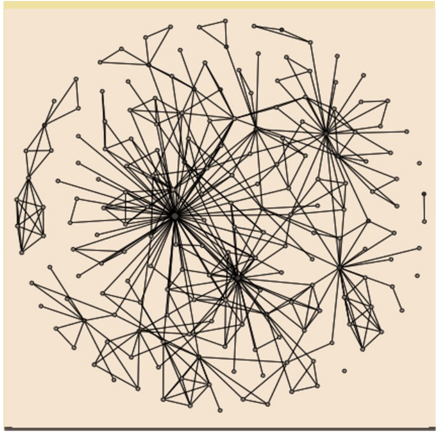
eScience Institute
ADVANCING DATA-INTENSIVE DISCOVERY IN ALL FIELDS

DEPARTMENT OF
STATISTICS



Unsupervised learning
in the age of Big DATA

Marina Meila

Department of Statistics

University of Washington

Supervised, Reinforcement, Unsupervised Learning

- We are witnessing an AI/ML revolution
  - this is led by Supervised and Reinforcement Learning
  - i.e. Prediction and Acting

- Unsupervised learning (clustering analysis, dimension reduction, explanatory models) in a much more primitive state of development
  - Everybody does them
  - Exploration, explanation, understanding
  - Is the next big challenge

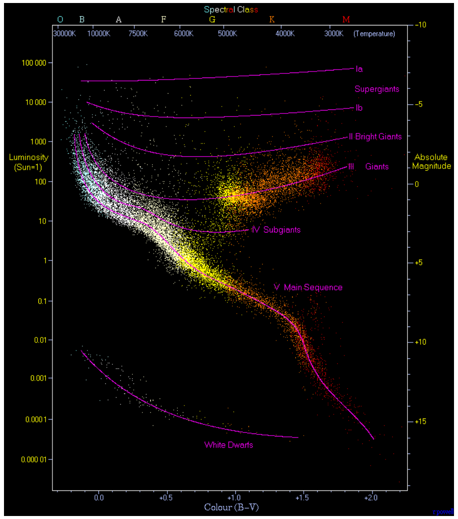
+

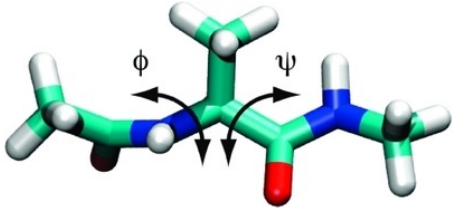
Unsupervised learning is the next big challenge

Research in my group

- Unsupervised learning at scale
  - Clustering
  - Dimension reduction
  - Models for preferences
- Mathematics/theory/theorems/models
  - validation/checking/guarantees
- Algorithms and computation
- Geometry
  - Non-linear dimension reduction
  - Topological data analysis
- Combinatorics
  - Graphs, rankings
  - Clustering

for the sciences





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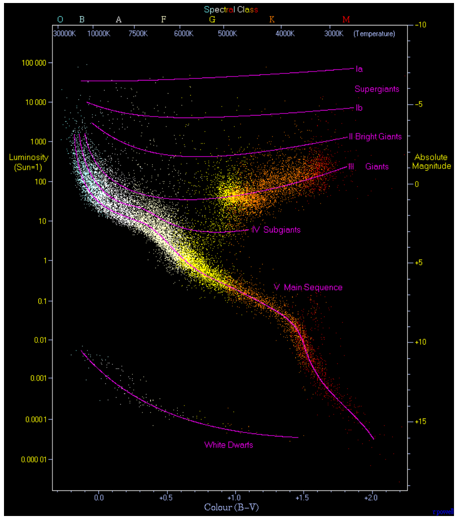

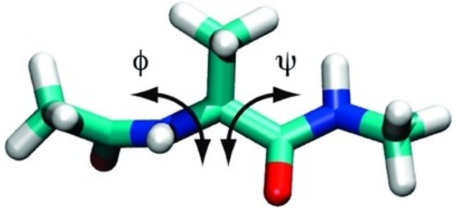

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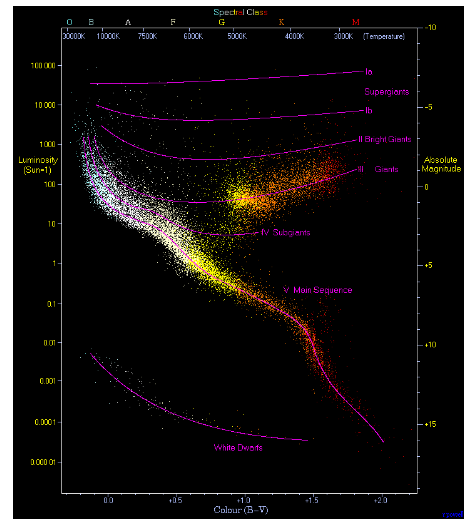

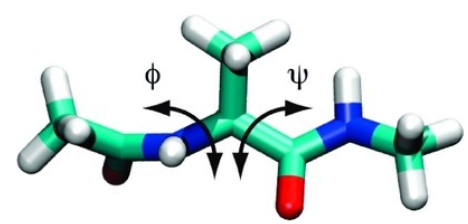

Machine Learning/AI in the picture

(statistics, optimization, theoretical computer science)

Artificial intelligence		Hard sciences
Speech recognition	Finance	Neuroscience
Image captioning	Health	Biology
Self driving cars	Power grid control	Chemistry
Translation	Robotics	Astronomy
Playing chess		Physics

"What a human can do in about 1 second"
-- Andrew Ng cca 2019

Machine Learning in the picture

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Playing chess		Physics

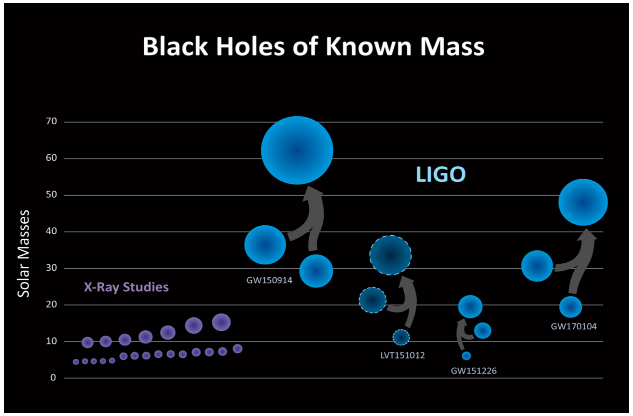
Correct?

Results EASY to validate

Results HARD to validate

Scientific discovery by machine learning and the mythical human "expert"

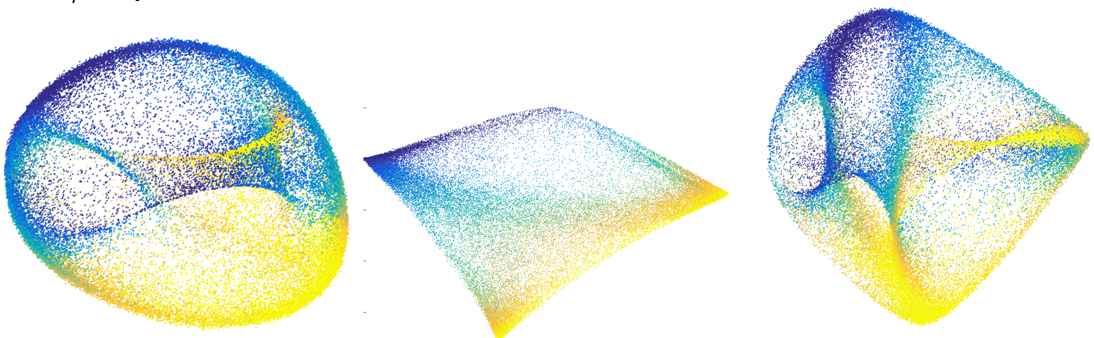
- Big data
  - Allows us to ask more detailed questions (e.g "personalized medicine")
  - Big data contains more complex patterns
  - Machine Learning discovers patterns fast
- Typically – validation by "domain experts"
- Often Hypotheses are cheap, experiments are expensive



Drowning in hypotheses. . .

Validation is the bottleneck

- Validation by visualization
- is qualitative not quantitative
- hard/impossible in dimension > 3



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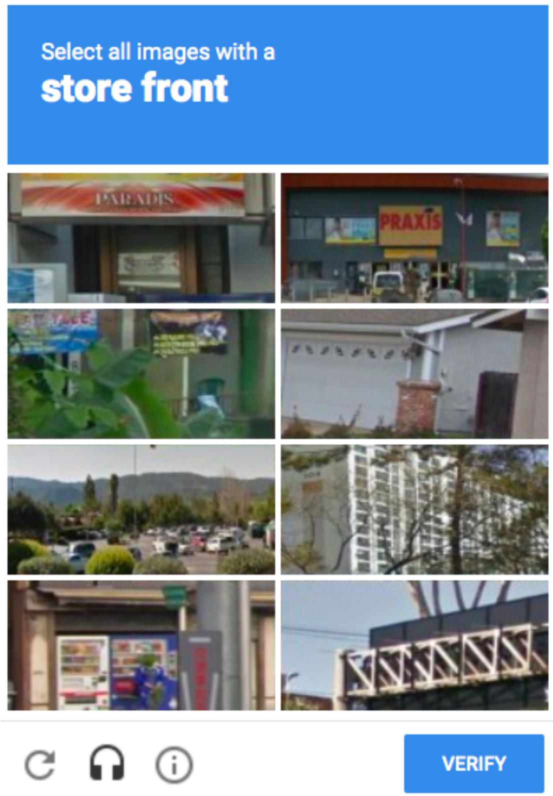

- can't be crowdsourced

Drowning in hypotheses. . .

