

معهد قطر لبحوث الحوسبة Qatar Computing Research Institute Member of Qatar Joundation مضوفي مؤسسة قطر

Reflections on Dimensionality Reduction for Visual Analytics: strengths, weaknesses and perspectives

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Joint work with: L. Allano, I. Espagnon, J.-D. Fekete, N. Heulot, S. Lespinats, H. Meyer-Baese, G. Sannie

Mascot-Num –Visualization methods for uncertainty studies – Institut Henri Poincare, Paris, May 22, 2017



• What is Dimensionality Reduction



- What is Dimensionality Reduction
- Strengths



- What is Dimensionality Reduction
- Strengths
- Weaknesses



- What is Dimensionality Reduction
- Strengths
- Weaknesses
- Turning weaknesses into strengths



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- Conclusion



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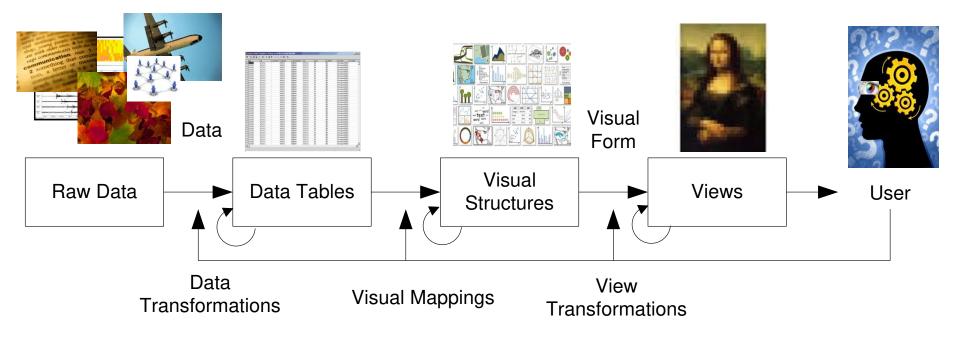


What is Dimensionality Reduction

- Strengths
- Weaknesses
- Turning weaknesses into strengths
- Conclusion
- Perspectives



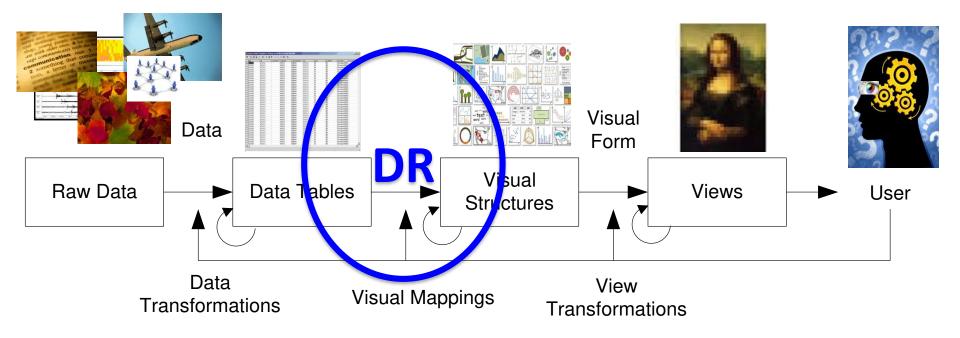
• DR in the visualization pipeline



S.K. Card, J. Mackinlay, B. Shneiderman, Information Visualization Readings in Information Visualization: Using Vision to Think. Morgan Kaufman 1998.



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• Data table

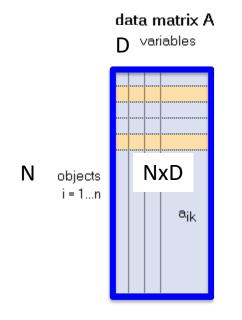
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	M5	0.8	4g	5	Round	\$13.89	Yes	183	Both	value
	M6	1	5g	6	Button	\$10.42	Yes	1043	Flat	
	M8	1.25	5g	8	Pan	\$11.98	No	298	Phillips	
	M10	1.5	6g	10	Round	\$16.74	Yes	488	Phillips	
	M12	1.75	7g	12	Pan	\$18.26	No	998	Flat	
	M14	2	7g	14	Rouna	\$21.19	No	235	Phillips	(item)
	M16	2	8g	16	Button	\$23.57	Yes	292	Both	(item)
	M18	2.1	8g	18	Button	\$25.87	No	664	Both	
	M20	2.4	8g	20	Pan	\$29.09	Yes	486	Both	
	M24	2.55	9g	24	Round	\$33.01	Yes	982	Phillips	
	M28	2.7	10g	28	Button	\$35.66	No	1067	Phillips	
	M36	3.2	12g	36	Pan	\$41.32	No	434	Both	
	M50	4.5	15g	50	Pan	\$44.72	No	740	Flat	



ce

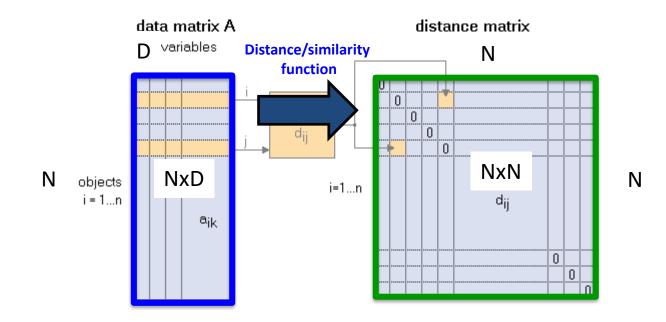


• From data table to similarity matrix



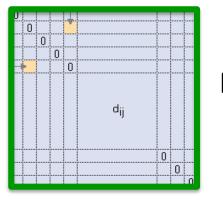


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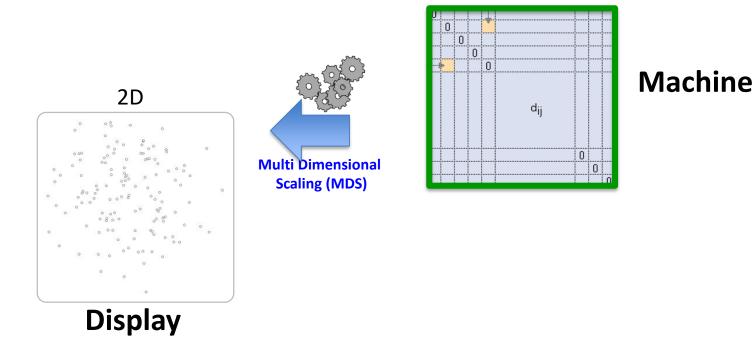


• From similarity matrix to scatterplot

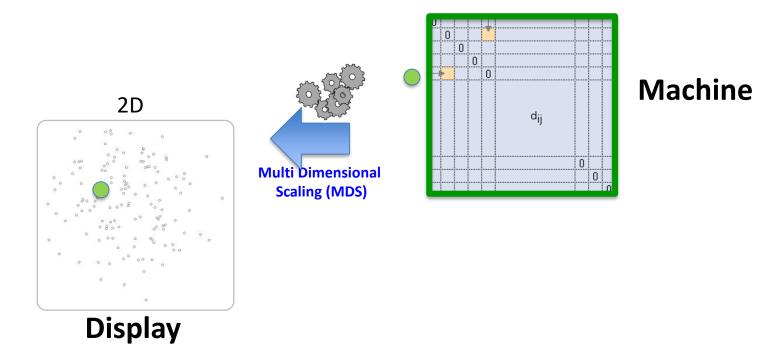


Machine

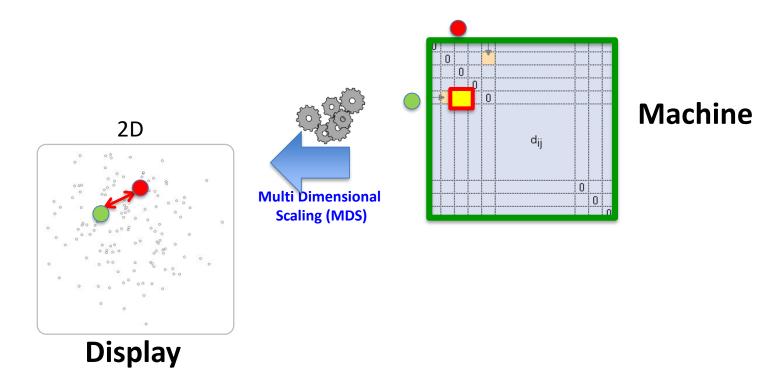




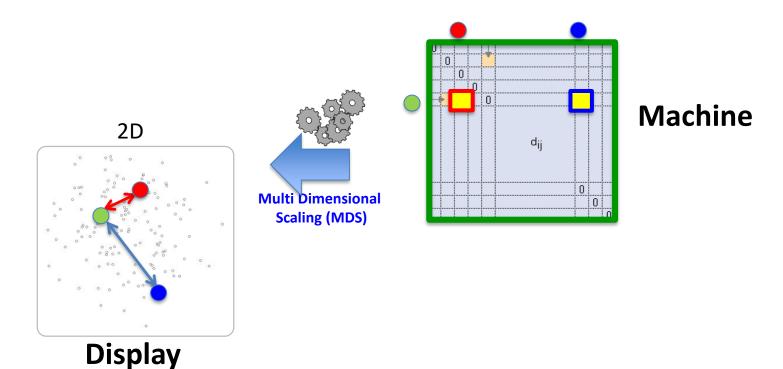










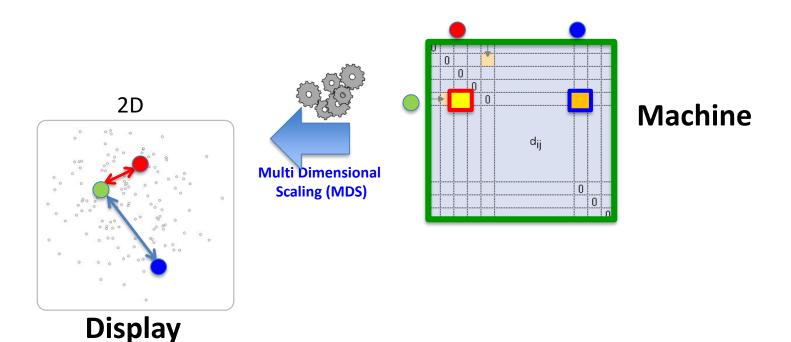




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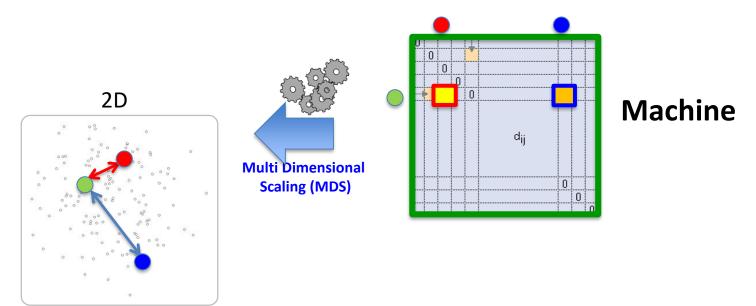


Benefits from Gestalt law of proximity





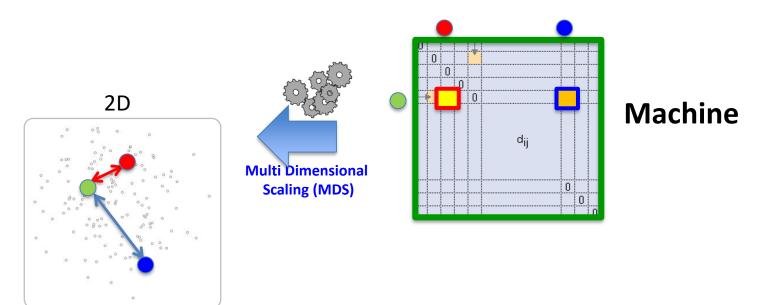
- Benefits from Gestalt law of proximity
 - spatial proximity => items **belong to same group**



Display



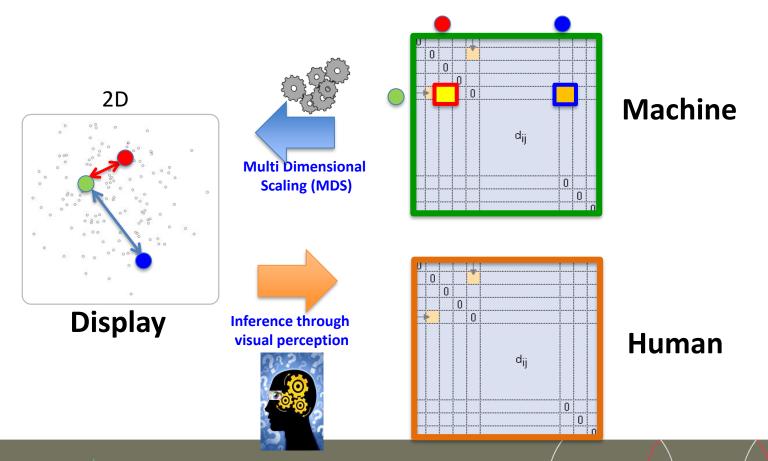
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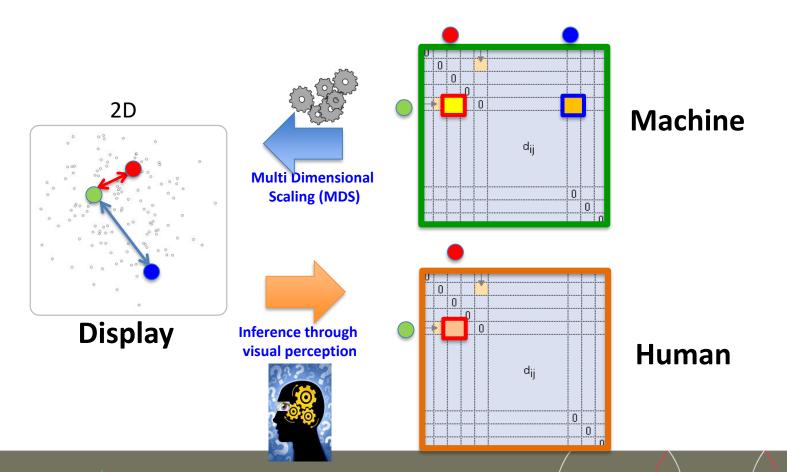


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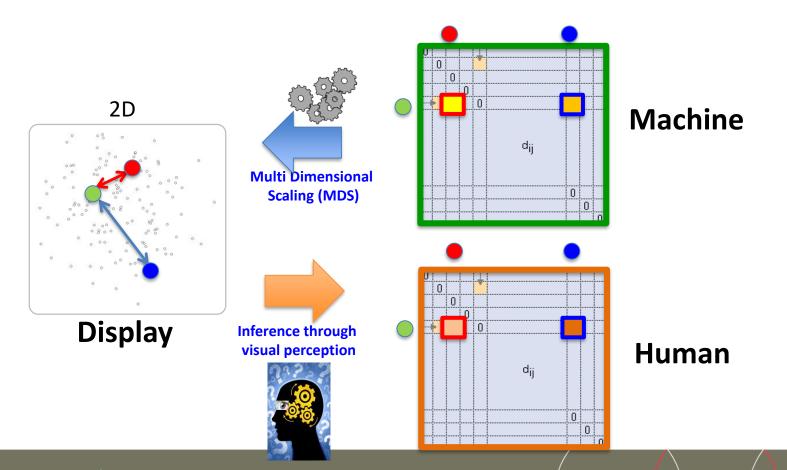


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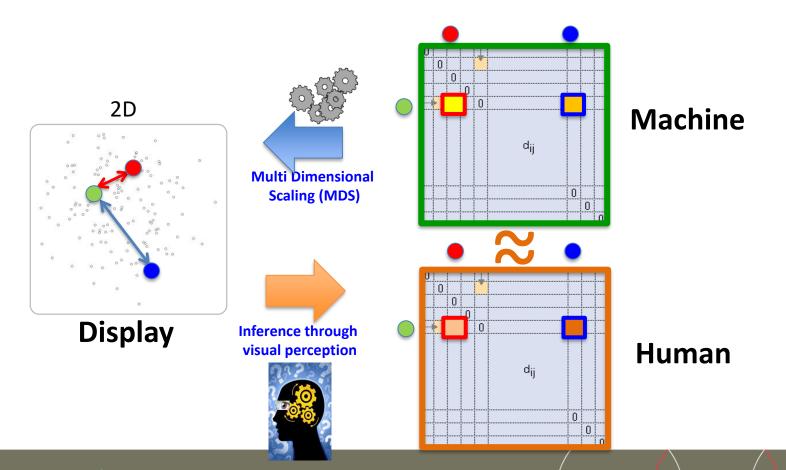


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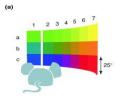
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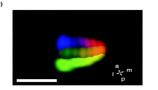


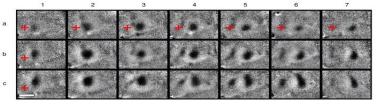




• Mammals' brains organize **similarities** to build **maps**



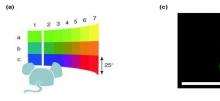


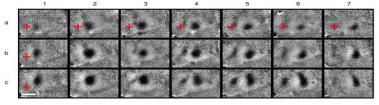


Retinotopic map of a mouse [Hübener 2003]



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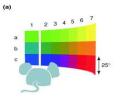


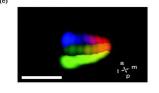
Retinotopic map of a mouse [Hübener 2003]

