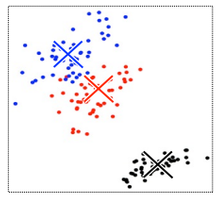
Data: Gaussian, synthetic
DR: MDS

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



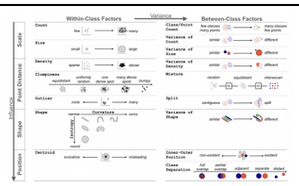
- rarely true for real datasets

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

Empirical Guidance on

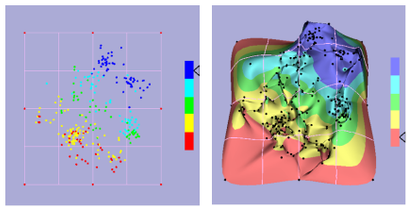
Scatterplot and Dimension Reduction Technique Choices



joint work with:
Michael Sedlmair, Melanie Tory

http://www.cs.ubc.ca/labs/imager/tr/2013/ScatterplotEval/

Empirical Guidance on Scatterplot and Dimension Reduction Technique Choices.
Sedlmair, Munzner, Tory. IEEE TVCG 19(12):2634-2643 (Proc. InfoVis 2013).



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).

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?
  - elsewhere: continue figuring out what people need
- (when do people need to use DR?)

Work in Progress

- DR in the Wild
  - multi-year cross-domain qualitative field study
- 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, deployed, adopted
    - ending point: stay tuned...

Conclusions

- cross-fertilization from attacking DR through different methodological angles
  - scratching own itches to find high-impact problems
    - 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
  - this talk: http://www.cs.ubc.ca/~tmm/talks.html#eda14
  - long version: http://www.cs.ubc.ca/~tmm/talks.html#utah13
  - http://www.cs.ubc.ca/group/infovis
    - papers, videos, open-source software (including Glimmer and DimStiller)
- acknowledgements
  - funding: NSERC Strategic Grant
  - joint work: all collaborators
    - Steven Bergner, Matthew Brehmer, Stephen Ingram, Veronika Irvine, Torsten Möller, Marc Olano, Michael Sedlmair, Andrada Tatu
  - 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 postdoc soon
  - http://www.cs.ubc.ca/~sfingram
  - available for hacker-analyst job in industry or research lab
    - in fall 2014 after postdoc