Validation is the bottleneck

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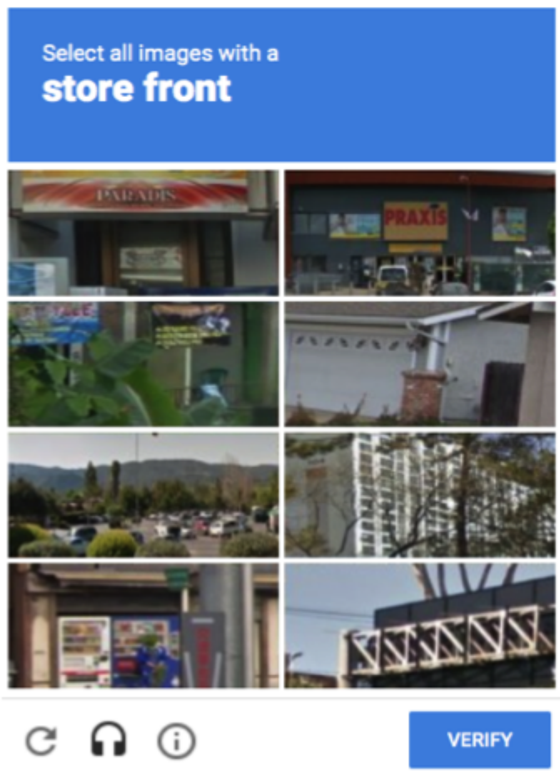
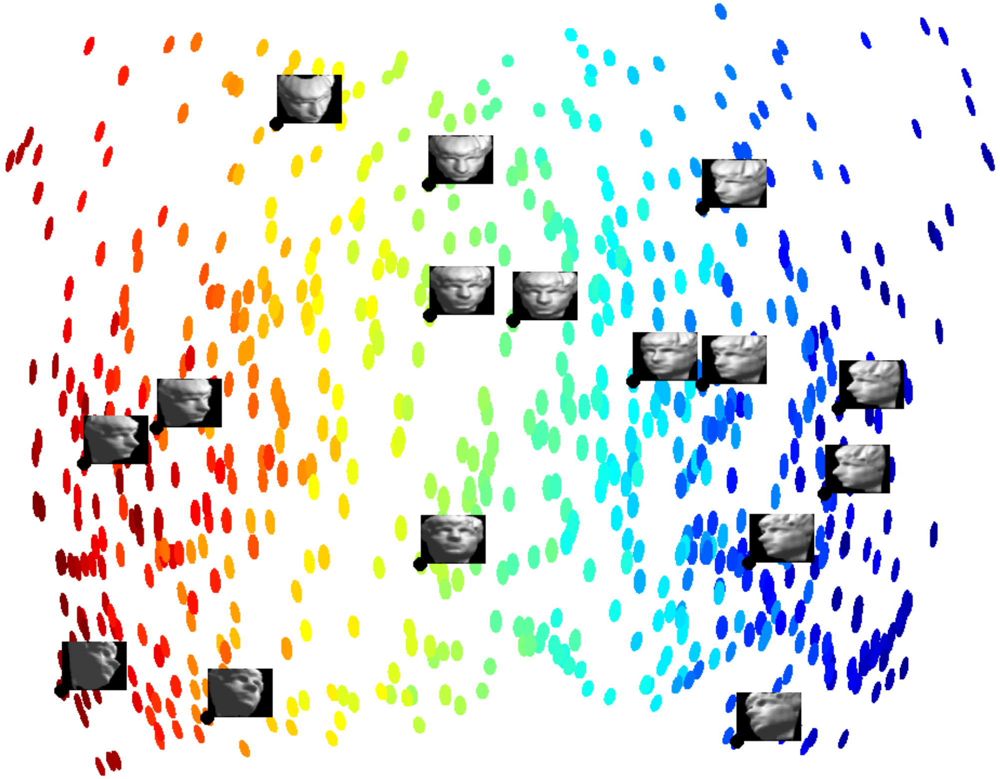


Select all
peptides that bind to this substrate

Select all images with
AGN (Active Galactic Nuclei)

Manifold Learning
non-linear dimension reduction

- When?
  - Data in high dimensions
  - Data can be described by a small number of parameters
  - Large sample size necessary – for consistency



Manifold Learning non-linear dimension reduction

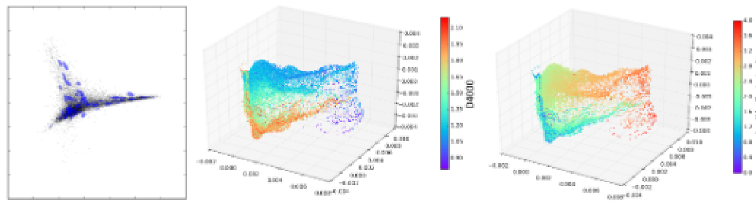
- When?
  - Data in high dimensions
  - Data can be described by a small number of parameters
  - Large sample size necessary – for consistency BIG DATA

- Problems?
- "Too expensive to perform for large data sets"
- Results not comparable between algorithms, "good only for visualization"

Manifold Learning and Clustering for Millions of Points

https://www.github.com/megaman

megaman: Manifold Learning for Millions of Points



build passing | pypi v0.1.1 | license BSD

`megaman` is a scalable manifold learning package implemented in python. It has a front-end API designed to be familiar to scikit-learn but harnesses the C++ Fast Library for Approximate Nearest Neighbors (FLANN) and the Sparse Symmetric Positive Definite (SSPD) solver Locally Optimal Block Precodition Gradient (LOBPCG) method to scale manifold learning algorithms to large data sets. On a personal computer megaman can embed 1 million data points with hundreds of dimensions in 10 minutes. megaman is designed for researchers and as such caches intermediary steps and indices to allow for fast re-computation with new parameters.

Package documentation can be found at http://mmp2.github.io/megaman/

You can also find our arXiv paper at http://arxiv.org/abs/1603.02763

Examples

- Tutorial Notebook

Installation with Conda

The easiest way to install `megaman` and its dependencies is with conda, the cross-platform package manager for the scientific Python ecosystem.