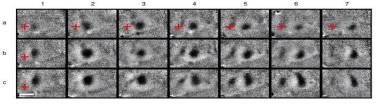
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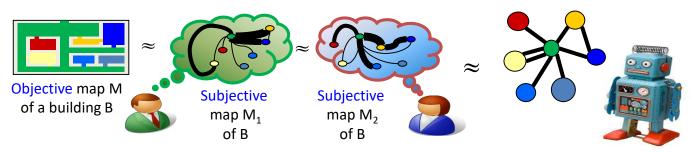






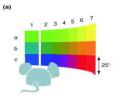
Retinotopic map of a mouse [Hübener 2003]

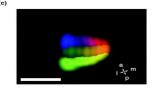
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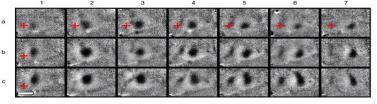




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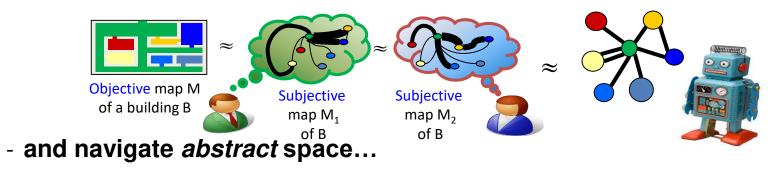






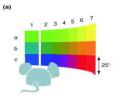
Retinotopic map of a mouse [Hübener 2003]

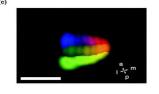
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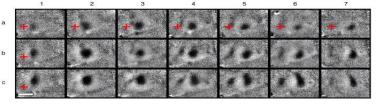




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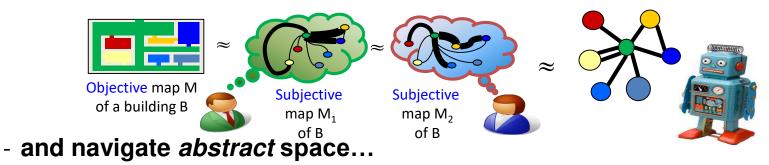






Retinotopic map of a mouse [Hübener 2003]

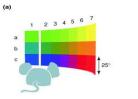
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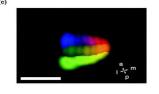


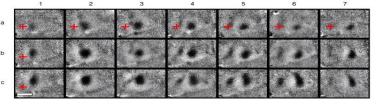
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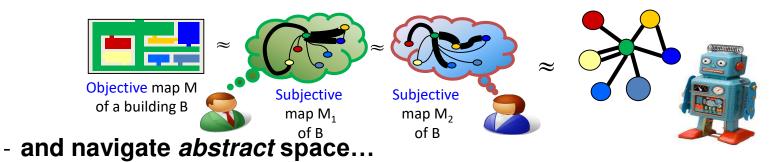






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Teleraedthsiaaealtgseslsolnhsparynetimikwyetrsneny

These letters make sense only *spatially arranged* in this way



• Correlation between spatial arrangement and additional information is crucial



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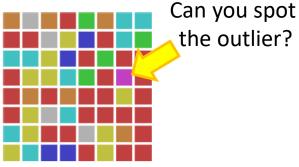




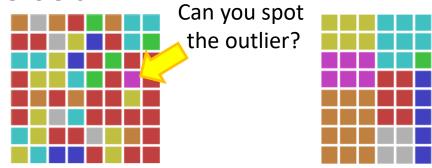
• Correlation between spatial arrangement and additional information is crucial

Can you spot the outlier?

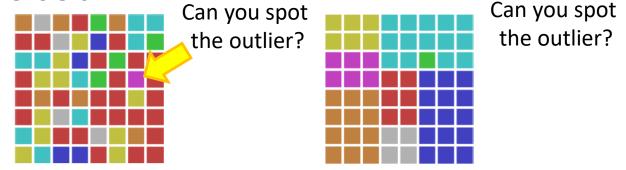




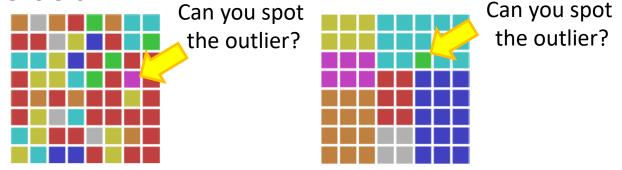




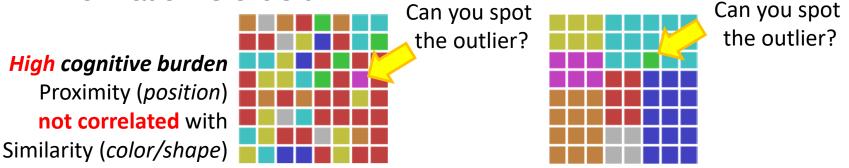




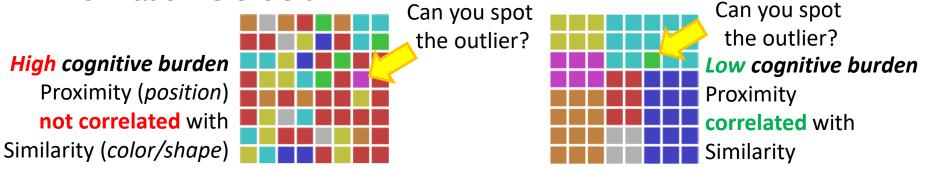










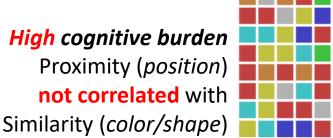




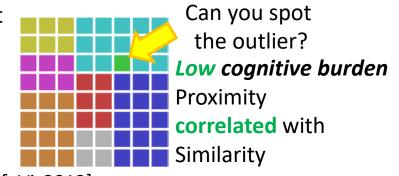




Correlation between spatial arrangement and additional information is crucial



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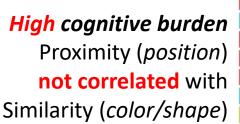


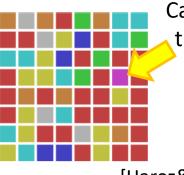
[Haroz&Whitney, InfoVis2012]

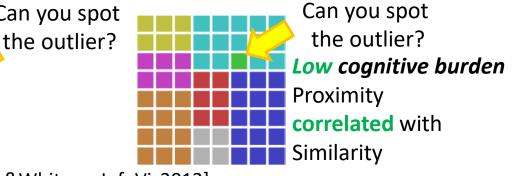




Correlation between spatial arrangement and additional information is crucial
 Can you spot
 Can you spot







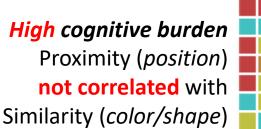
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Error in Position? or error in Color?

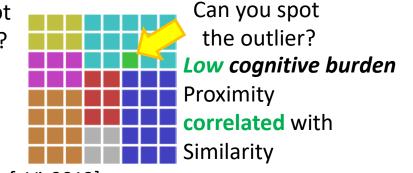




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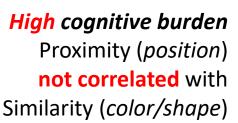
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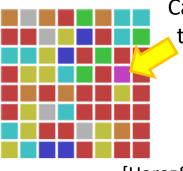
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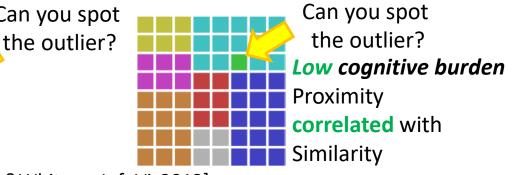




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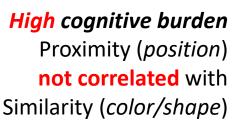
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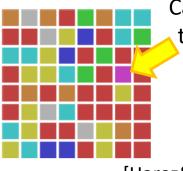






Correlation between spatial arrangement and additional information is crucial
 Can you spot
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Can you spot the outlier?

[Haroz&Whitney, InfoVis2012]

Error in *Position?* or error in *Color?*





Position and Color are coherent with external information

the outlier?

correlated with

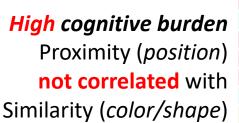
Proximity

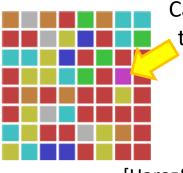
Similarity

Low cognitive burden



Correlation between spatial arrangement and additional information is crucial
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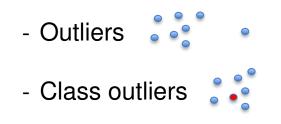




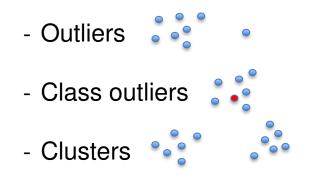
Many interesting (abstract) patterns are similarity-based

- Outliers

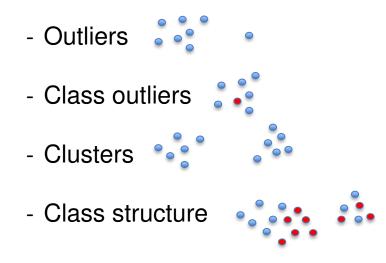




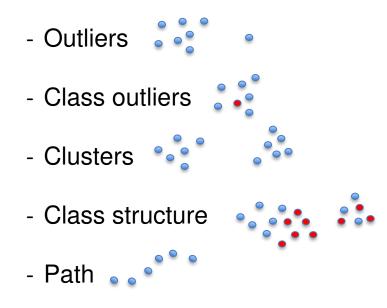






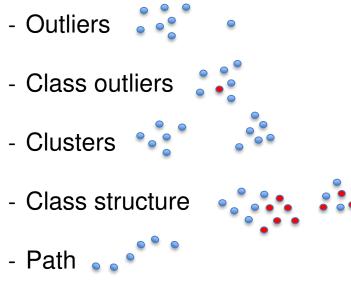








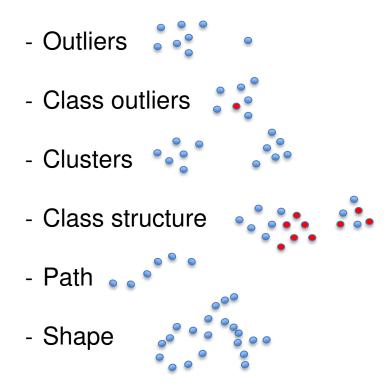
Many interesting (abstract) patterns are similarity-based



- Shape



Many interesting (abstract) patterns are similarity-based



• DR preserve similarities so is likley to preserve these patterns



Outline

- What is Dimensionality Reduction
- Strengths

Weaknesses

- Turning weaknesses into strengths
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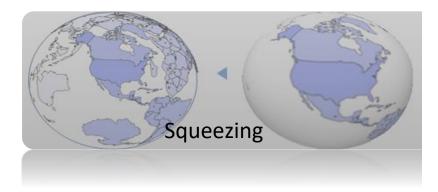


Mapping distortions prevent perfect similarity preserving





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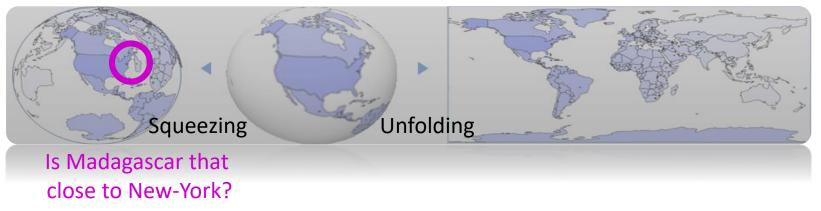
False neighbors





Mapping distortions prevent perfect similarity preserving

False neighbors

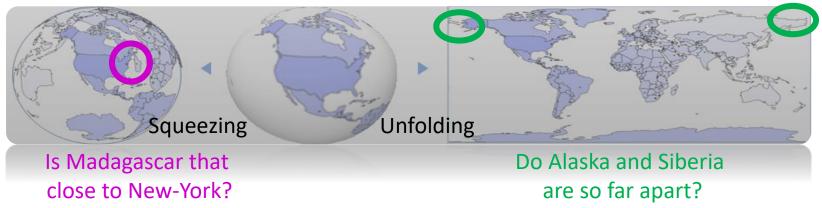




Mapping distortions prevent perfect similarity preserving

False neighbors

Missed neighbors

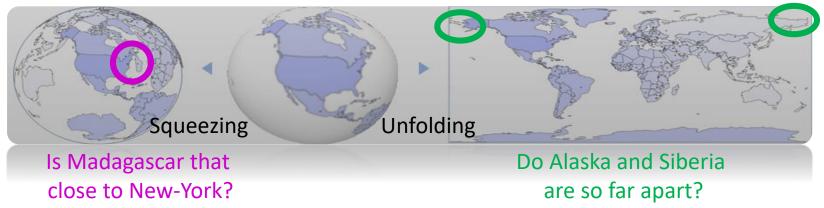


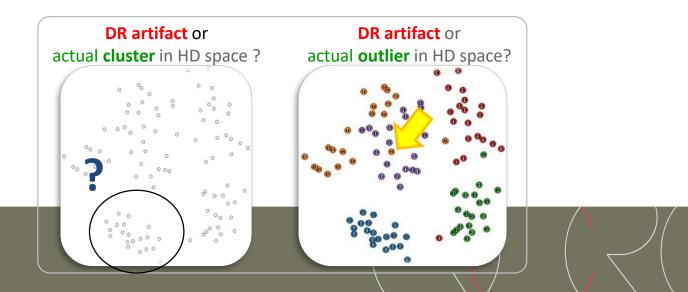


Mapping distortions prevent perfect similarity preserving

False neighbors

Missed neighbors







Mapping distortions prevent perfect similarity preserving



- Mapping distortions prevent perfect similarity preserving
- Inference of HD patterns from 2D ones very likely to be wrong



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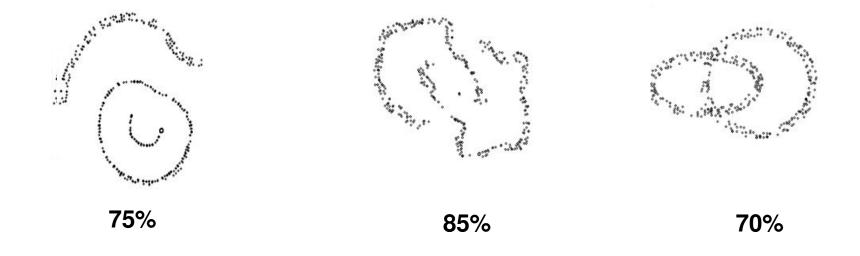
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 - reduced
 - or overcome



• Displaying map accuracy as a number





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70%

- Support selection of the most accurate map



• Displaying map accuracy as a number



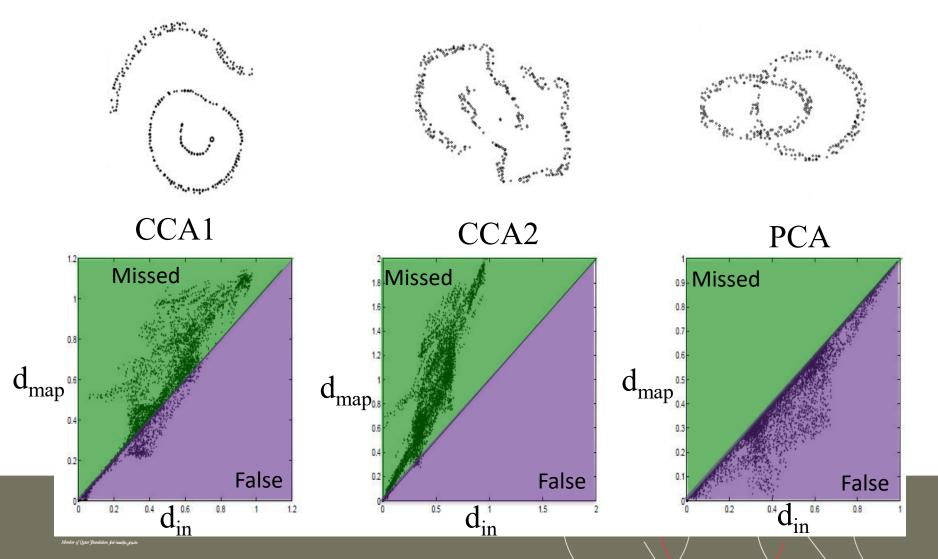


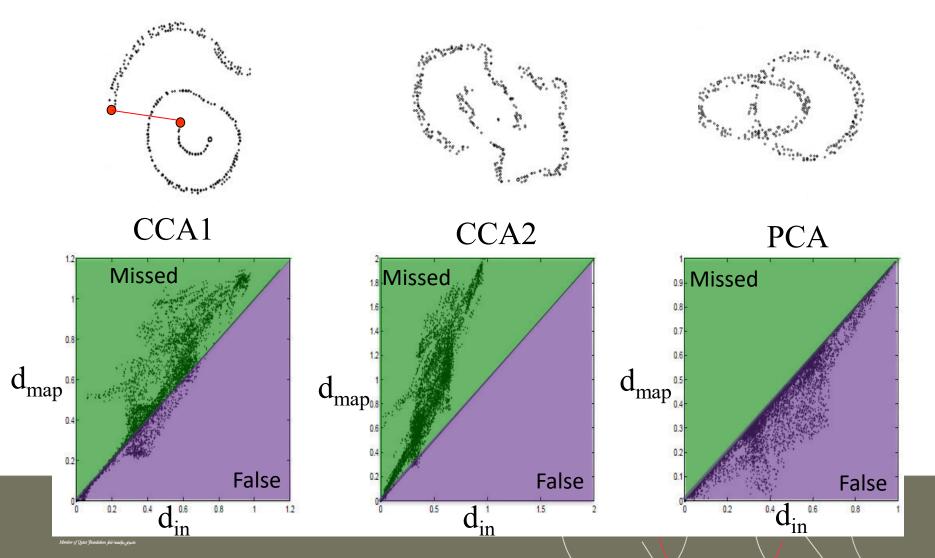


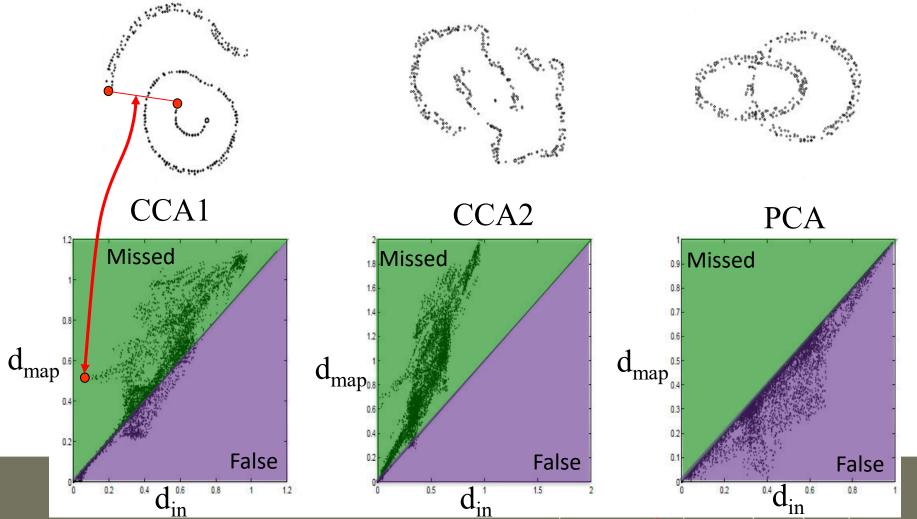
70%

- Support selection of the most accurate map
- Do not support interpretation even of the most accurate map
 - Are the 15% remaining distortions spread all over the map or concentrated somewhere???