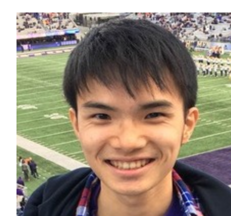
James McQueen

Jake VanderPlas

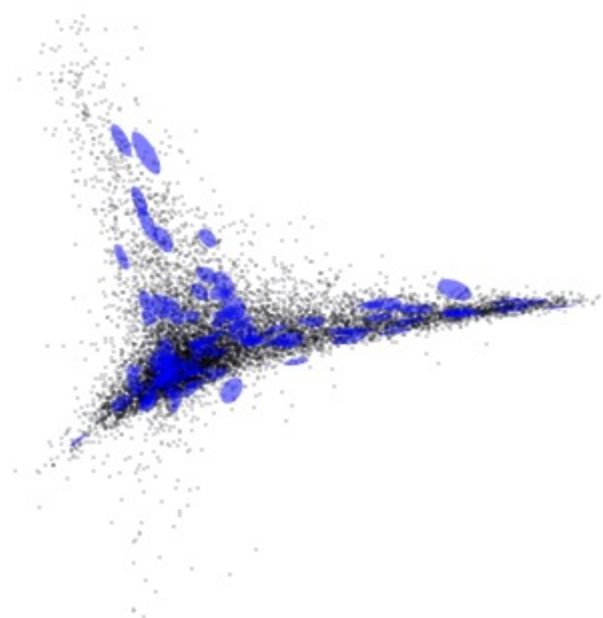
Jerry Zhang

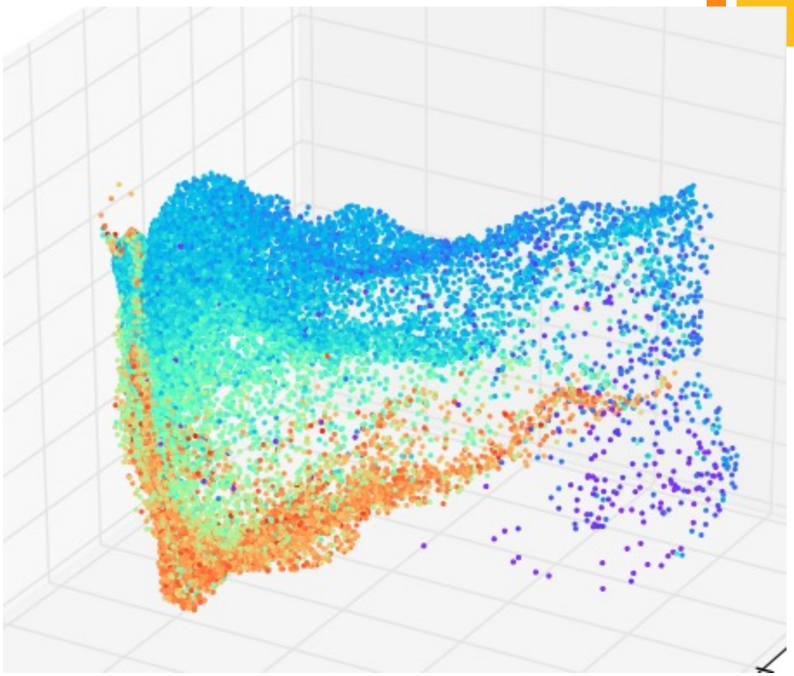
Grace Telford

Yu-chia Chen



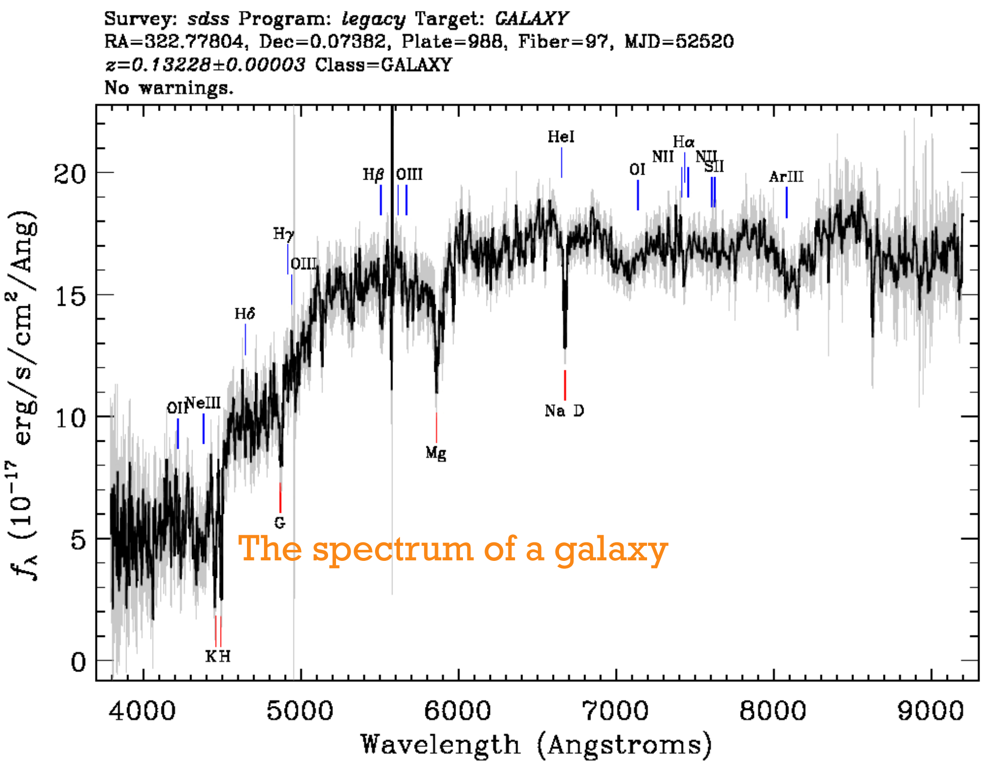
Manifold Learning for Millions of Points

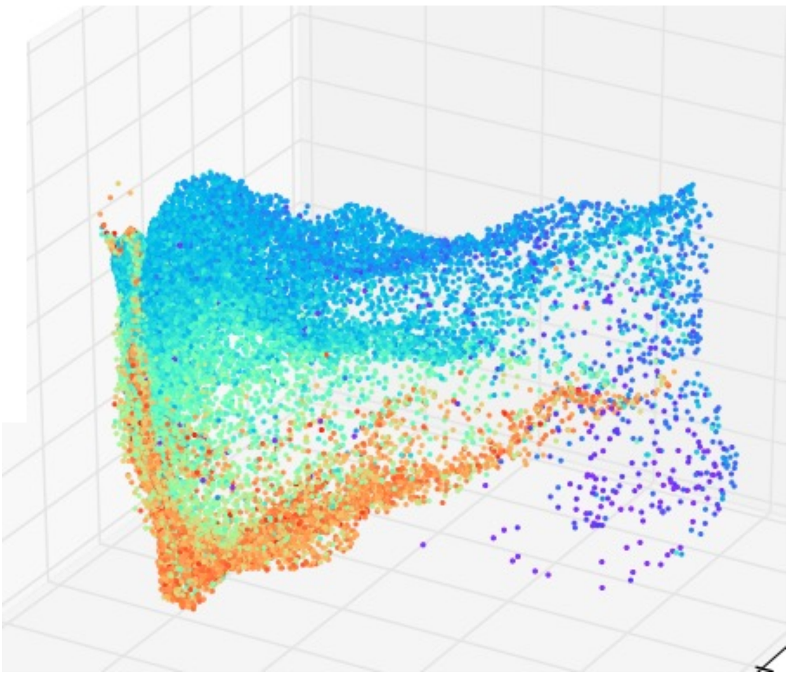


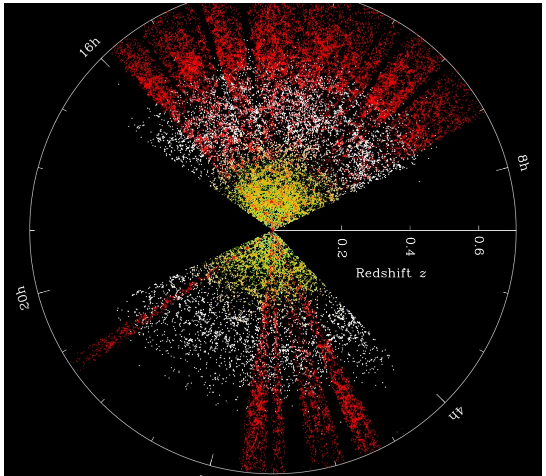


- English words and phrases taken from Google news (3,000,000 phrases originally represented in 300 dimensions by the Deep Neural Network word2vec [Mikolov et al]
- Main sample of galaxy spectra from the Sloan Digital Sky Survey (675,000 spectra originally in 3750 dimensions).
  preprocessed by Jake VanderPlas, figure by Grace Telford

Galaxy spectra from the Sloan Digital Sky Survey (675,000 spectra originally in 3750 dimensions).



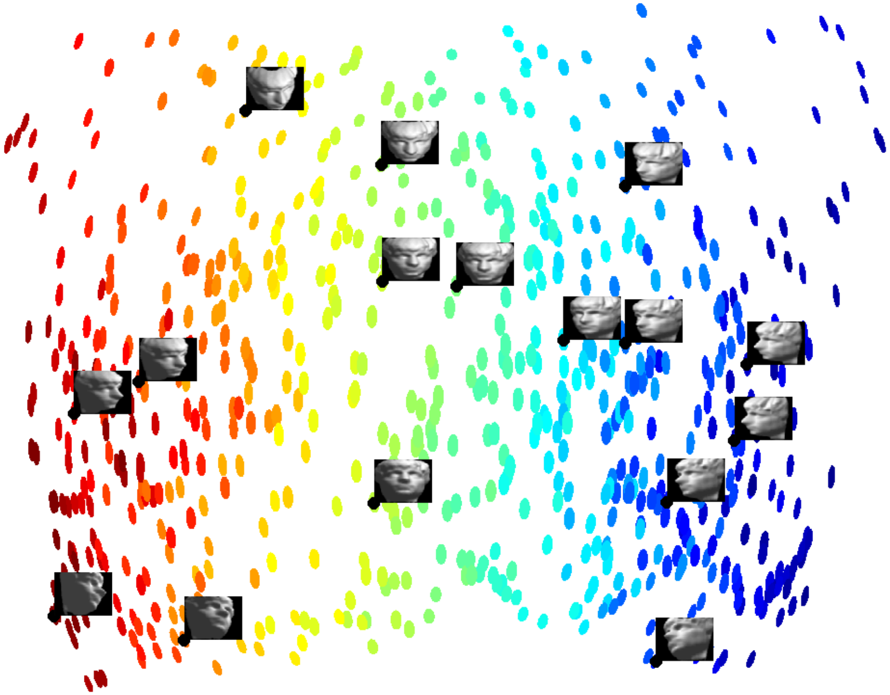




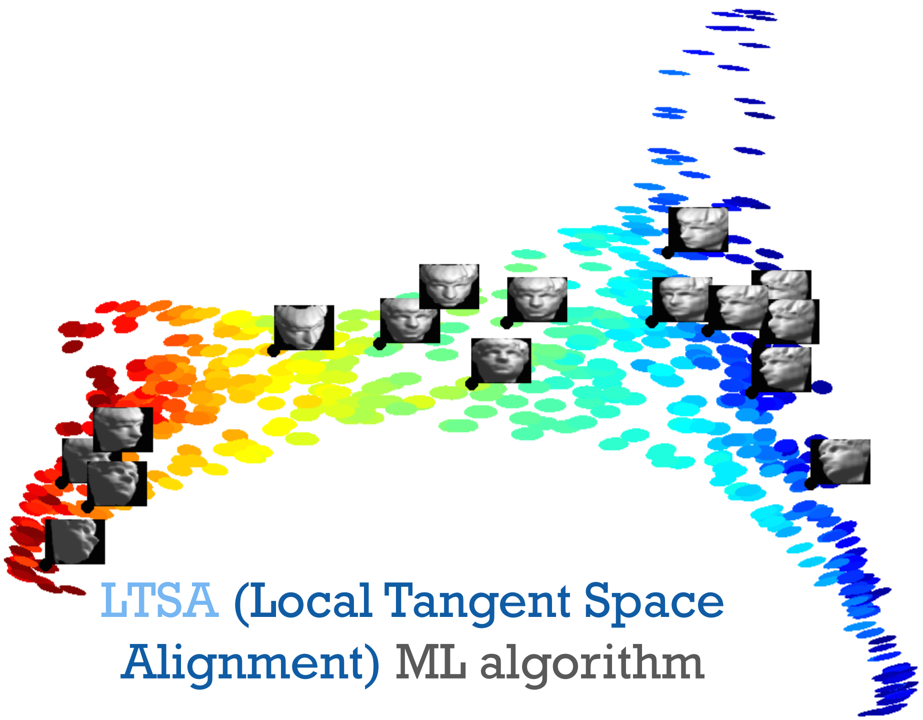
Sloan Digital Sky Survey: where the spectra are from in the Universe

Distortions in Manifold Learning and how to remove them

- We estimate the distortion! (called push-forward Riemannian metric)

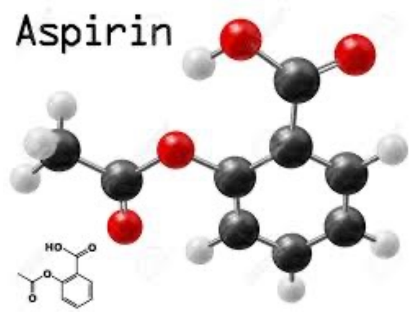


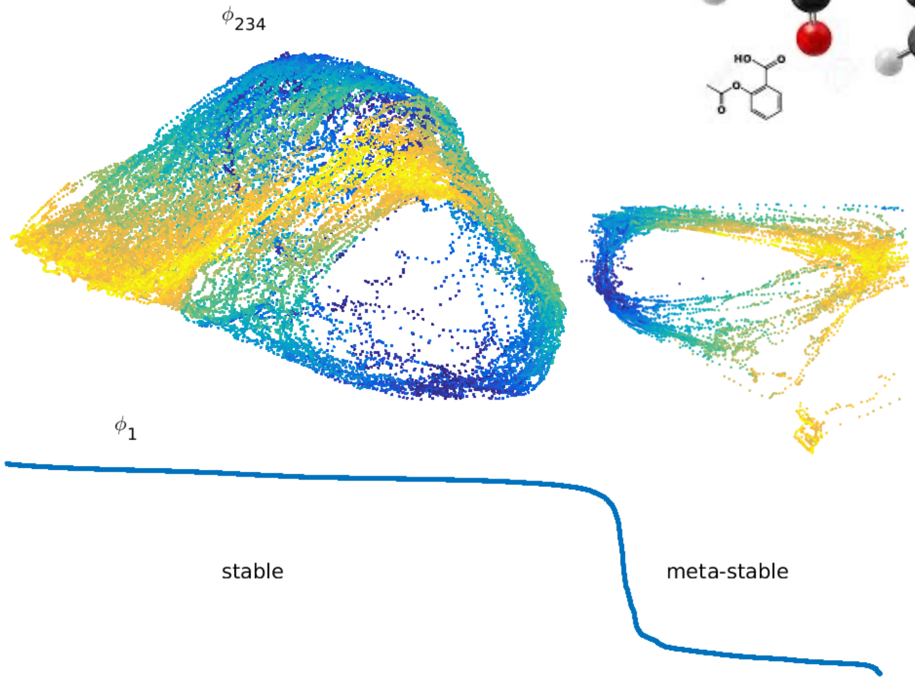
Isomap ML algorithm



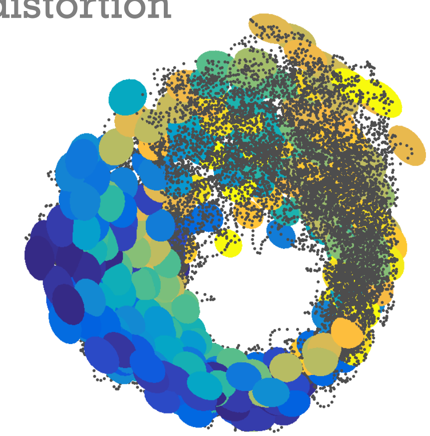
LTSA (Local Tangent Space Alignment) ML algorithm

Exploring the configurations of small molecules





Riemann metric measures geometric distortion

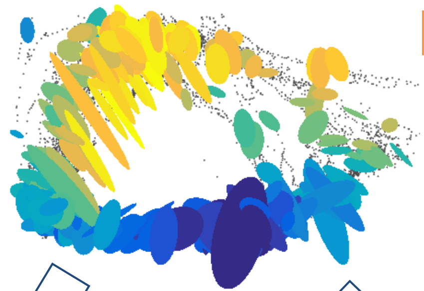


- Configuration space of the Aspirin molecule (210,000 states x 21 atoms x 3 dim) after non-linear embedding with Diffusion Maps, colored by the torsion of the CH_3-C=O bond.

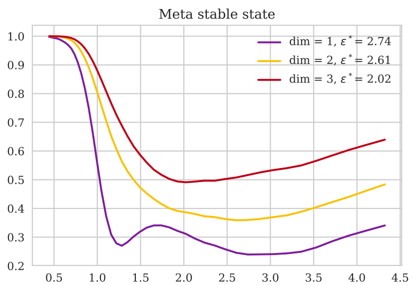
With Alexandre Tkatchenko and Stefan Chmiela.

Argonne NATIONAL LABORATORY “Polymorphic landscapes of molecular crystals” with
Tkatchenko, R. DiStasio, A. Vasquez-Mayagoitia

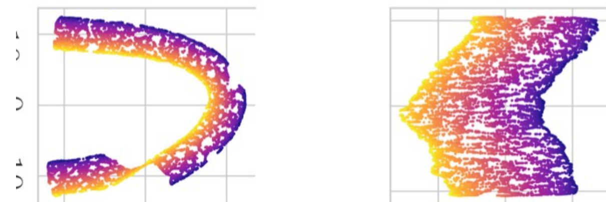
Estimate
Riemannian metric



Optimize
neighborhood size
[NIPS 2016]

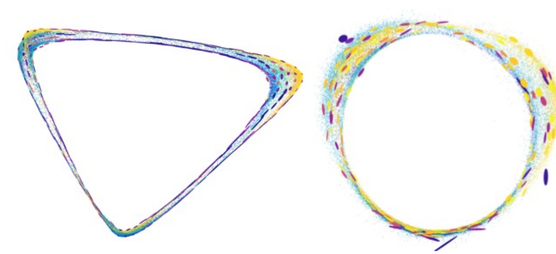


Choose independent e-vectors
[NeurIPS 2019]

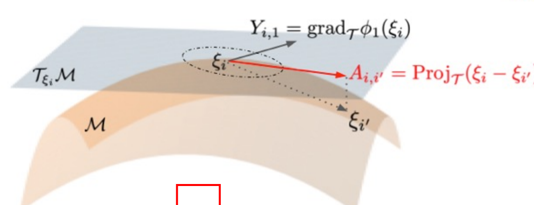


Distances,
angles, areas
preserved

Riemannian relaxation
[NIPS 2015]

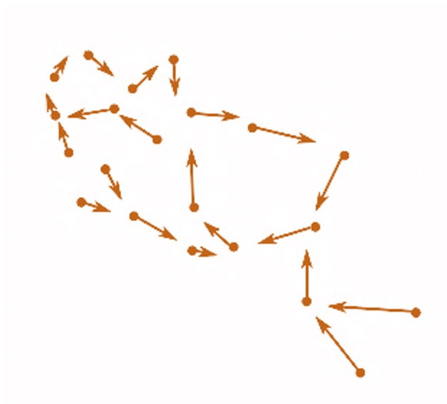


Vector fields
preserved

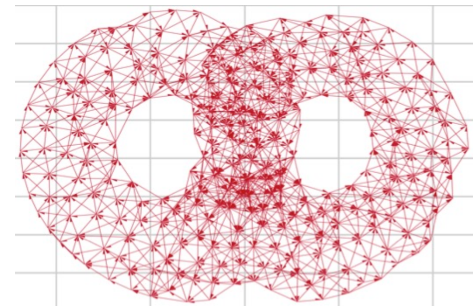


Coordinates with physical meaning

Directed graph embedding
Manifold + vector field [NIPS 2011]