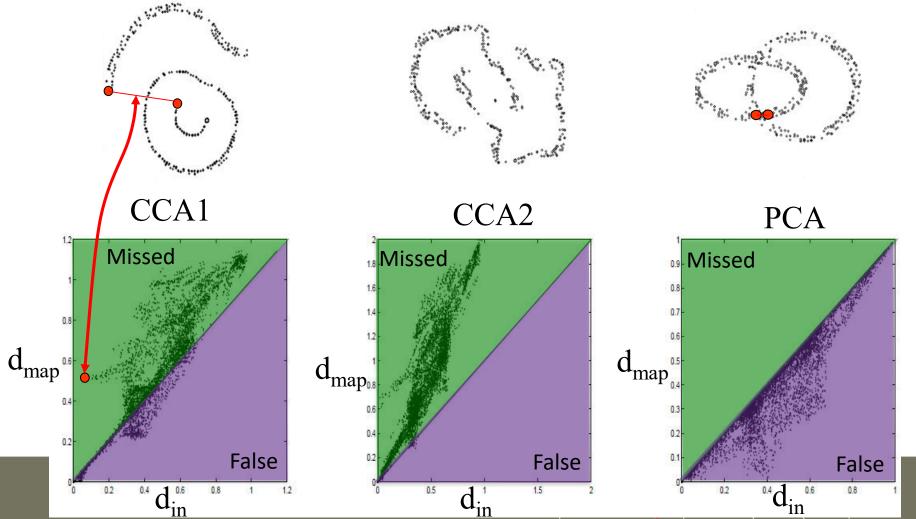




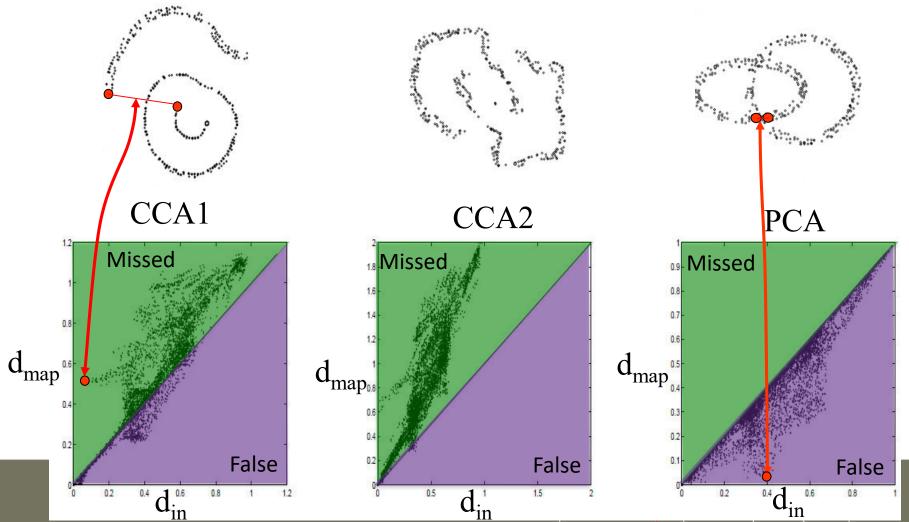




موفى Annher of Ostar Foundation بلغ مستقرب



موفى Annher of Ostar Foundation بلغ مستقرب



موفى مؤسسة- قطر Member of Qatar Foundation

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Turning weaknesses into strengths

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Use distortions within the map to recover HD patterns

Original



Original	Miss
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	o
0 0 0 (4 ¥ 4) 0 0 0 0 0	°°°(∠¥) ▲°°°°°
00000000000	°° ∧ ▲ ° ° ° ° ° ° ° °
0 0 0 0 0 0 0 0 0 0 0	00 0000000
0 0 0 0 0 0 0 0 0 0 0	° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° °
0 0 0 0 0 0 0 0 0 0 0	° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° ° °
0 0 0 0 0 0 0 0 0 0 0	000000000
0 0 0 0 0 0 0 0 0 0 0	° ₀ 00 0000000
0 0 0 0 0 0 0 0 0 0 0	° ₀ 000000000
0 0 0 0 0 0 0 0 0 0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0



Original	Miss	False
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		



Original	Miss	False	Miss&False
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			



Use distortions within the map to recover HD patterns

Original	Miss	False	Miss&False	Miss Shuffled
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				No
0 0 0 0 0 0 0 0 0 0 0	• • • • • • • • • • • • • • • • • • •	0 0 0 0 0 0 0 0 0 0 0 0		distortion False

Perceptually uniform color map



Use distortions within the map to recover HD patterns

Original	Miss	False	Miss&False	Miss Shuffled
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			0 0	No distortion False

Perceptually uniform color map

Three graphical inference rules based on the colored map

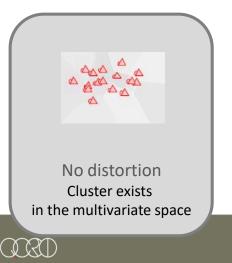


Use distortions within the map to recover HD patterns

Original	Miss	False	Miss&False	Miss Shuffled
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				No distortion False

Perceptually uniform color map

Three graphical inference rules based on the colored map



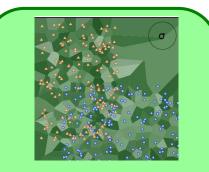
Use distortions within the map to recover HD patterns

Original	Miss	False	Miss&False	Miss Shuffled
$\begin{array}{cccccccccccccccccccccccccccccccccccc$				No
		$\begin{array}{cccccccccccccccccccccccccccccccccccc$		distortion False

Perceptually uniform color map

Three graphical inference rules based on the colored map





True overlap Both classes overlap in the multivariate space

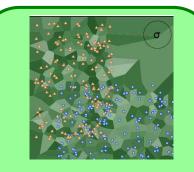
Use distortions within the map to recover HD patterns

Original	Miss	False	Miss&False	Miss Shuffled
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$				No
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			000000000000000000000000000000000000000	distortion False

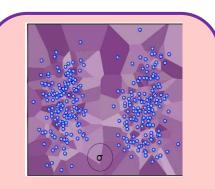
Perceptually uniform color map

Three graphical inference rules based on the colored map



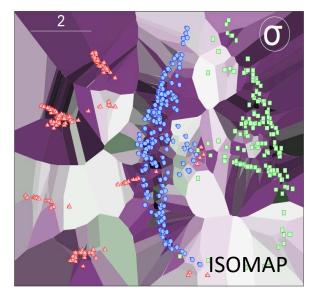


True overlap Both classes overlap in the multivariate space



True separation Both clusters are separated in the multivariate space

Use distortions within the map to recover HD patterns



CheckViz OilFlow data (N=1000, D=12) Miss Shuffled

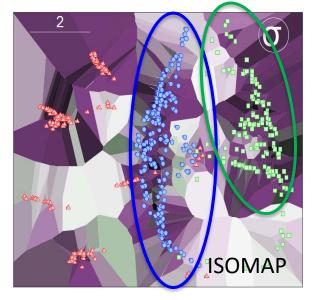
False

distortion



Turning weaknesses into strengths

Use distortions within the map to recover HD patterns



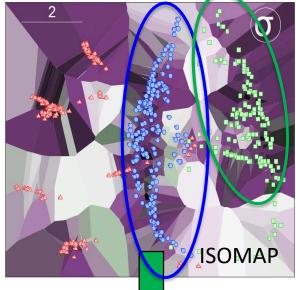
OilFlow data (N=1000, D=12) Miss Shuffled

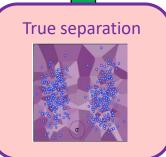
CheckViz



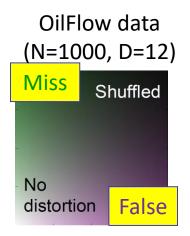
Turning weaknesses into strengths

Use distortions within the map to recover HD patterns



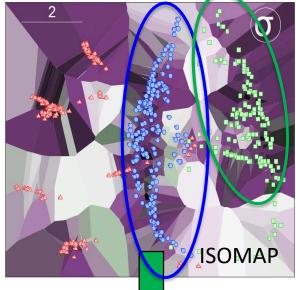


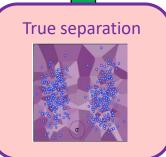
CheckViz



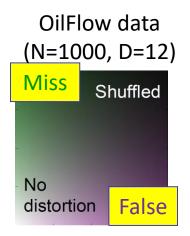
Turning weaknesses into strengths

Use distortions within the map to recover HD patterns



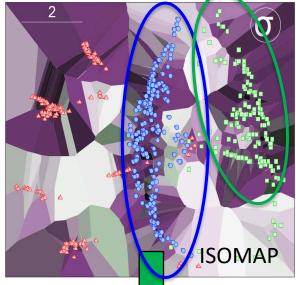


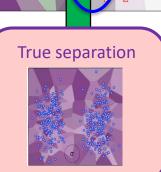
CheckViz



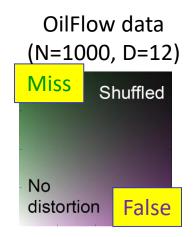
Turning weaknesses into strengths

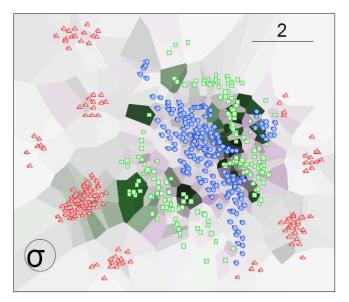
Use distortions within the map to recover HD patterns





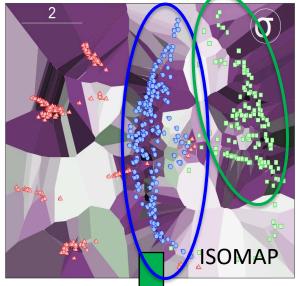
CheckViz

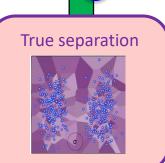




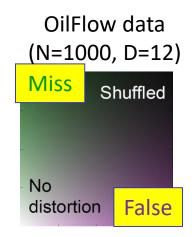
Turning weaknesses into strengths

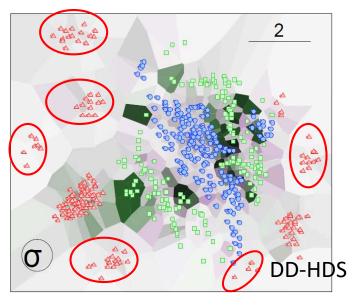
Use distortions within the map to recover HD patterns