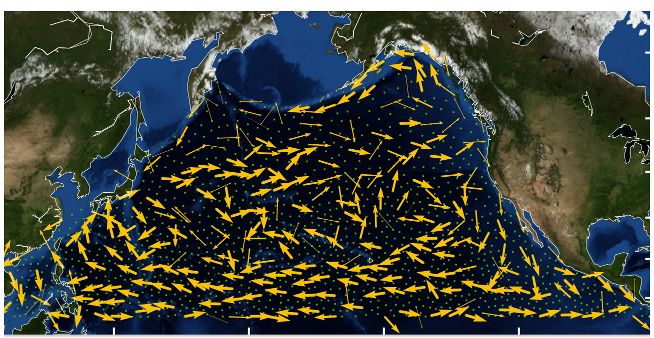


1-Laplacian estimation

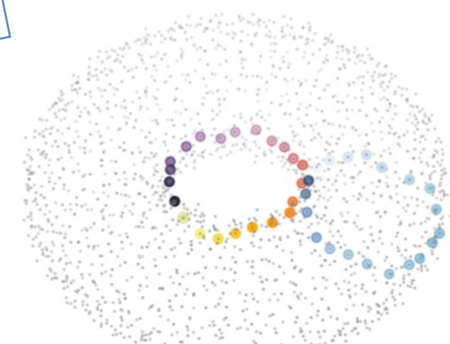


Helmholtz-Hodge
decomposition

Smoothed vector fields

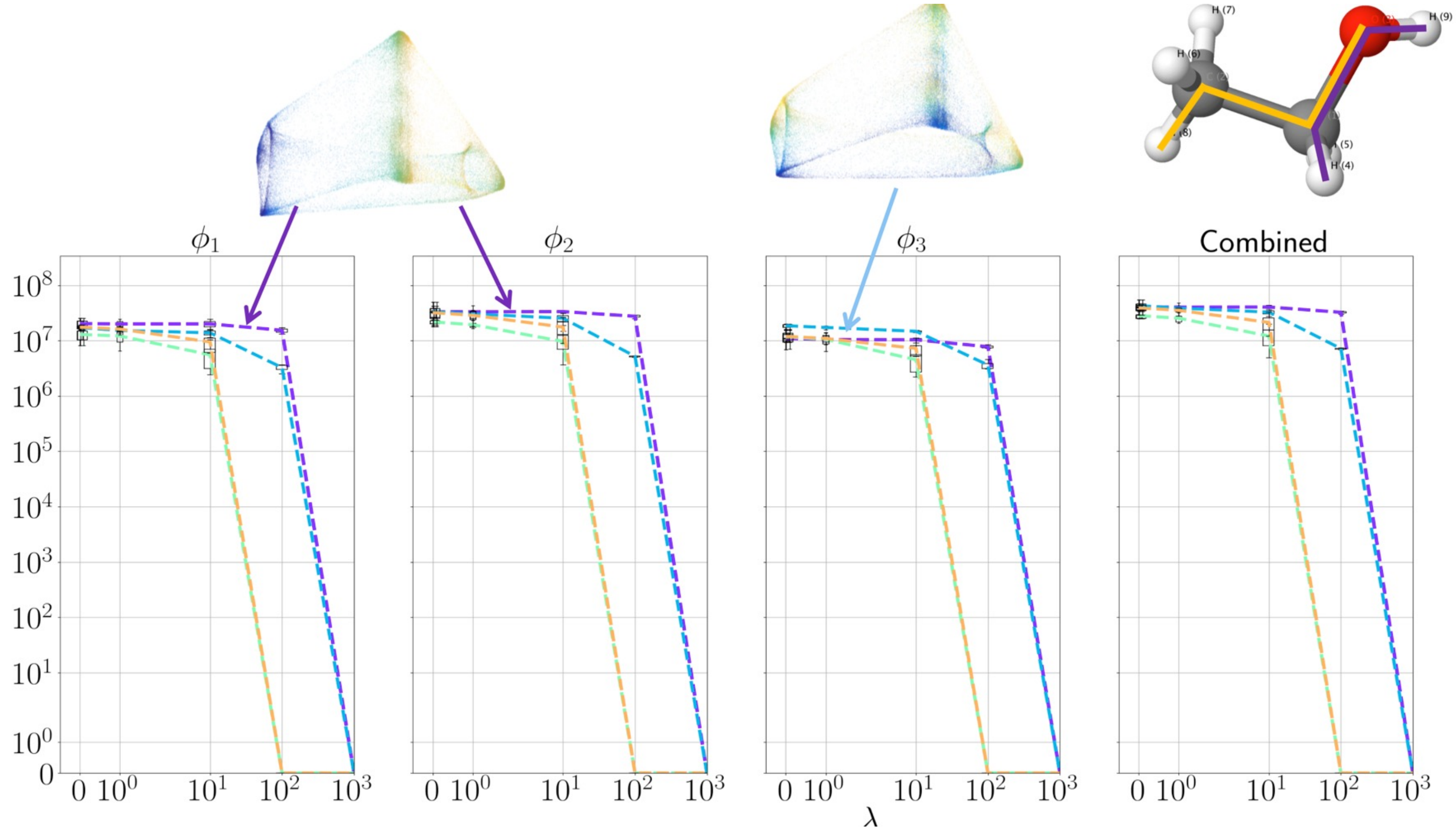


Independent loops
(H_1 basis)



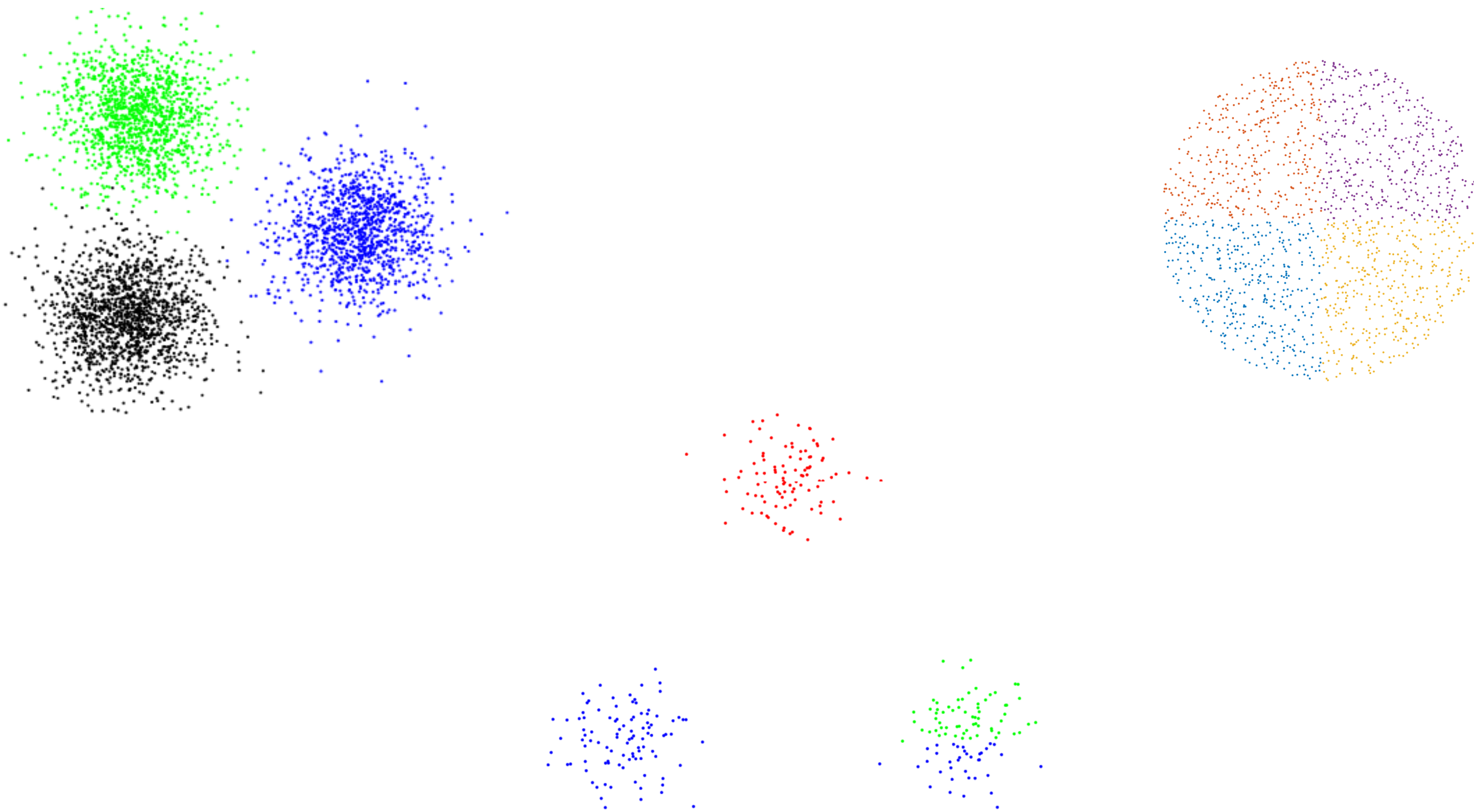
(In progress)

ManifoldLasso: coordinates with physical meaning



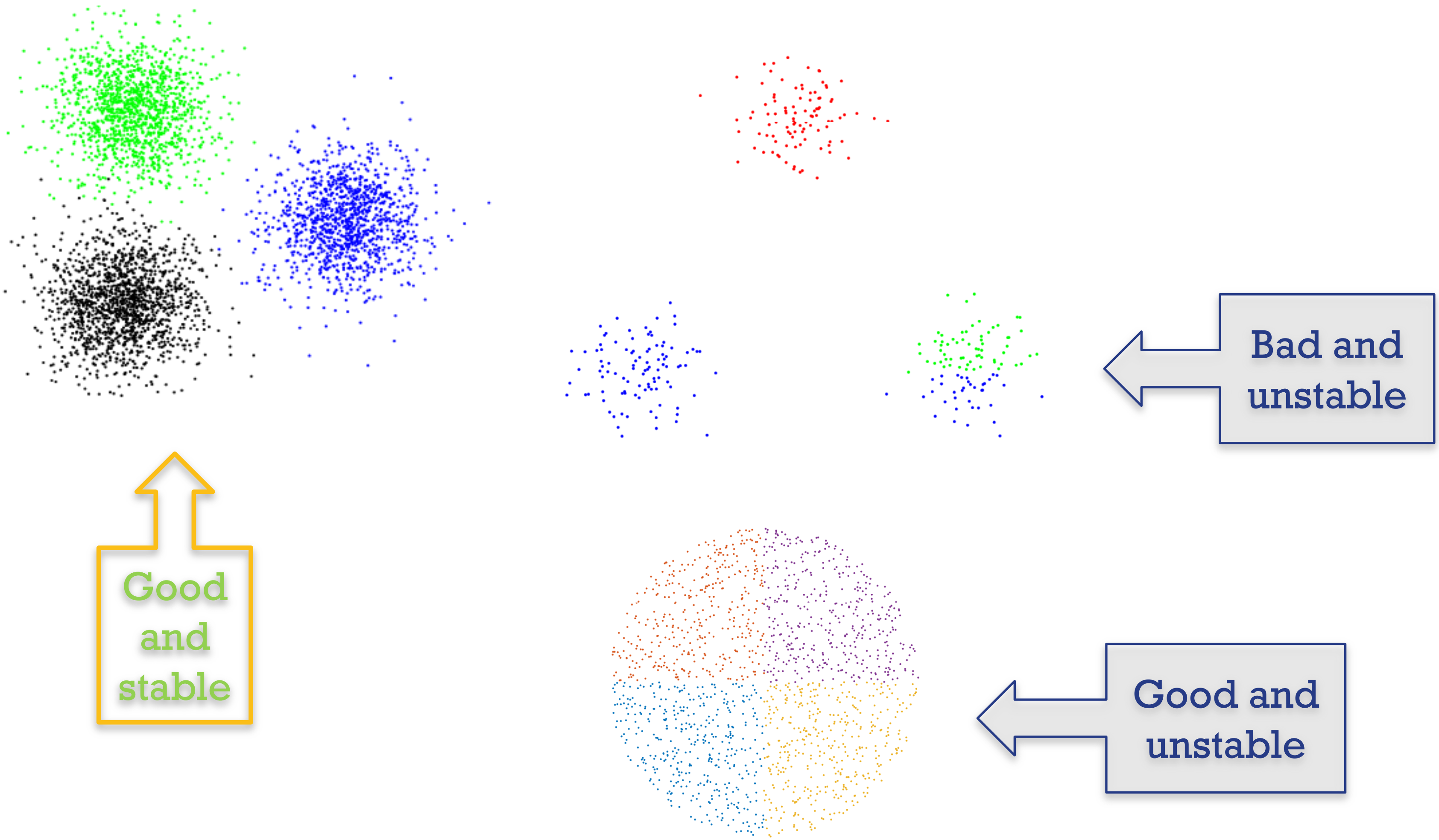
Model free guarantees for clustering

- Given a "good" clustering C of a data set, prove that there is no other good clustering C' too different from C



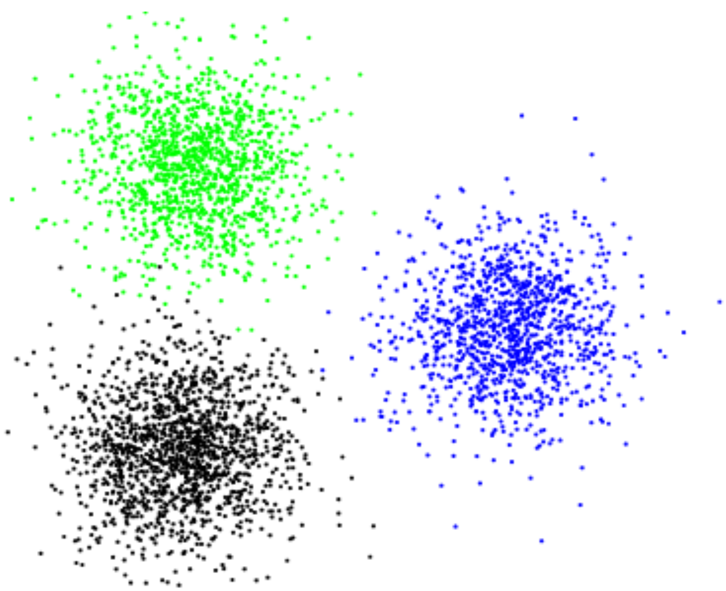
Model free guarantees for clustering

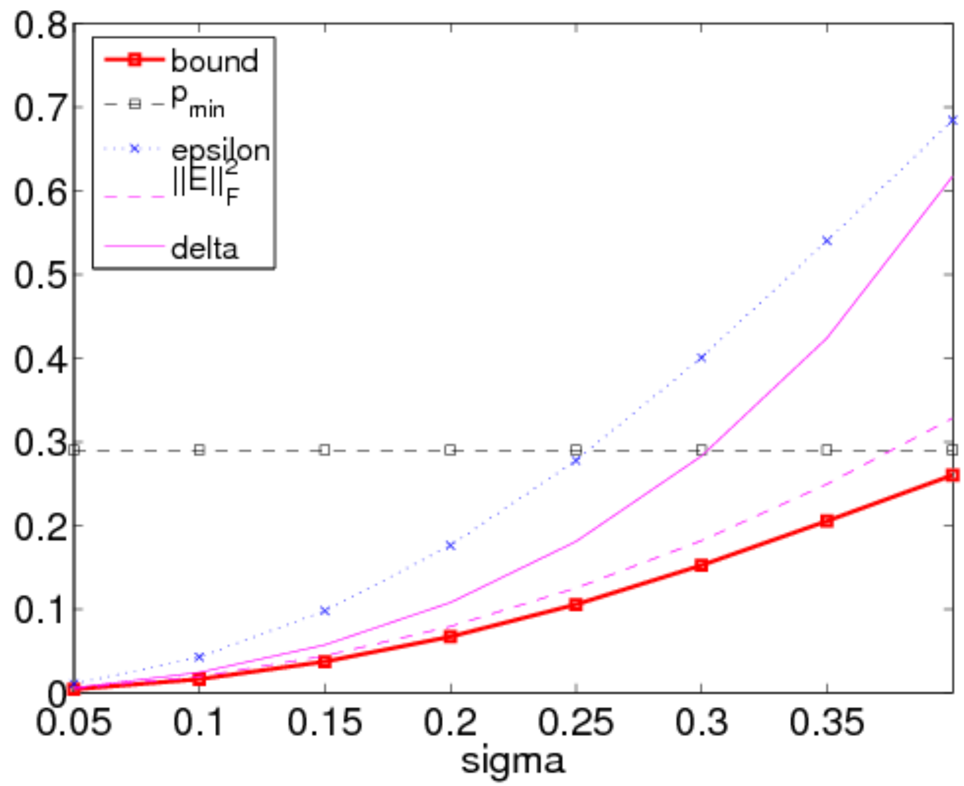
- Given a "good" clustering C of a data set, prove that there is **no other good clustering C'** too different from C



Model free guarantees for clustering

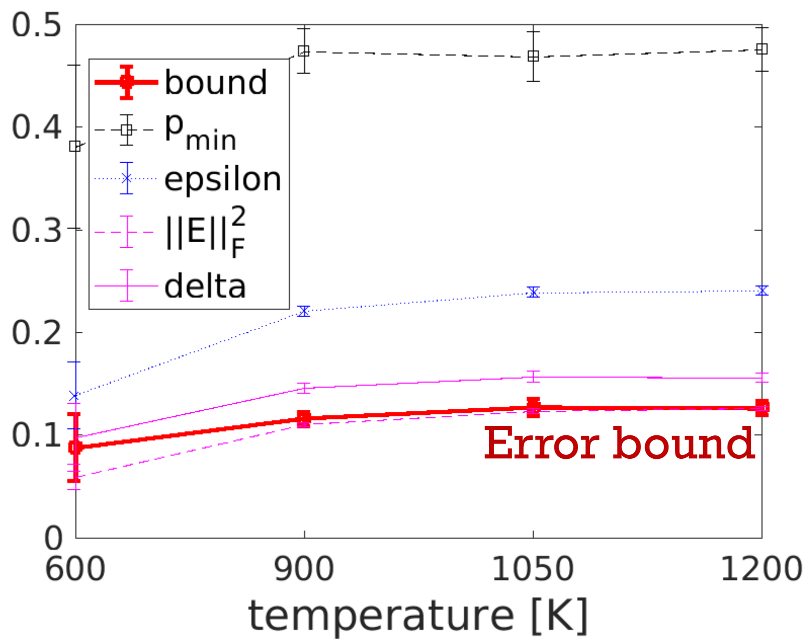
- Framework:
- Given a "good" clustering C of a data set, prove that there is no other good clustering C' too different from C