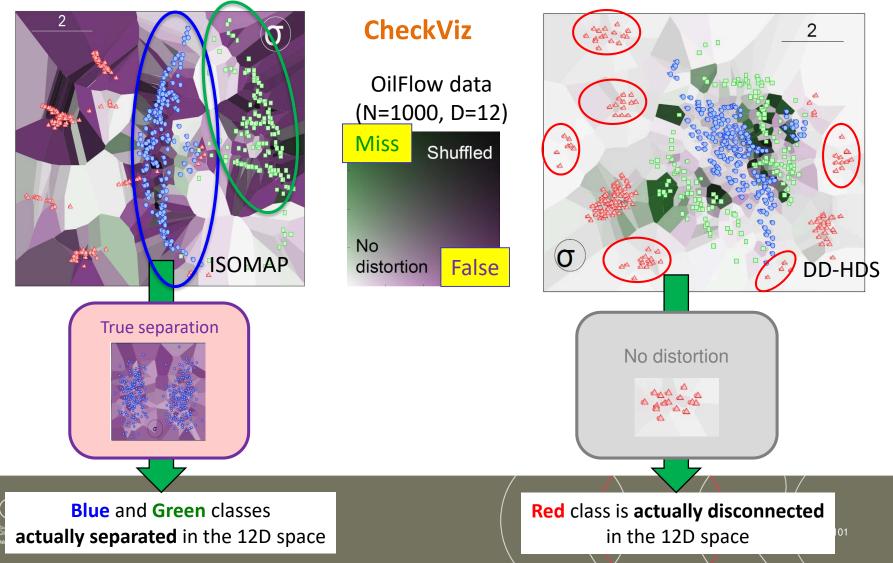


CheckViz





Turning weaknesses into strengths



















• Displaying original similarities within the map itself



ProxiViz



• Displaying original similarities within the map itself

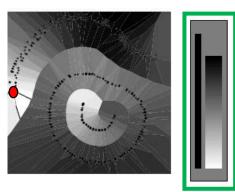


ProxiViz

• Displaying original similarities within the map itself

ProxiViz



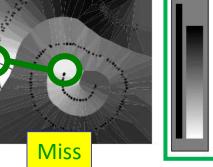






• Displaying original similarities within the map itself









• Displaying original similarities within the map itself









• Displaying original similarities within the map itself



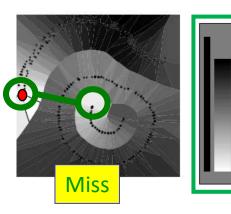


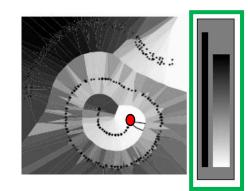




• Displaying original similarities within the map itself





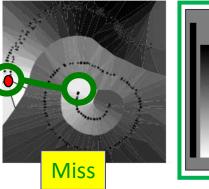


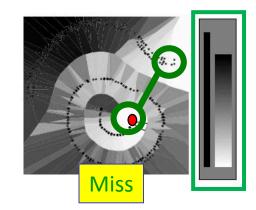


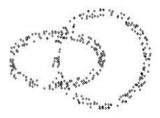


Displaying original similarities within the map itself



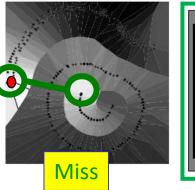


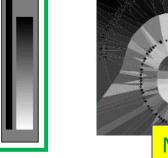


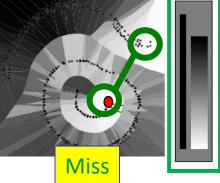


Displaying original similarities within the map itself

Model Model Model Model Model Model Model





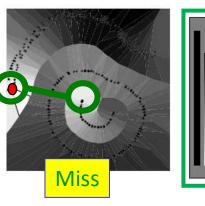




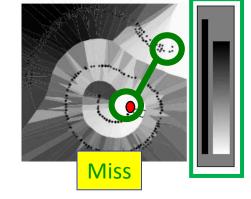


Displaying original similarities within the map itself

Model Model Model Model Model Model Model

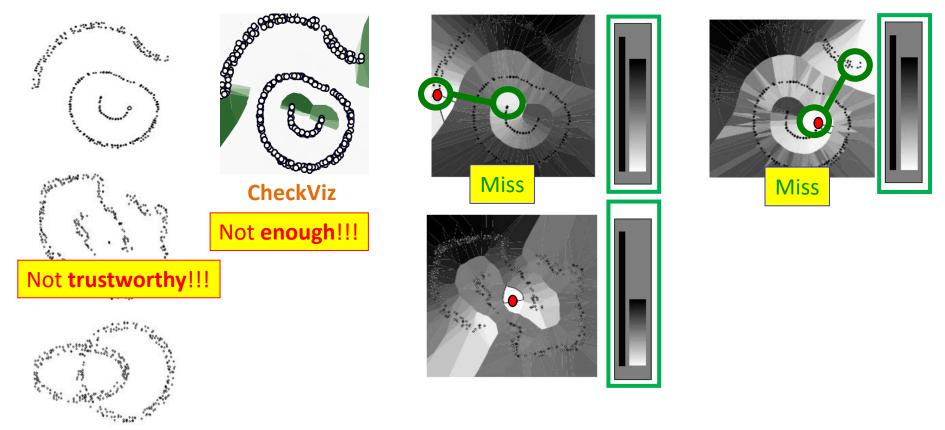






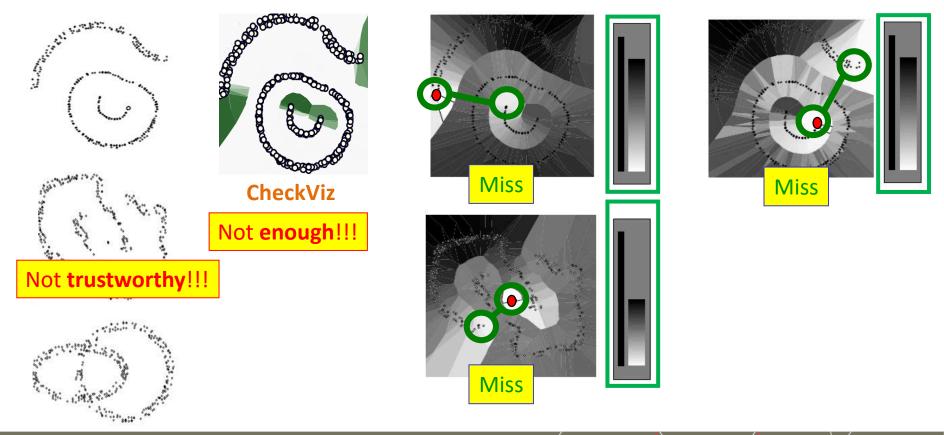


• Displaying original similarities within the map itself



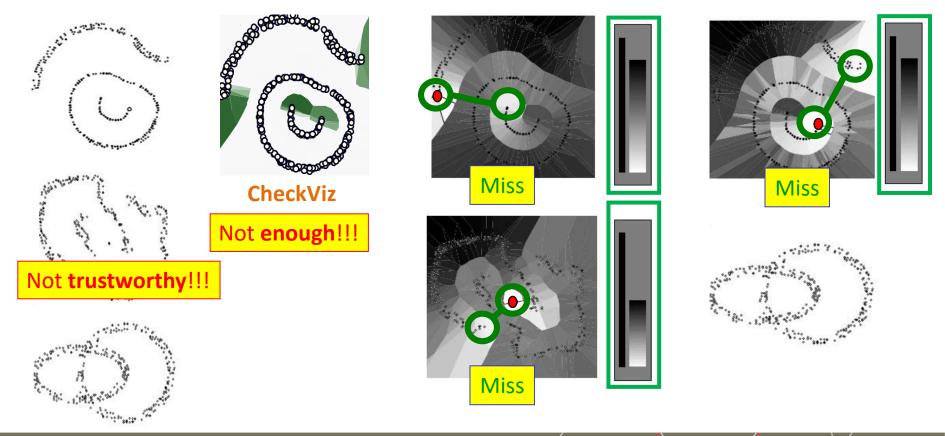


Displaying original similarities within the map itself



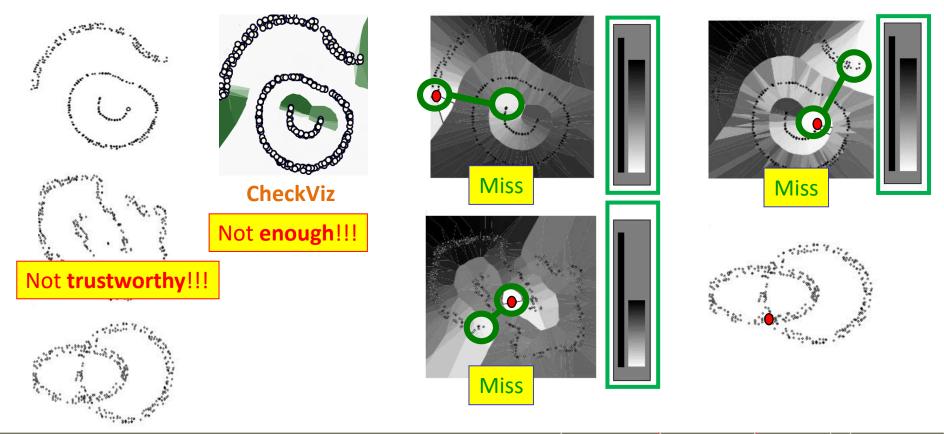


• Displaying original similarities within the map itself



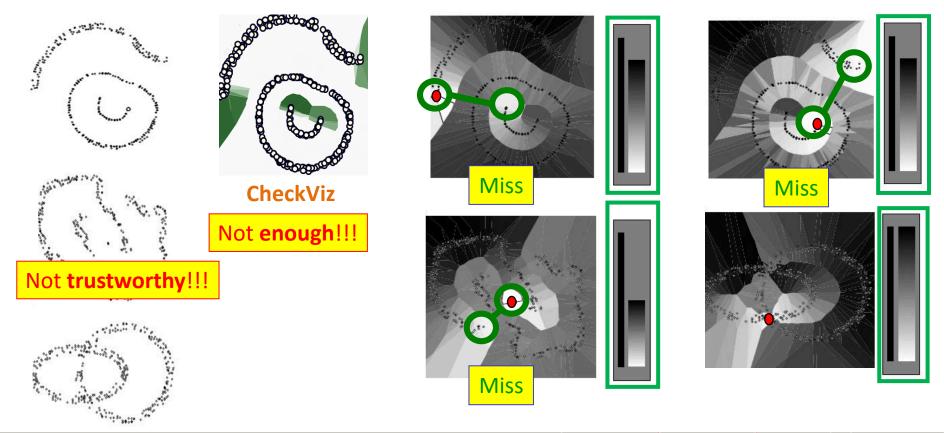


• Displaying original similarities within the map itself



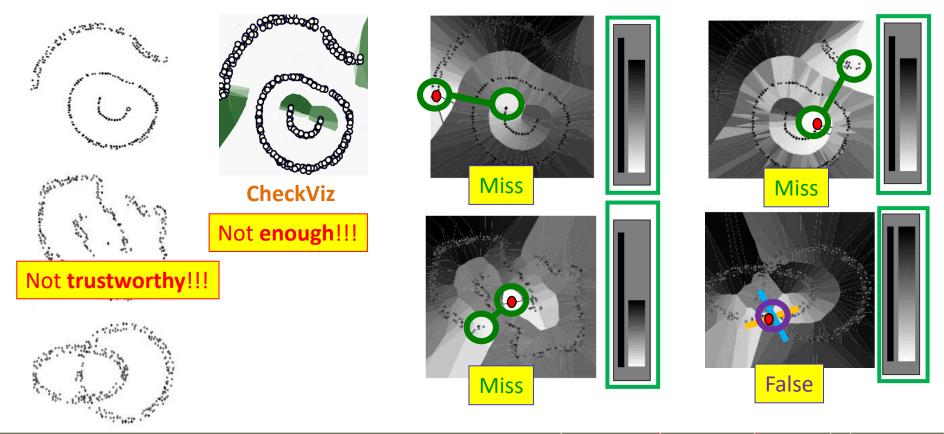


• Displaying original similarities within the map itself





• Displaying original similarities within the map itself



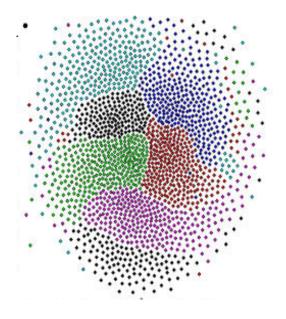


• Displaying original similarities within the map itself ISOLET data (D=617, N=1800, C=6)



• Displaying **original similarities within the map itself** ISOLET data (**D=617**, N=1800, C=6)

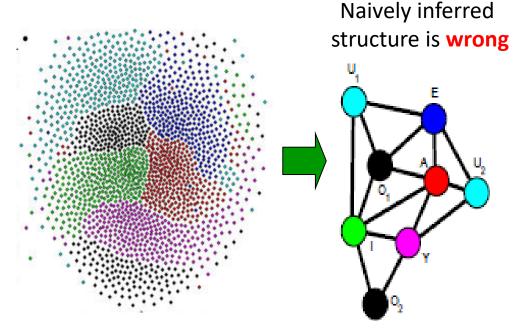
CCA projection





• Displaying original similarities within the map itself ISOLET data (D=617, N=1800, C=6)

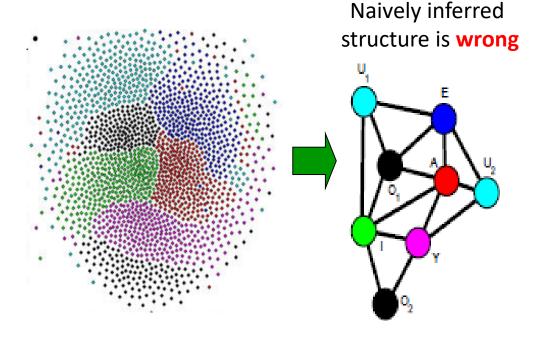
CCA projection

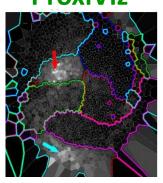




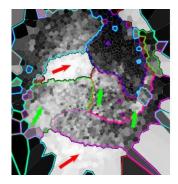
Displaying original similarities within the map itself
 ISOLET data (D=617, N=1800, C=6)
 ProxiViz

CCA projection





Within-class proximity



Between-class proximity

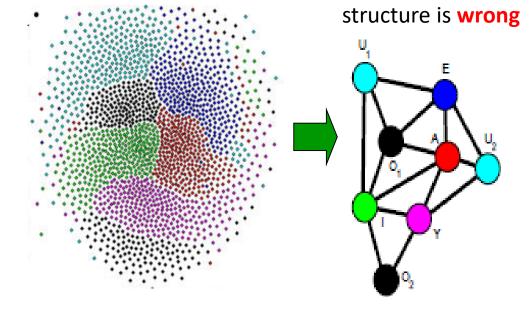


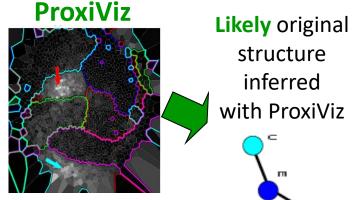
· Displaying original similarities within the map itself

Naively inferred

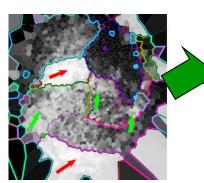
ISOLET data (**D=617**, N=1800, C=6)

CCA projection





Within-class proximity



Between-class proximity

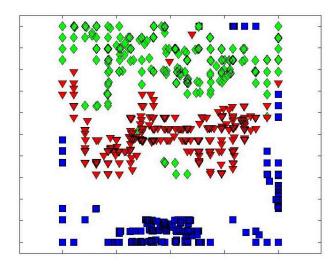


structure

inferred

• Displaying original similarities within the map itself OIL FLOW data (D=12, N=1000, C=3)

GTM

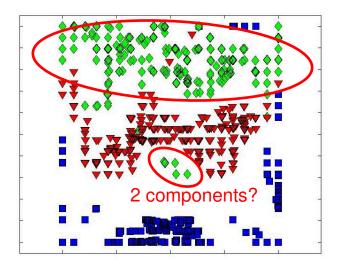




• Displaying original similarities within the map itself OIL FLOW data (D=12, N=1000, C=3)

Query

GTM

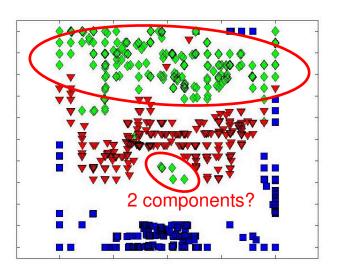


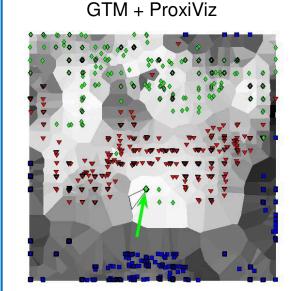


Displaying original similarities within the map itself
 OIL FLOW data (D=12, N=1000, C=3)

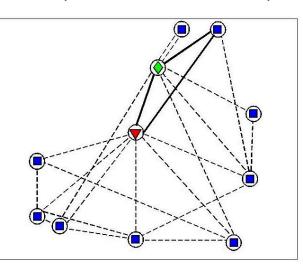
Query

GTM



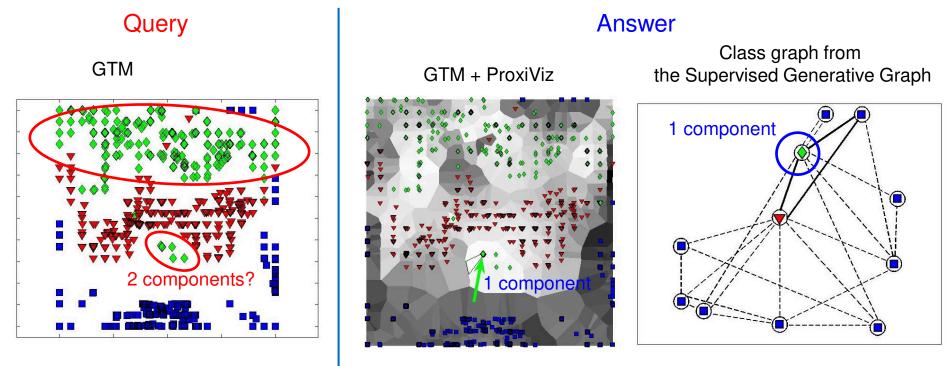


Class graph from the Supervised Generative Graph





• Displaying original similarities within the map itself OIL FLOW data (D=12, N=1000, C=3)





ProxiLens Heulot, Aupetit, Fekete. ProxiLens: Interactive Exploration of High-Dimensional Data using Projections EuroVis 2013 Workshop on Visual analytics using Multidimensional Projections, Leipzig, Germany, June 2013

Turning weaknesses into strengths

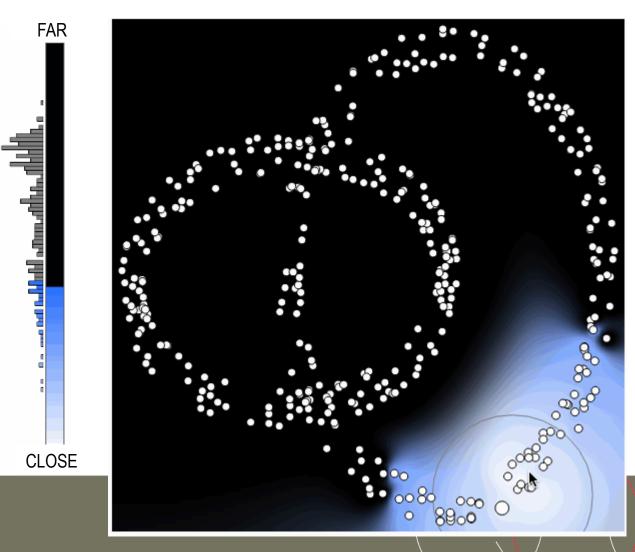
• Displaying original similarities within a lens to navigate



ProxiLens Heulot, Aupetit, Fekete. ProxiLens: Interactive Exploration of High-Dimensional Data using Projections EuroVis 2013 Workshop on Visual analytics using Multidimensional Projections, Leipzig, Germany, June 2013

Turning weaknesses into strengths

• Displaying original similarities within a lens to navigate

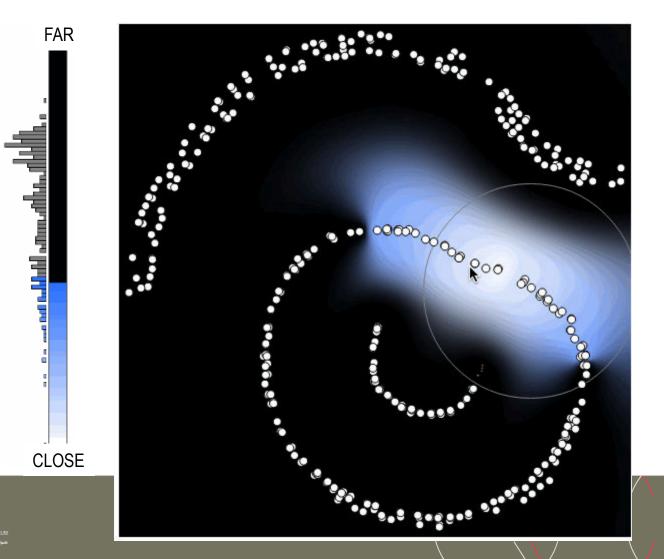




ProxiLens Heulot, Aupetit, Fekete. ProxiLens: Interactive Exploration of High-Dimensional Data using Projections EuroVis 2013 Workshop on Visual analytics using Multidimensional Projections, Leipzig, Germany, June 2013

Turning weaknesses into strengths

• Displaying original similarities within a lens to navigate



MD-Brush Michaël Aupetit, Nicolas Heulot, Jean-Daniel Fekete. A multidimensional brush for scatterplot data analytics Poster at IEEE VIS 2014 conference, Paris, France, November 2014

Turning weaknesses into strengths

• Displaying original similarities within a lens to brush MD data



HDBrush Michaël Aupetit, Nicolas Heulot, Jean-Daniel Fekete. A multidimensional brush for scatterplot data analytics Poster at IEEE VIS 2014 conference, Paris, France, November 2014

Turning weaknesses into strengths

• Displaying original similarities within a lens to brush HD data

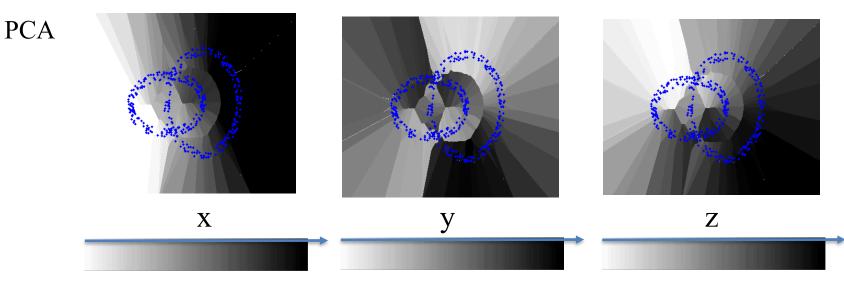
A multidimensional brush for scatterplot data analytics