Clustering with data driven guarantees

$CH_3Cl+Cl^- \leftarrow\rightarrow CH_3Cl+Cl^-$
MD simulation at T=900K
6 atoms x 3 dim



with Jim Pfaendtner and Chris Fu

Modeling Preferences

Burger preferences
$n = 6, N = 600$

```
med-rare med rare ...
done med-done med ...
med-rare rare med ...
```

Elections Ireland, $n = 5, N = 1100$

```
Roch Scal McAl Bano Nall
Scal McAl Nall Bano Roch
Roch McAl
```

College programs $n = 533, N = 53737, t = 10$

```
DC116 DC114 DC111 DC148 DB512 DN021 LM054 WD048 LM020 LM050
WD028
DN008 TR071 DN012 DN052
FT491 FT353 FT471 FT541 FT402 FT404 TR004 FT351 FT110 FT352
```

- Preference data is
  - Discrete
  - Many valued
  - Non-Euclidean
  - Has algebraic/combinatorial structure
- Goal: do "statistics as usual" on large preference data
  - .e.g what is the mean? Variance?
  - Clustering? Regression? Bayesian inference?
  - Estimate the structure of preferences

+ Statistics with rankings

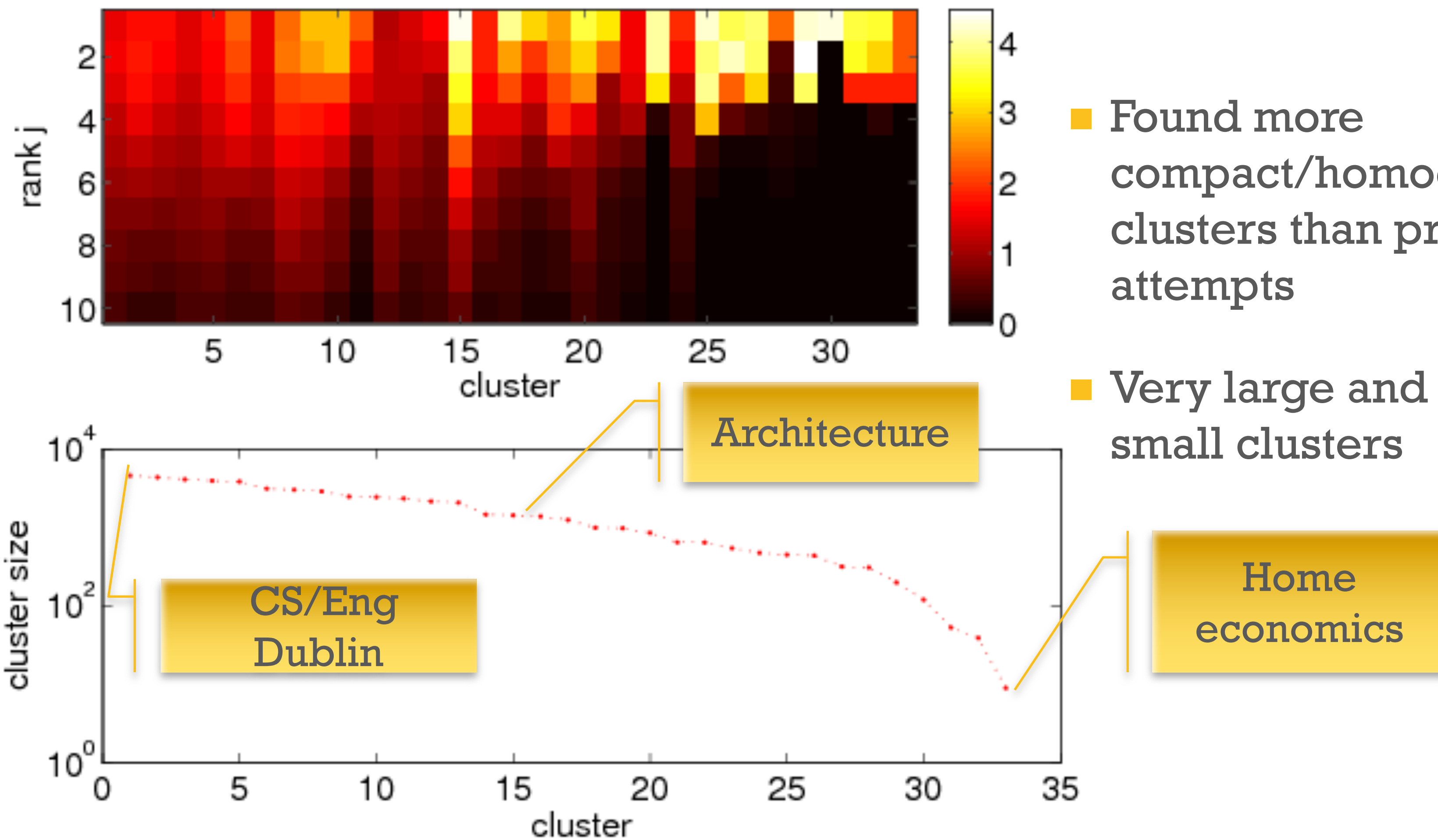
- Modeling permutations by counting inversions
  - Flexible models, with interpretable parameters
  - Allow for efficient computation when consensus exists
  - Adapt to various types of missing data (e.g. top-k rankings, ratings, pairwise comparisons)

- Software github.com/mmp2/dpmm-gmm
  - C+matlab code performing Bayesian non-parametric clustering for ranked data

College programs $n = 533$, $N = 53737$, $t = 10$

```
DC116 DC114 DC111 DC148 DB512 DN021 LM054 WD048 LM020 LM050
WD028
DN008 TR071 DN012 DN052
FT491 FT353 FT471 FT541 FT402 FT404 TR004 FT351 FT110 FT352
```

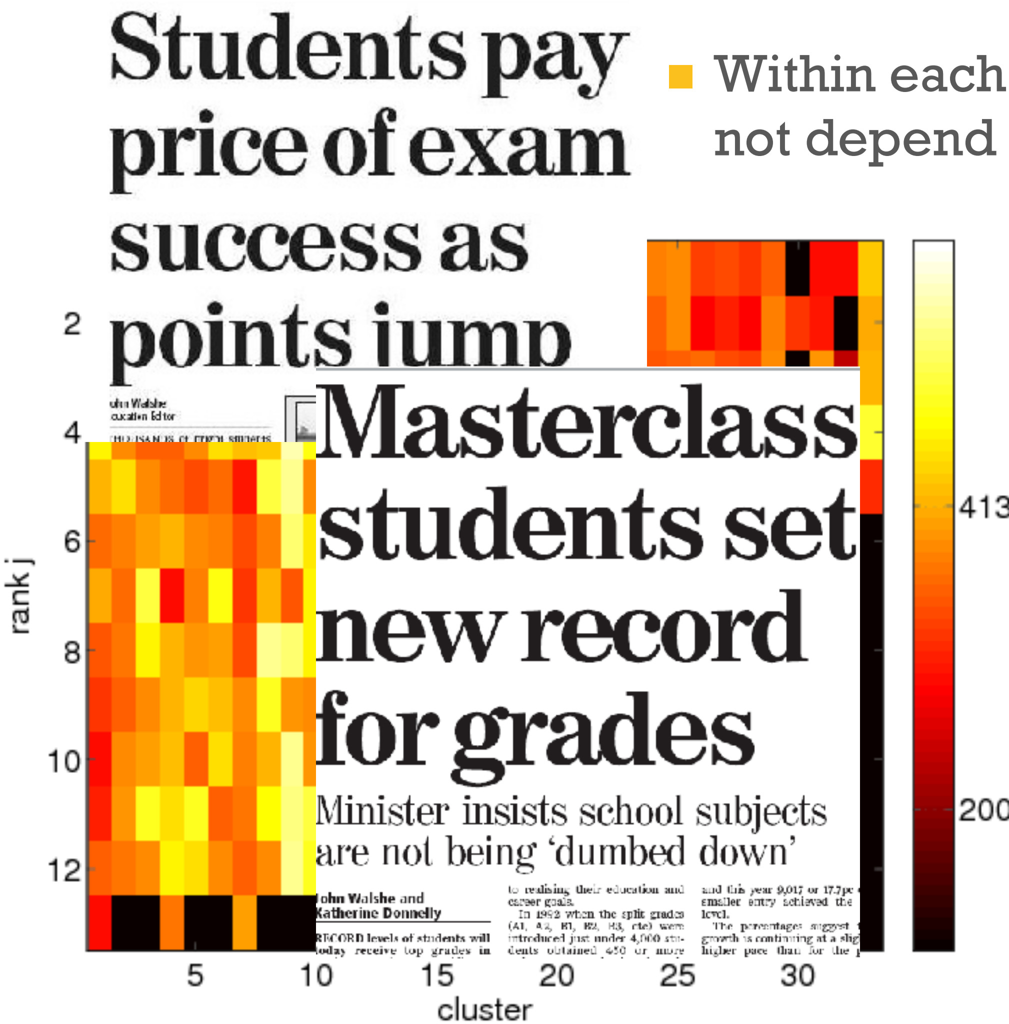
Degree programs preference data: the clusters found

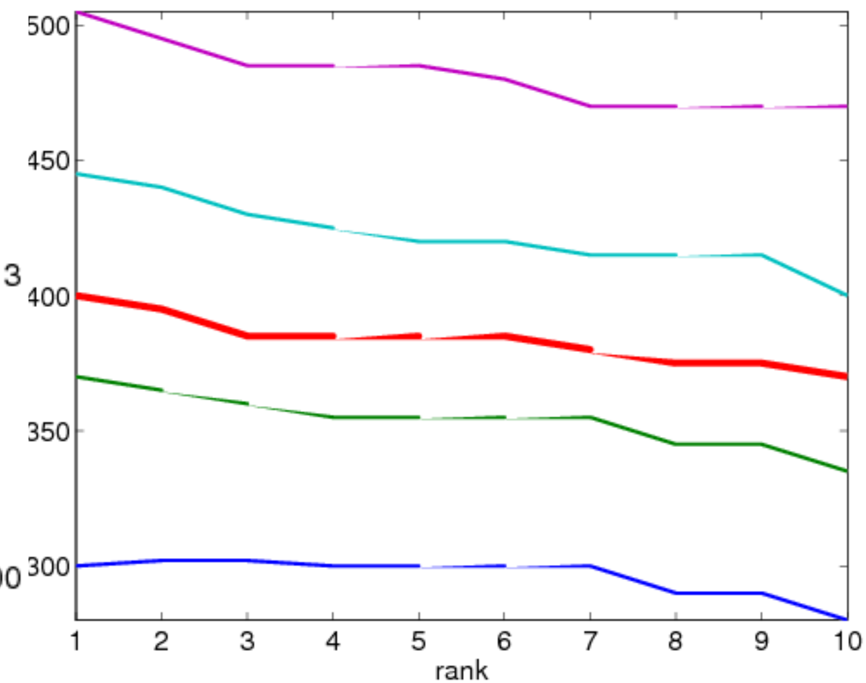


- Found more compact/homogeneous clusters than previous attempts
- Very large and very small clusters

Degree programs preference data: points vs. preferences

- Within each cluster, preferences do not depend on "grades/points" only



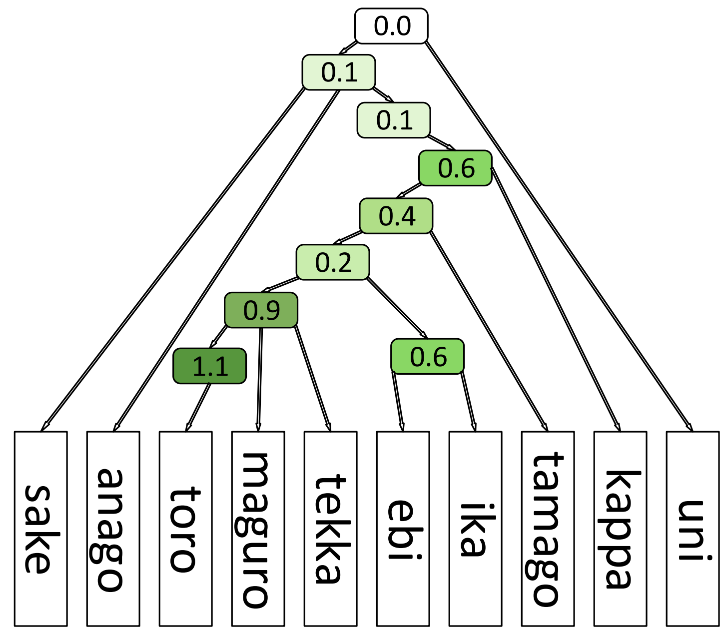


The Structure of preferences

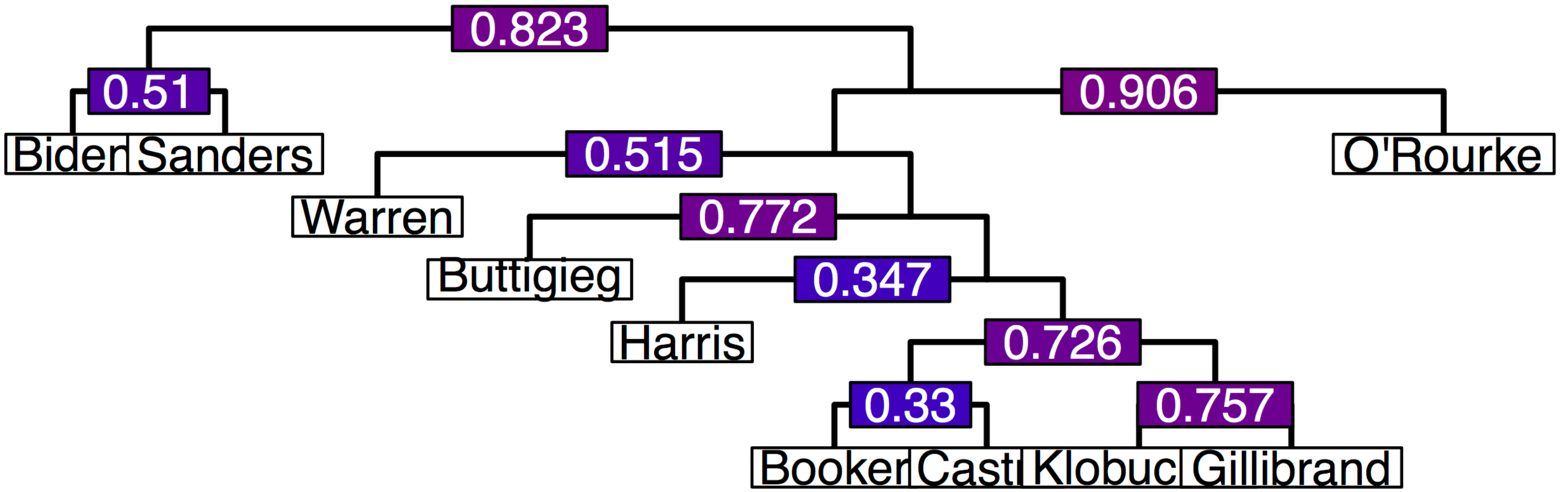
$N = 5000$ people ranked $n = 12$ types of sushi

sake |ebi |ika |uni |tamago |kappa-maki |tekka-maki |anago |toro |maguro
ebi |kappa-maki |tamago |ika |toro |maguro |tekka-maki |anago |sake |uni
toro |ebi |maguro |ika |tekka-maki |uni |sake |anago |kappa-maki |tamago
tekka-maki |tamago |sake |ebi |ika |kappa-maki |maguro |toro |uni |anago
tamago |maguro |kappa-maki |ebi |sake |anago |uni |tekka-maki |toro |ika
uni |toro |ebi |anago |maguro |tekka-maki |ika |sake |kappa-maki |tamago
maguro |ika |toro |tekka-maki |ebi |uni |sake |tamago |anago |kappa-maki

- Preferences have **hierarchical structure**
- This was **estimated from data** (along with consensus and dispersions)
- Current work: **partial rankings**
  sake | ebi,ika |
  uni | toro,ebi,anago | maguro,tekka-maki |



The Structure of preferences



- Applied to peer review, surveys, social choice
- Upcoming Electoral Geometry and Gerrymandering group

Summary -- next challenges

- Finding explanations / descriptions
  - Unsupervised learning
- Validation
  - Of explanations
  - Of scientific hypotheses
  - Is much more costly than generating hypotheses (requires more data, new experiments, expert involvement)

Summary -- next challenges

- Finding explanations / descriptions
  - Unsupervised learning
- Validation
  - Of explanations
  - Of scientific hypotheses
  - Is much more costly than generating hypotheses (requires more data, new experiments, expert involvement)
- With BIG Data – machines must assist humans in validation process
- Mathematics must assist human intuition with non-Euclidean data
- Theory must assist computation (and conversely)

Ongoing and future projects

- Discovery in Materials Science and Molecular Chemistry, Active learning for material discovery (solar cells materials) (Alex)
- Discovering the structure of point clouds = geometric data analysis (James, Weicheng)
  - interpretable coordinates,
  - ML with vector fields,
  - finding the boundary of the data manifold,
  - manifolds with noise,
  - finding the loop basis and prime manifold decomposition
- Networks – which graph properties are stable/statistically significant?
- Modeling preferences and applications to peer review
- Clustering with data driven guarantees

…at the scale of the current data

What do my students do?

- Implement in python
- Apply to scientific data/problems (data analysis)
- Develop algorithms and methods
- Think geometrically
- Prove consistency or (sometimes) use other people's proofs

What do they need to know?

- Be a reliable programmer
- 580s (some), multivariate analysis, non-parametric statistics
- Optimization/combinatorics/graph theory/CS algorithms/differential geometry – depending on the research topic
- Select ML areas (e.g sparse regression) – go deeper as needed
- Willingness to learn new math or ML

Thank You!