Michaël Aupetit – QCRI, Doha Nicolas Heulot – IRT SystemX, Université Paris-Saclay Jean-Daniel Fekete – INRIA AVIZ, Université Paris-Saclay

Contact: michael.aupetit@gmail.com

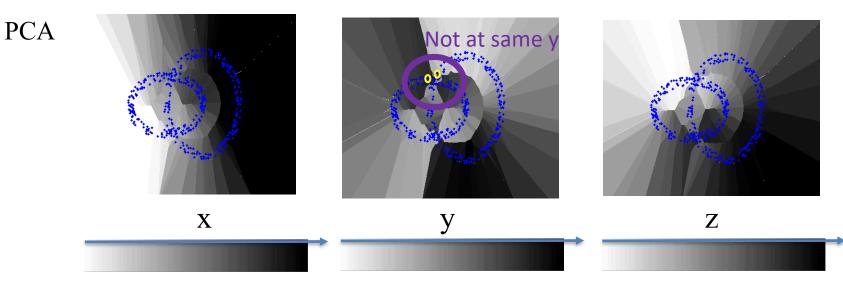


- Displaying original variable within the map itself
- Can detect correlations between variables



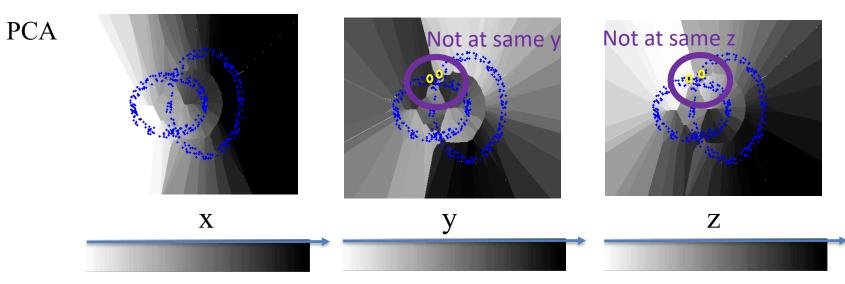


- Displaying original variable within the map itself
- Can detect correlations between variables



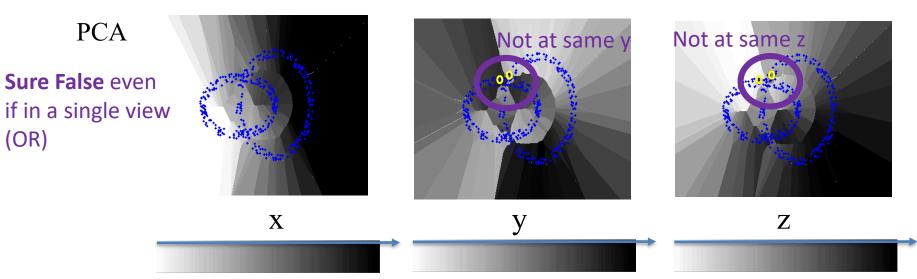


- Displaying original variable within the map itself
- Can detect correlations between variables



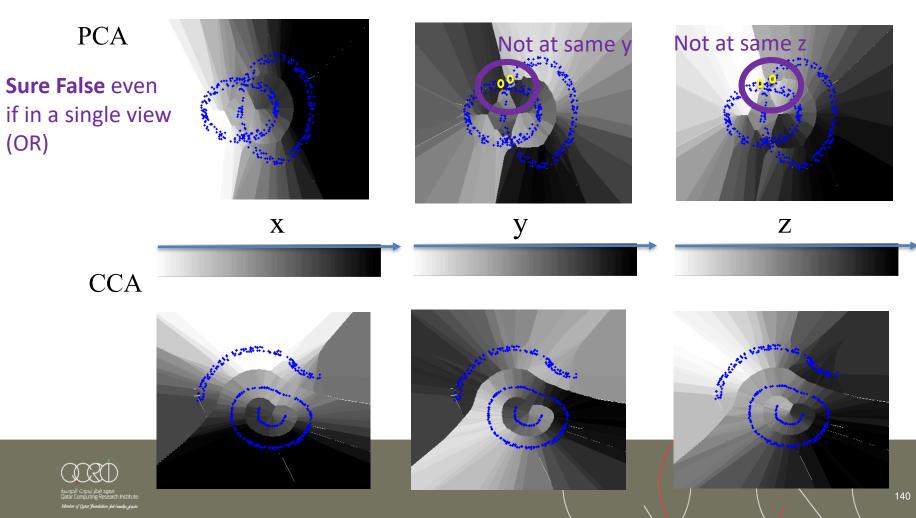


- Displaying original variable within the map itself
- Can detect correlations between variables

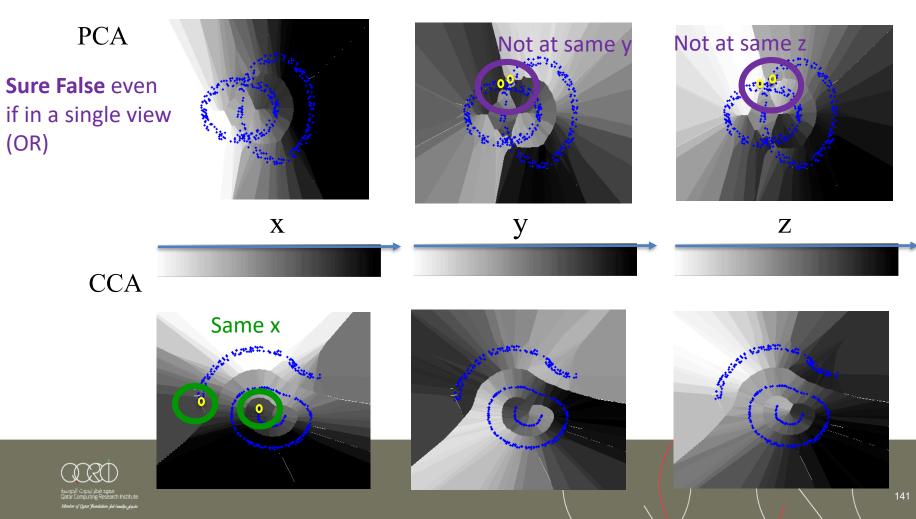




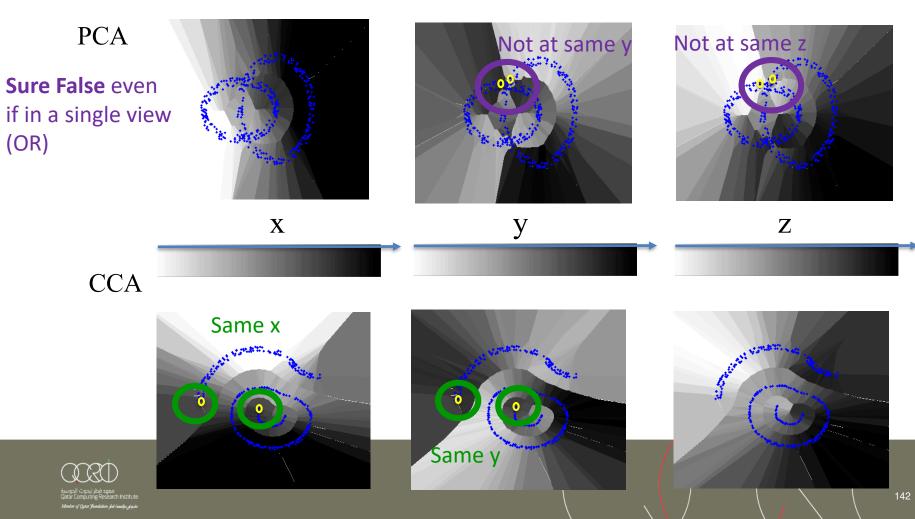
- Displaying original variable within the map itself
- Can detect correlations between variables



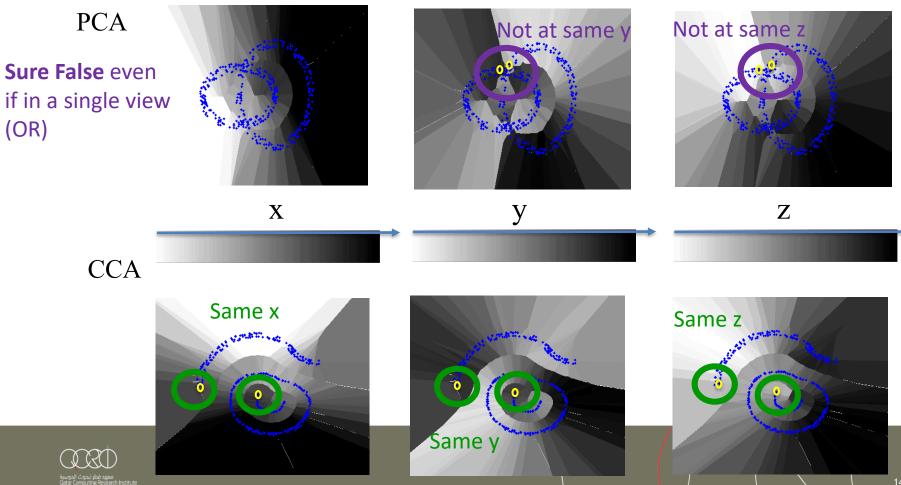
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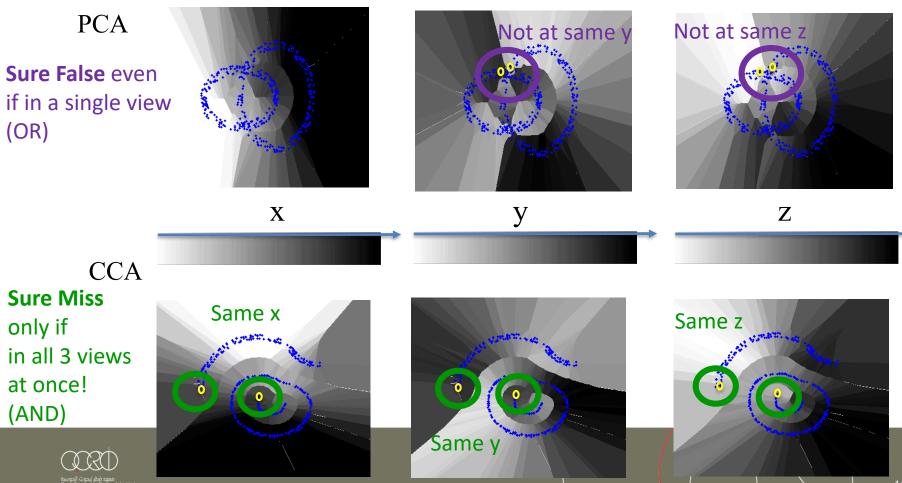
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- Can detect correlations between variables

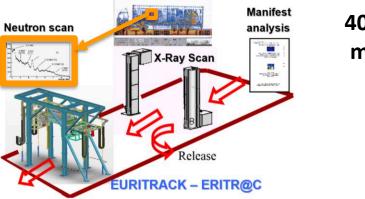








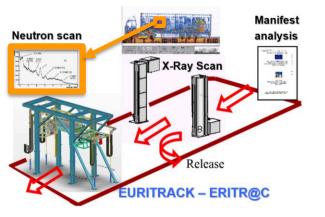
Displaying out-of-sample instance within the map itself



40 reference materials



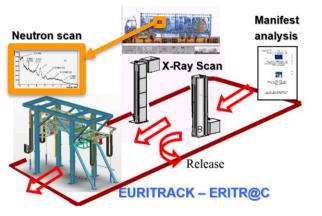
Displaying out-of-sample instance within the map itself



40 reference materials Wood furniture Textile Metal box Plastic boxes

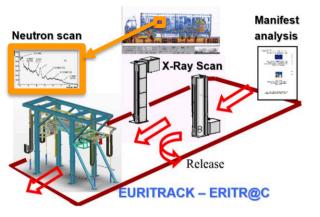
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40 reference materials	15D chemical signature
Wood furniture	
Textile	
Metal box	
Plastic boxes	

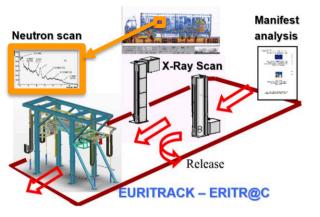




40 reference materials	15D chemical signature
Wood furnitur	e ser
Textile	
Metal box	
Plastic boxes	

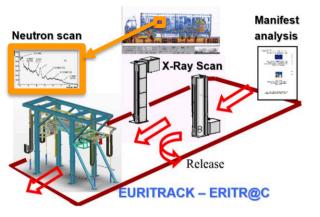


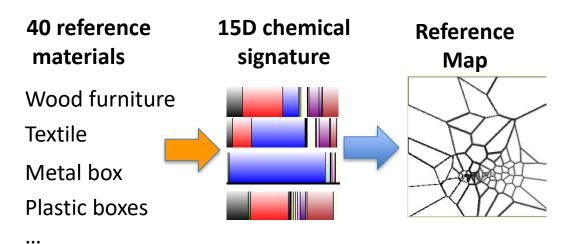
...



40 reference materials	15D chemical signature	Reference Map
Wood furniture Textile Metal box Plastic boxes		



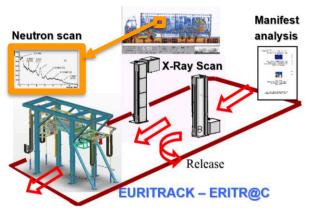


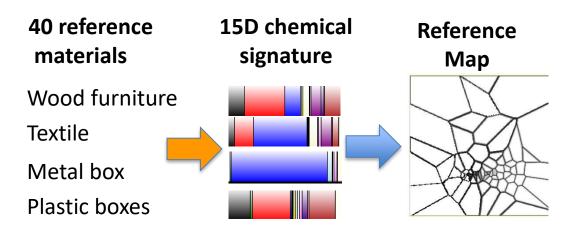




...

Displaying out-of-sample instance within the map itself



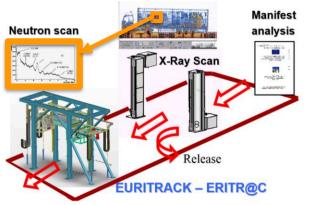


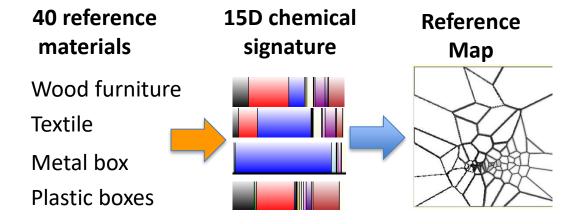
New content

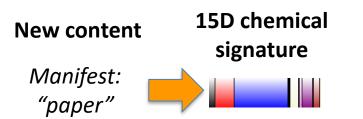
Manifest: "paper"



. . .

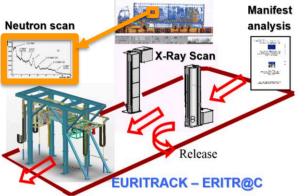


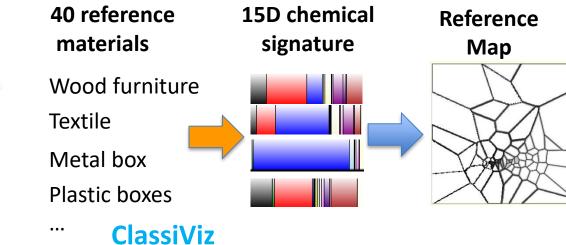






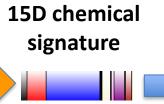
Displaying out-of-sample instance within the map itself

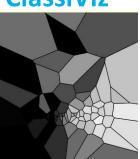






Manifest: "paper"

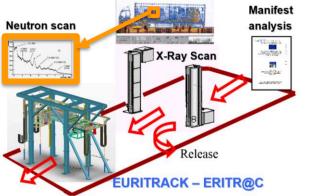


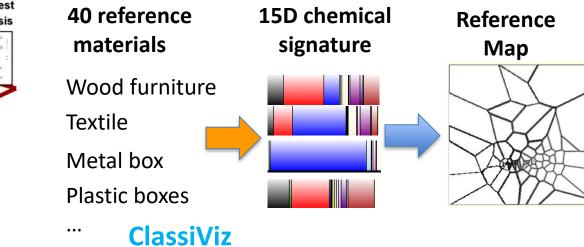


Similarity to reference is color-coded



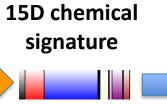
Displaying out-of-sample instance within the map itself

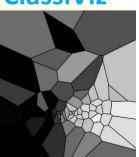






Manifest: "paper"

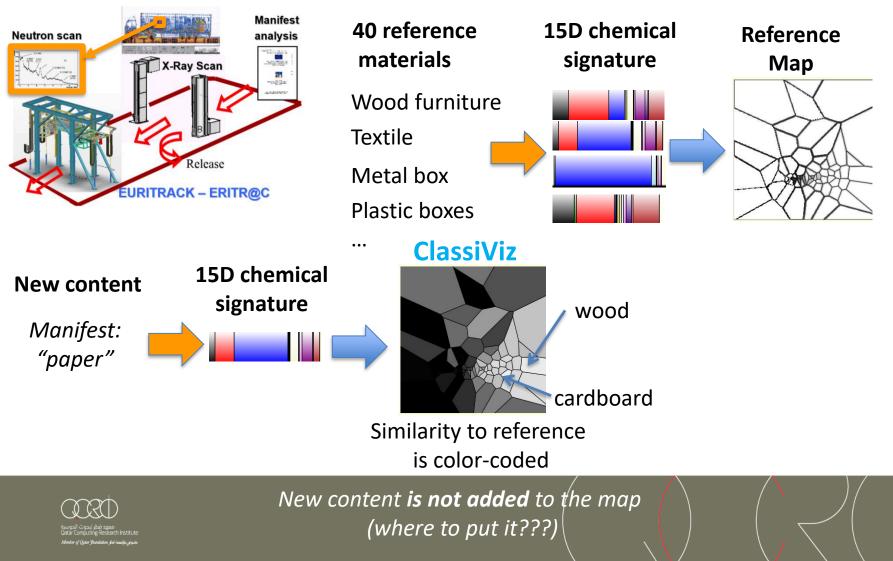


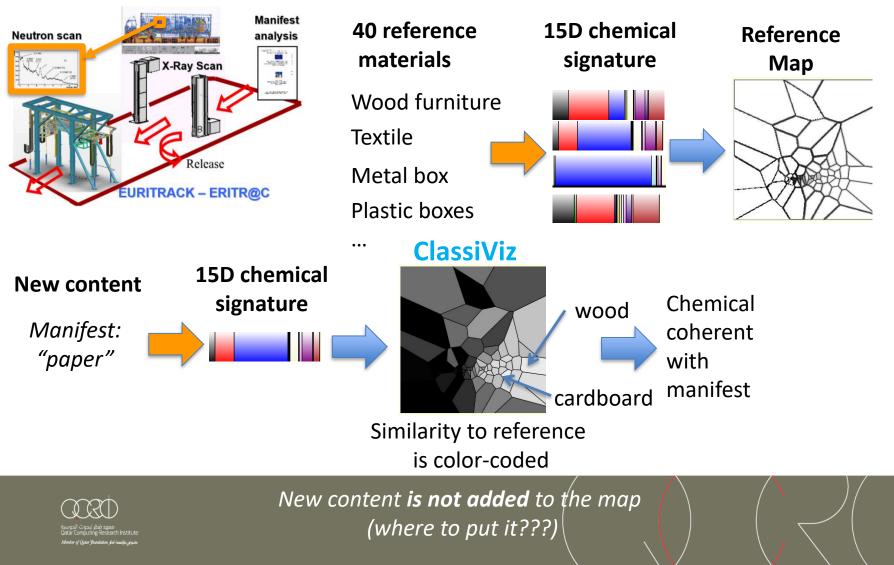


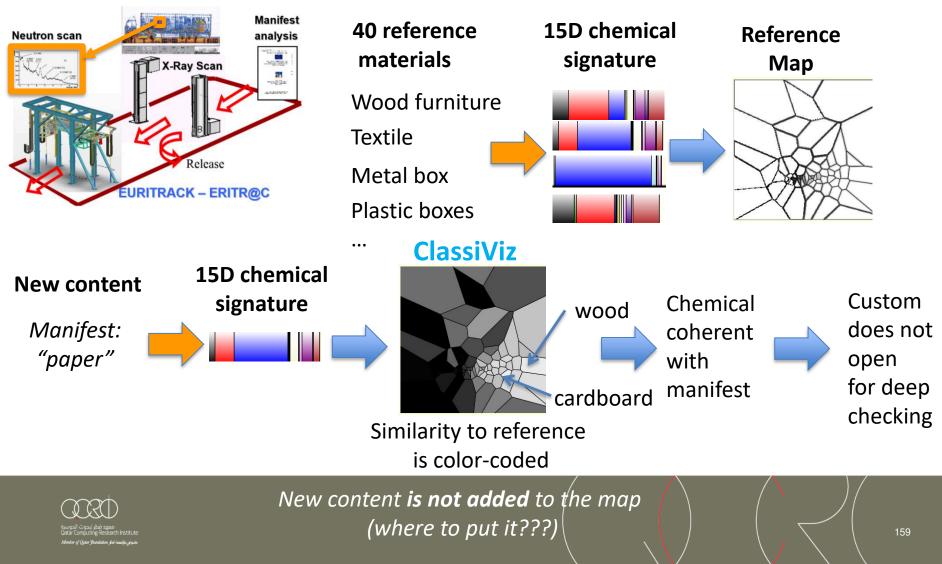
Similarity to reference is color-coded



New content **is not added** to the map (where to put it???)







Display distortions



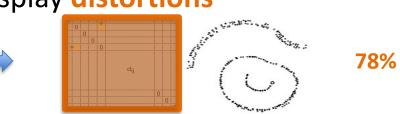
dij





Display distortions



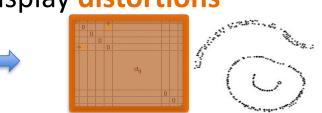




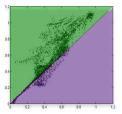
Display distortions



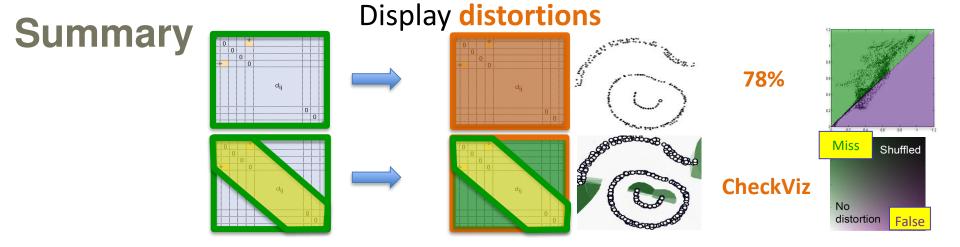
dij



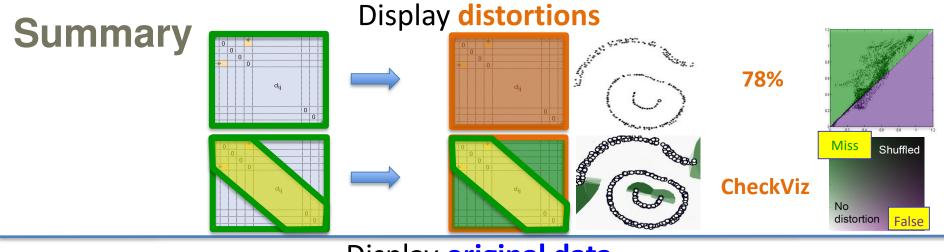




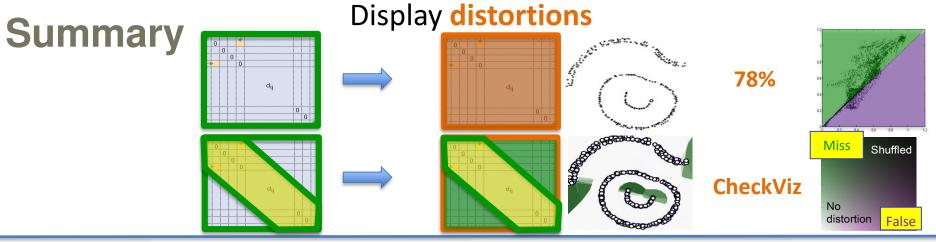


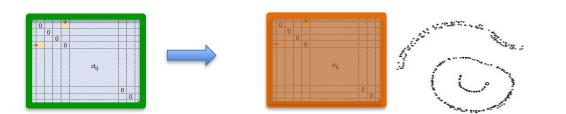




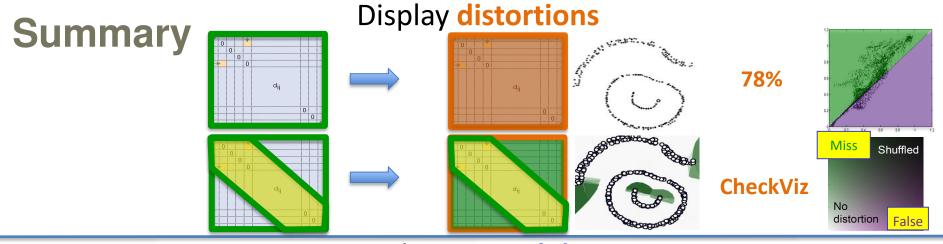


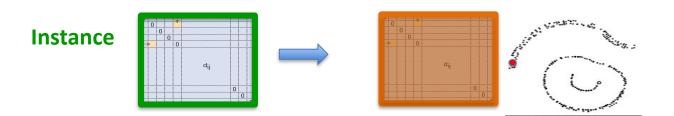




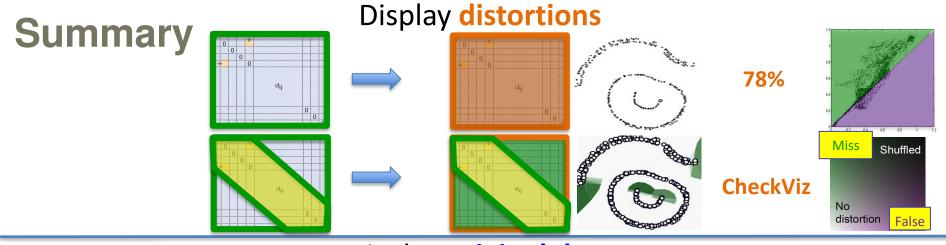


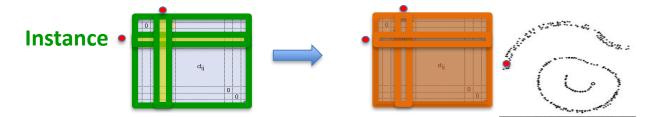




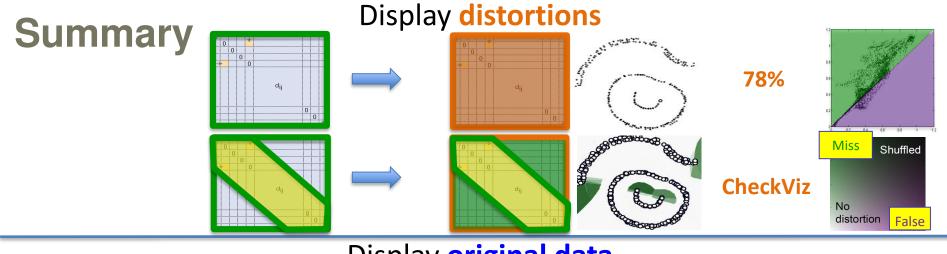


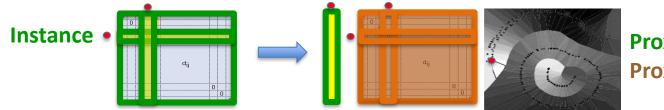






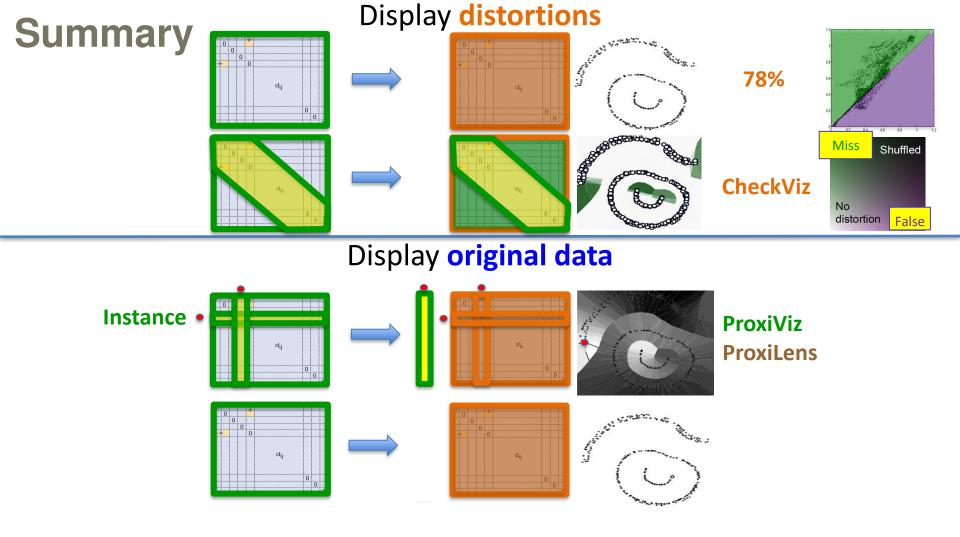




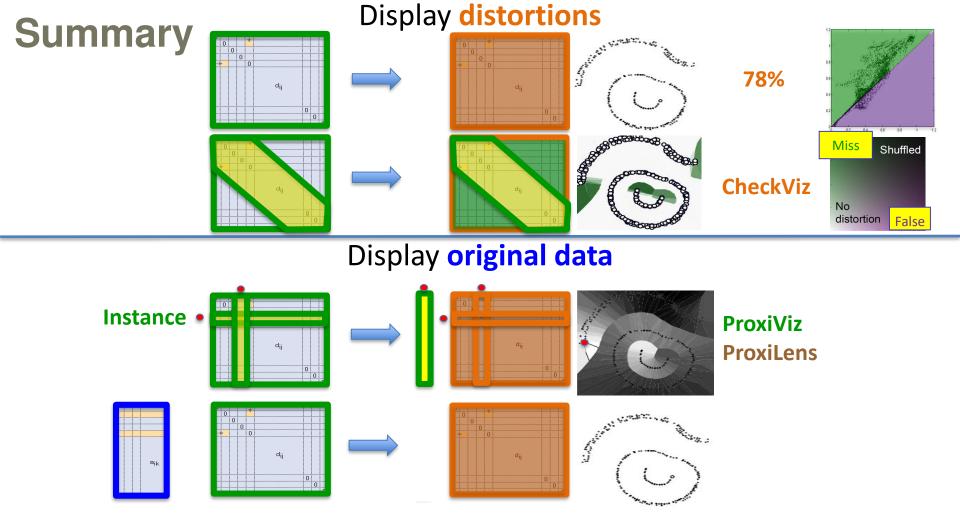




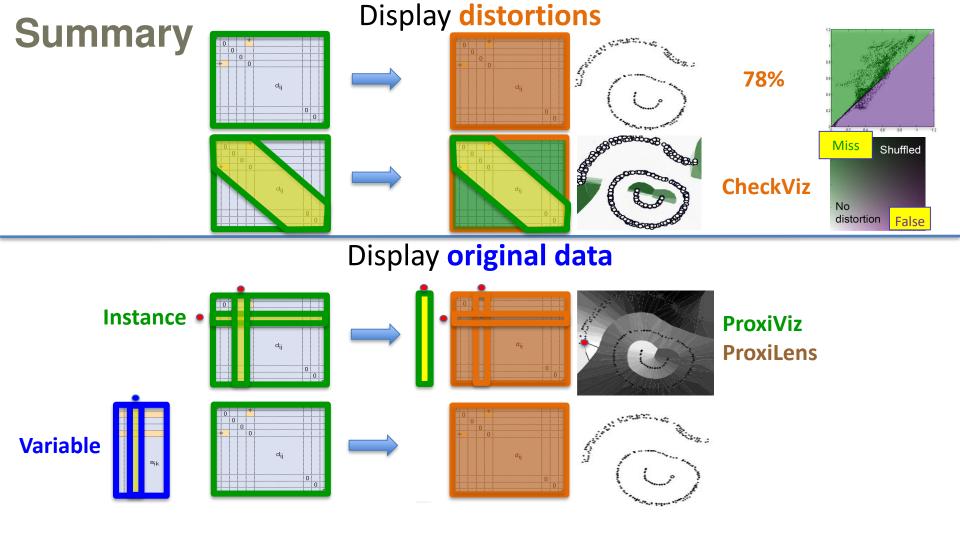




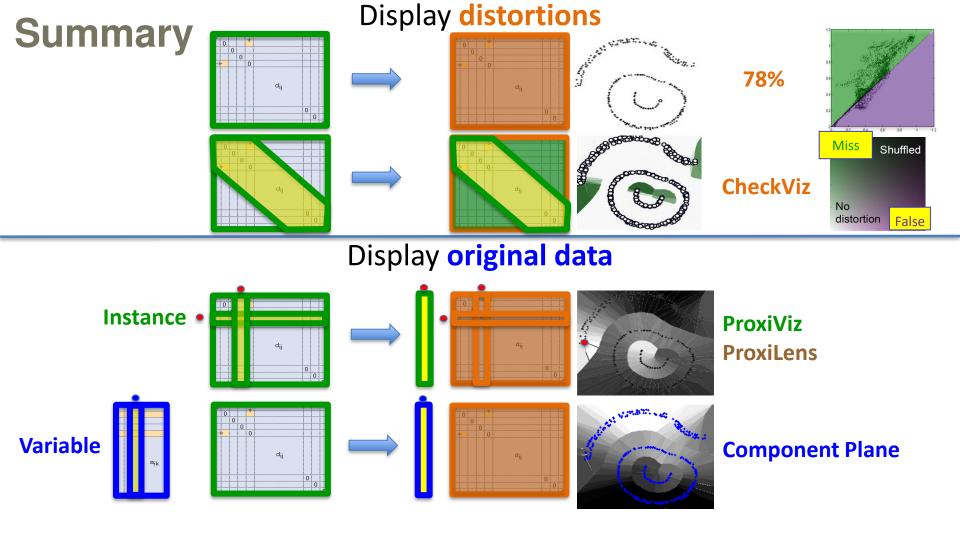




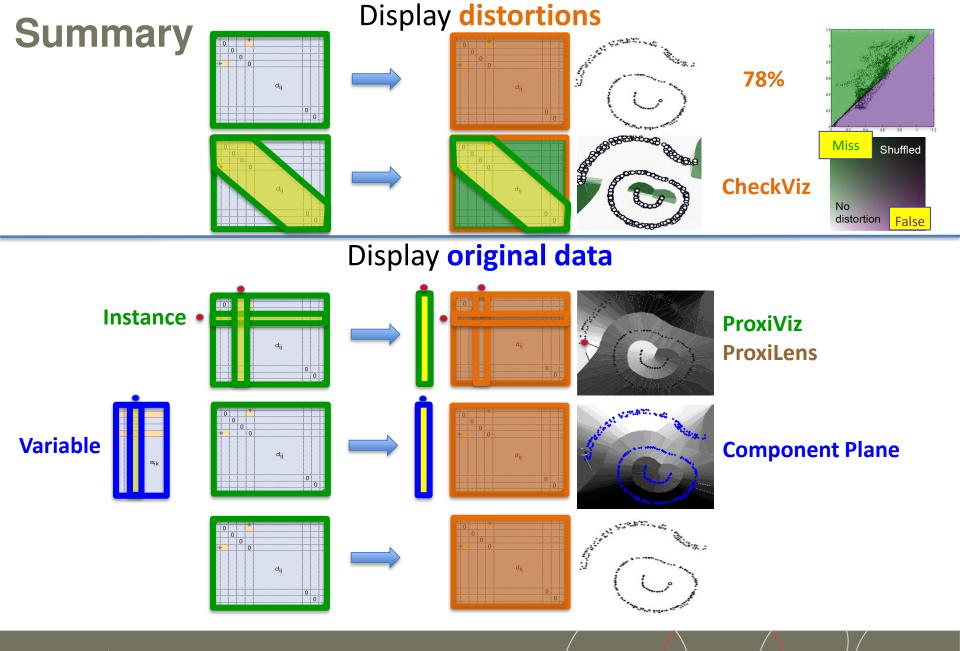




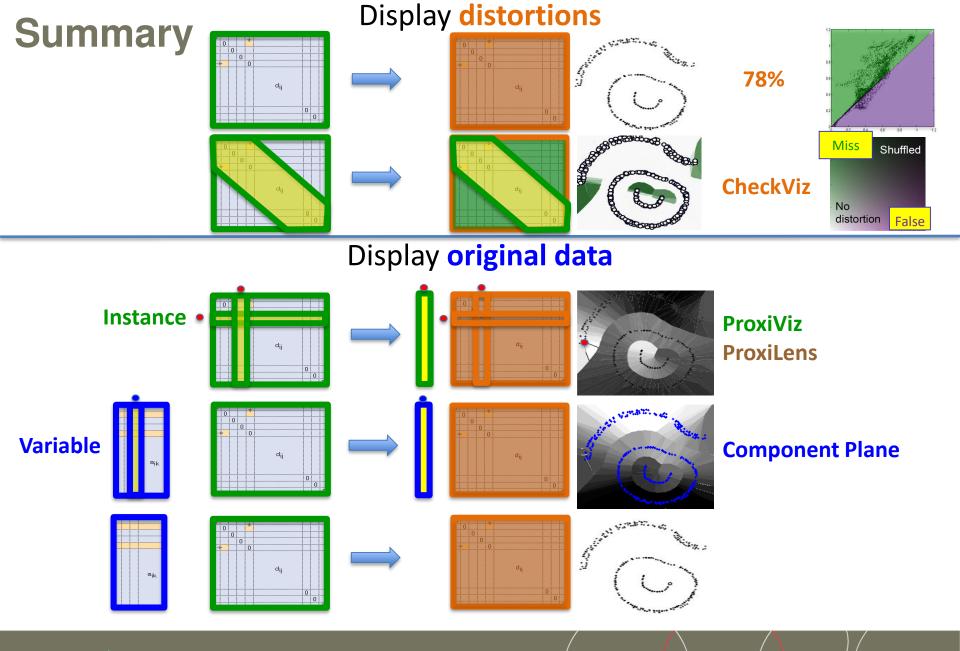




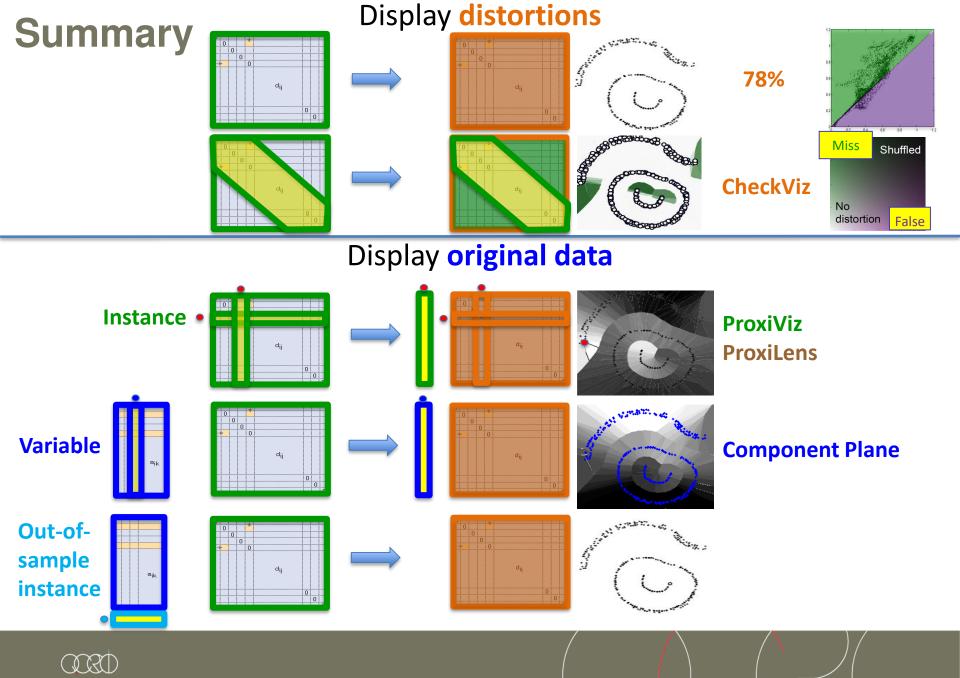




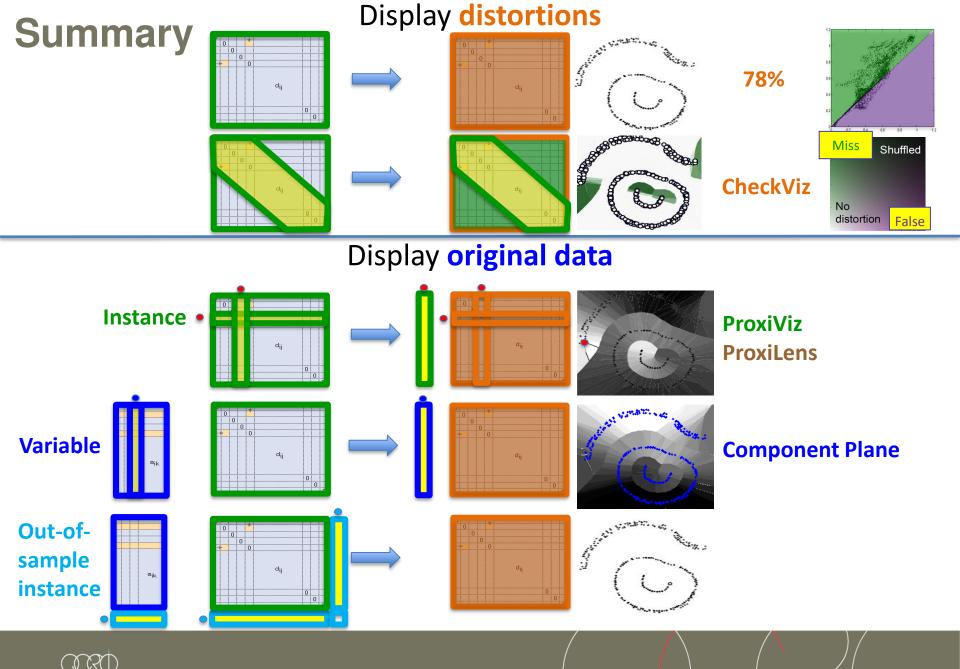


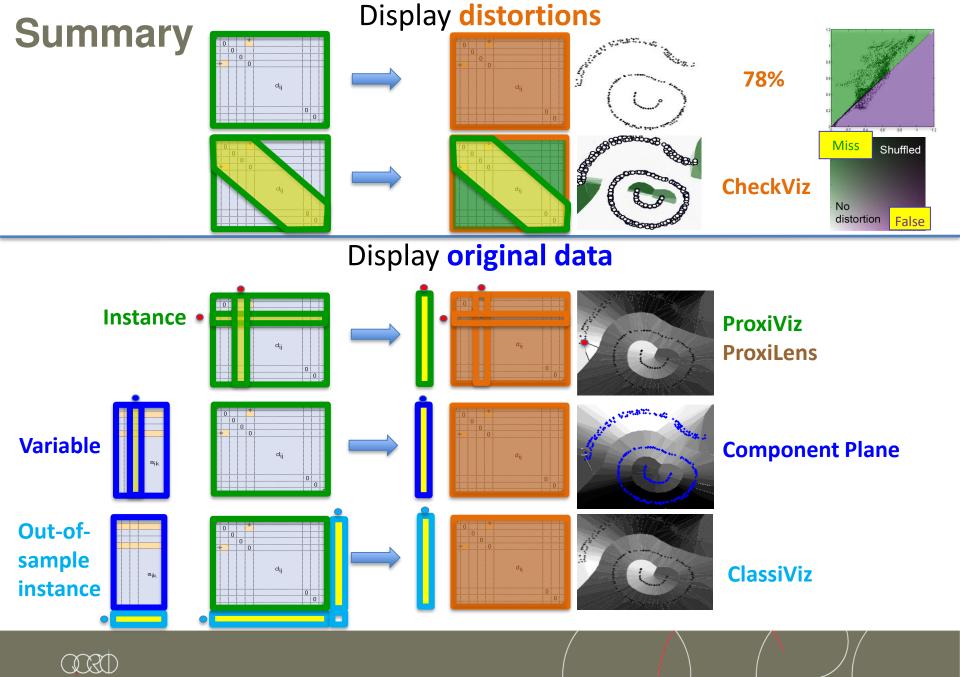


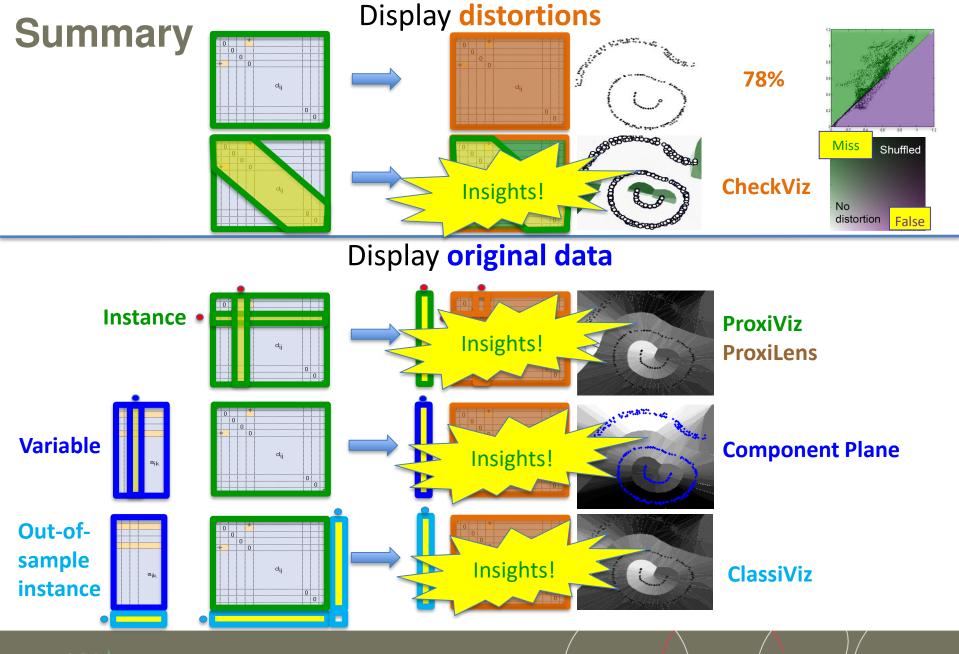




معهد قطر لبدوث الدوسية Qatar Computing Research Institute Member of Oster Newsletion Institute

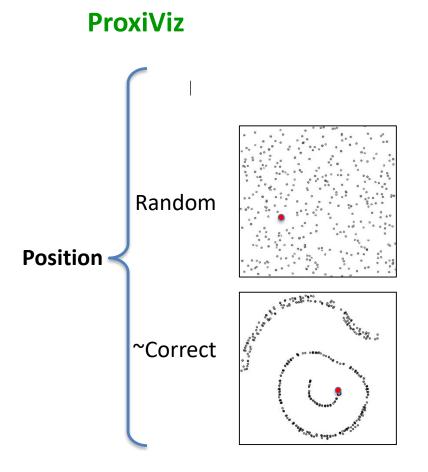






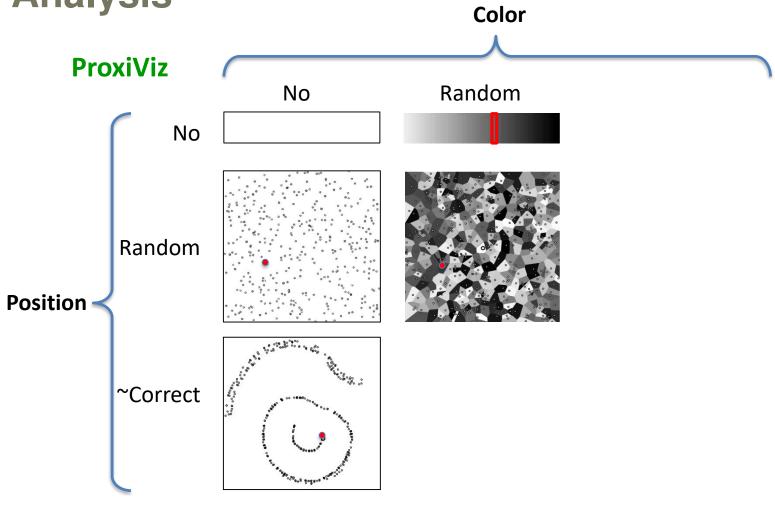
مربع المعرفة المعنى إسرائيل المحمد المحمد

Analysis

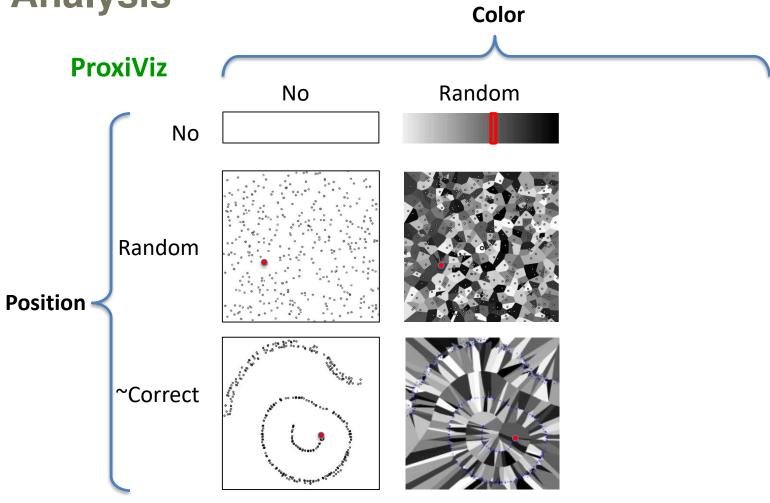




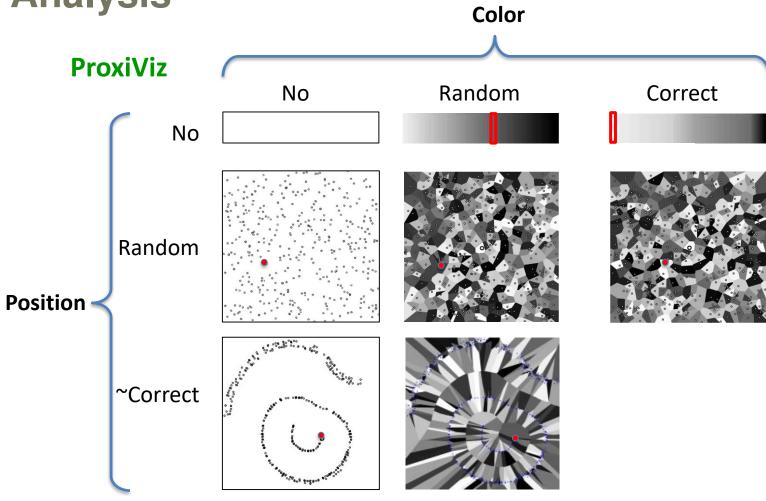
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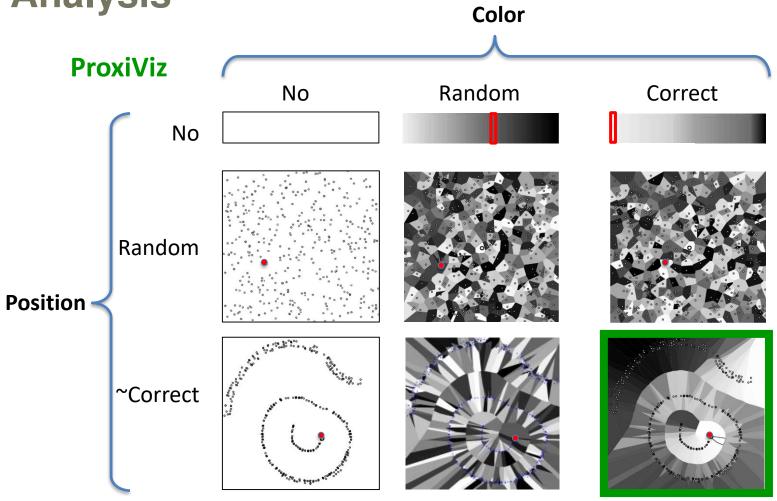




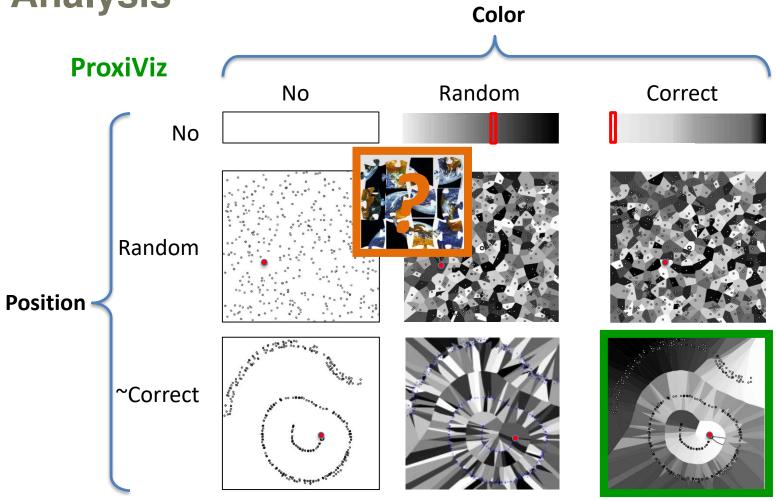




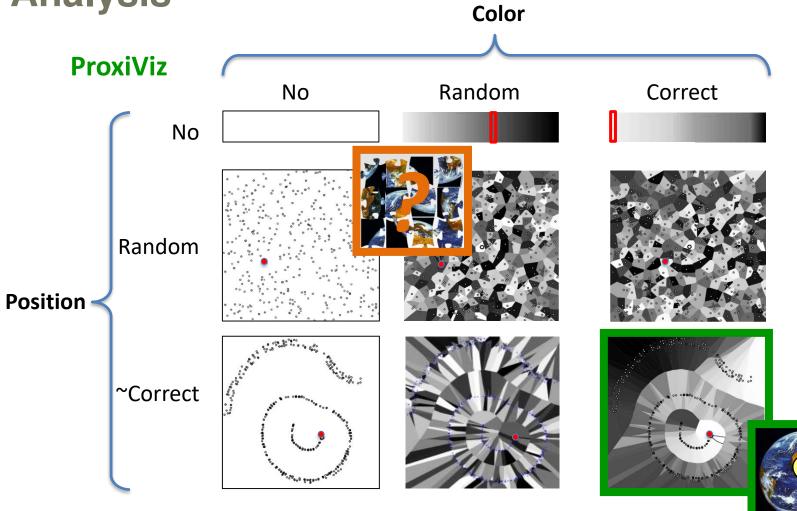




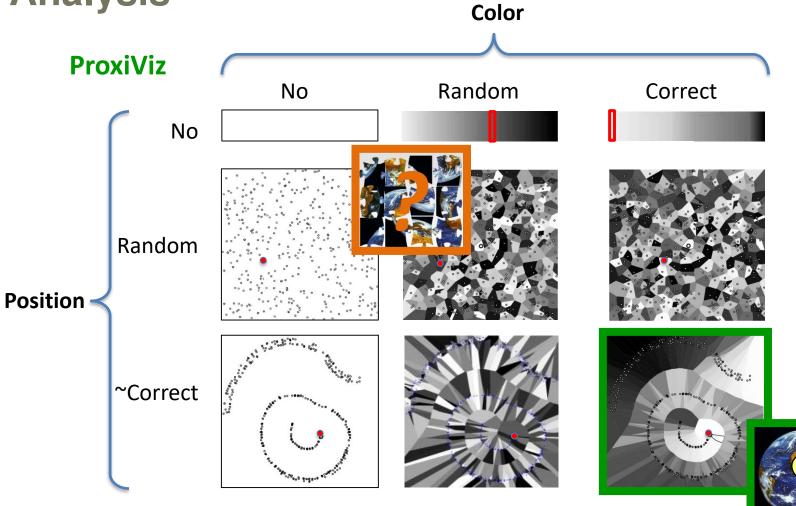










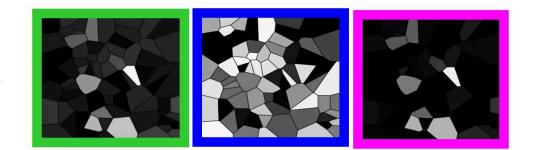


 Correlation between position and color is crucial to detect patterns



ClassiViz

Random

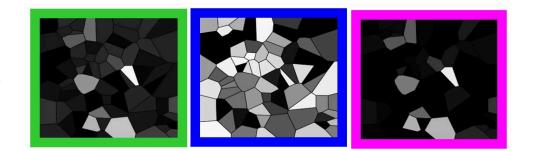






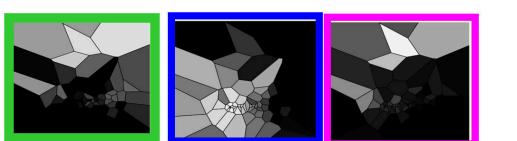
ClassiViz

Random





MDS (DD-HDS)

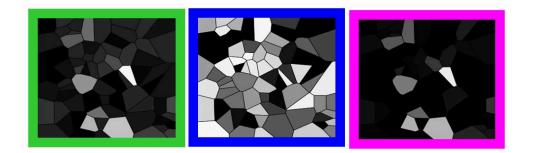




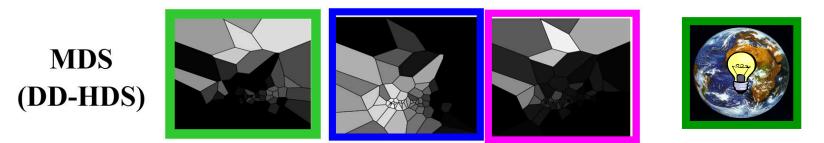


ClassiViz

Random





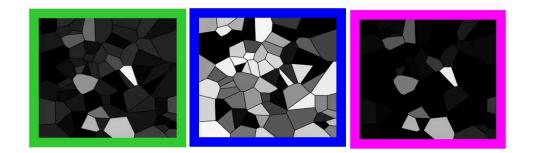


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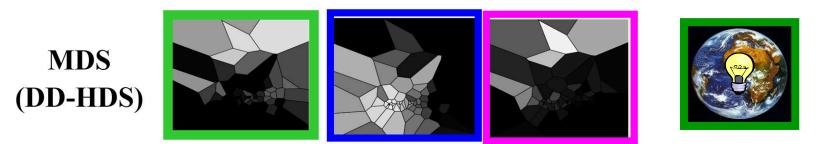


ClassiViz

Random





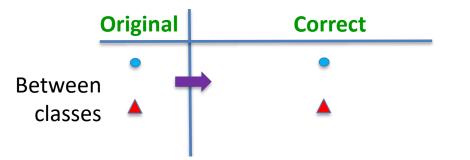


Correlation between position and color is crucial to lower cognitive load and ease decision



Turning weaknesses into strengths

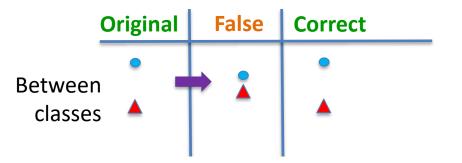
Mapping labeled data using distortions





Turning weaknesses into strengths

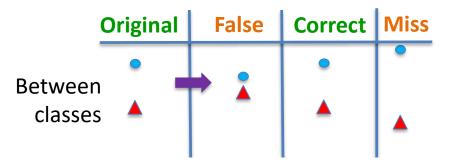
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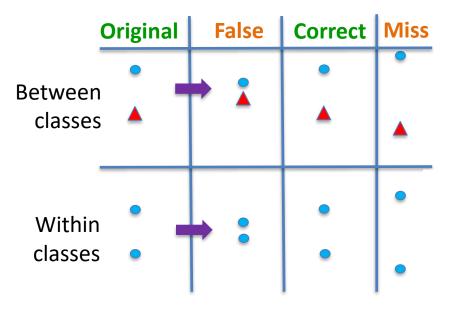
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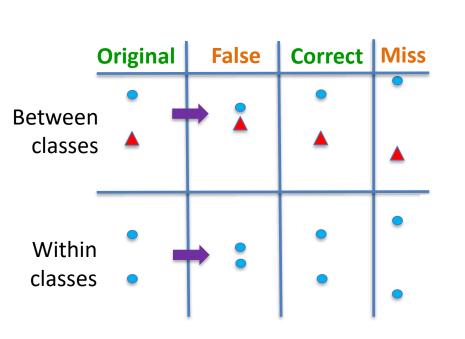
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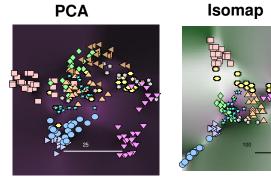


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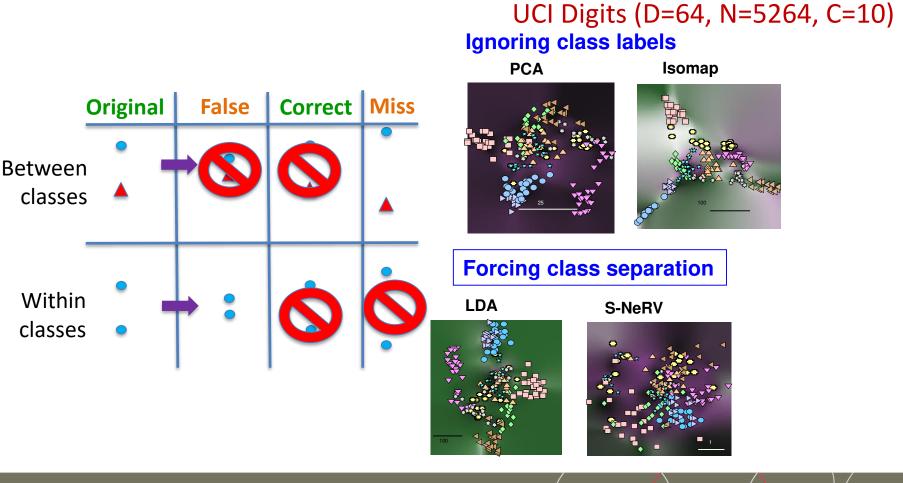
UCI Digits (D=64, N=5264, C=10) Ignoring class labels





Turning weaknesses into strengths

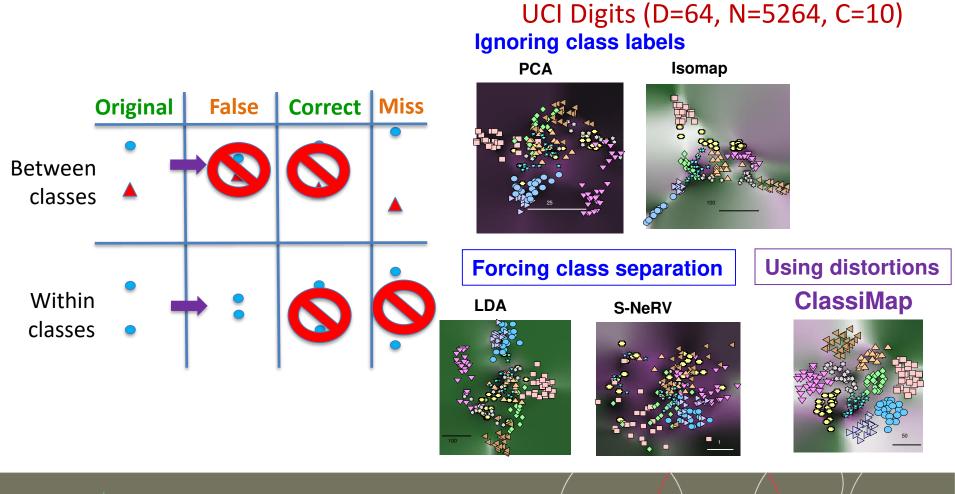
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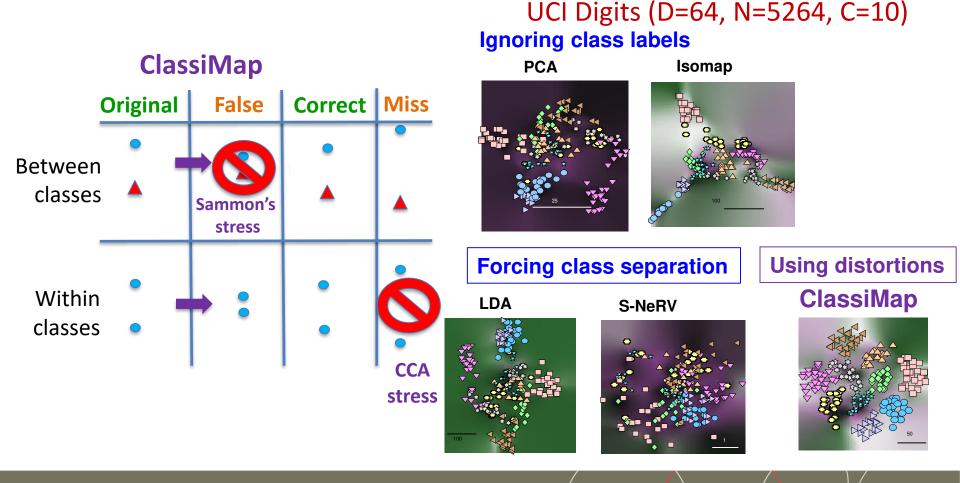
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Turning weaknesses into strengths

Mapping labeled data using distortions



Outline

- What is Dimensionality Reduction
- Strengths
- Weaknesses
- Turning weaknesses into strengths
- Conclusion
- Perspectives





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- Maps are useless without additional information
 - Can generate false pattern
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- Maps are not an end but a mean to support user decision





• Formalization needed to go beyond similarity-based distortions



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 - \circ Outliers
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 - \circ Clusters
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 - o Class structure...
 - What is the impact of similarity distortions on specific pattern detection?
 - Can we design DR techniques tuned to optimize preservation of specific patterns?

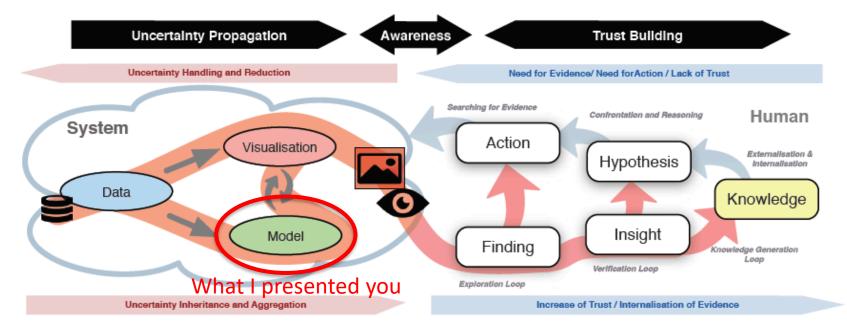


Worth reading

IEEE TRANSACTIONS ON VISUALIZATION AND COMPUTER GRAPHICS, VOL. 22, NO. 1, JANUARY 2016

The Role of Uncertainty, Awareness, and Trust in Visual Analytics

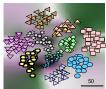
Dominik Sacha, Hansi Senaratne, Bum Chul Kwon, Member, IEEE, Geoffrey Ellis, and Daniel A. Keim, Member, IEEE



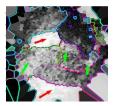




[CheckViz] Lespinats, Aupetit. *CheckViz: Sanity Check and Topological Clues for Linear and Non-Linear Mappings*. Computer Graphics Forum 30(1): 113-125 (2011)



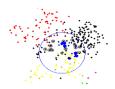
[ClassiMap] Lespinats, Aupetit, Meyer-Baese. ClassiMap: *A New Dimension Reduction Technique for Exploratory Data Analysis of Labeled Data*. IJPRAI 29(6) (2015)



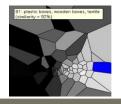
[**ProxiViz**] Aupetit. *Visualizing distortions and recovering topology in continuous projection techniques.* Neurocomputing 70(7-9): 1304-1330 (2007)



[ProxiLens] Heulot, Aupetit, Fekete. *ProxiLens: Interactive Exploration of High-Dimensional Data using Projections* EuroVis 2013 Workshop on Visual analytics using Multidimensional Projections, Leipzig, Germany, June 2013



[HDBrush] Aupetit, Heulot, Fekete. *A multidimensional brush for scatterplot data analytics* Poster at IEEE VIS 2014 conference, Paris, France, November 2014



[ClassiViz] Aupetit, Allano, Espagnon, Sannie. Visual Analytics to Check Marine Containers in the Eritr@c Project EuroVAST (2010)

معهد فط ليدوث الدوست معامد فط ليدوث الدوست Gatar Computing Research Institute Montor of Quer Kinodation Jei عليه

Thank you !

Q&A

- How users perceive these maps, how long it takes them to learn how to use these techniques. For instance Euritrac ClassiViz -> qualitatively but not quantitatively evaluated
- Compare with Nonato connected missed with edge bundle, compare to color coding -> yes, all at one glance while proxiviz requires selecting a focus point, but proxiviz shows the actual data (1 row of the similarity matrix), not a summary (= no free lunch), what is best for users?
- Multi scale topological structure in HD used to enrich map -> yes, could be used to enrich and interact with data
- Dual problem between graph drawing drawing all edges, and approach here where we only draw missed neighbors -> interesting remark, would need more formalism to better understand relations between both approaches

<u>maupetit@hbku.edu.qa</u> <u>https://about.me/michaelaupetit</u>

