Inference, Computation, & Dynamic Visualization for Convex Clustering

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June 5, 2018

Motivation: Clustering & Biclustering

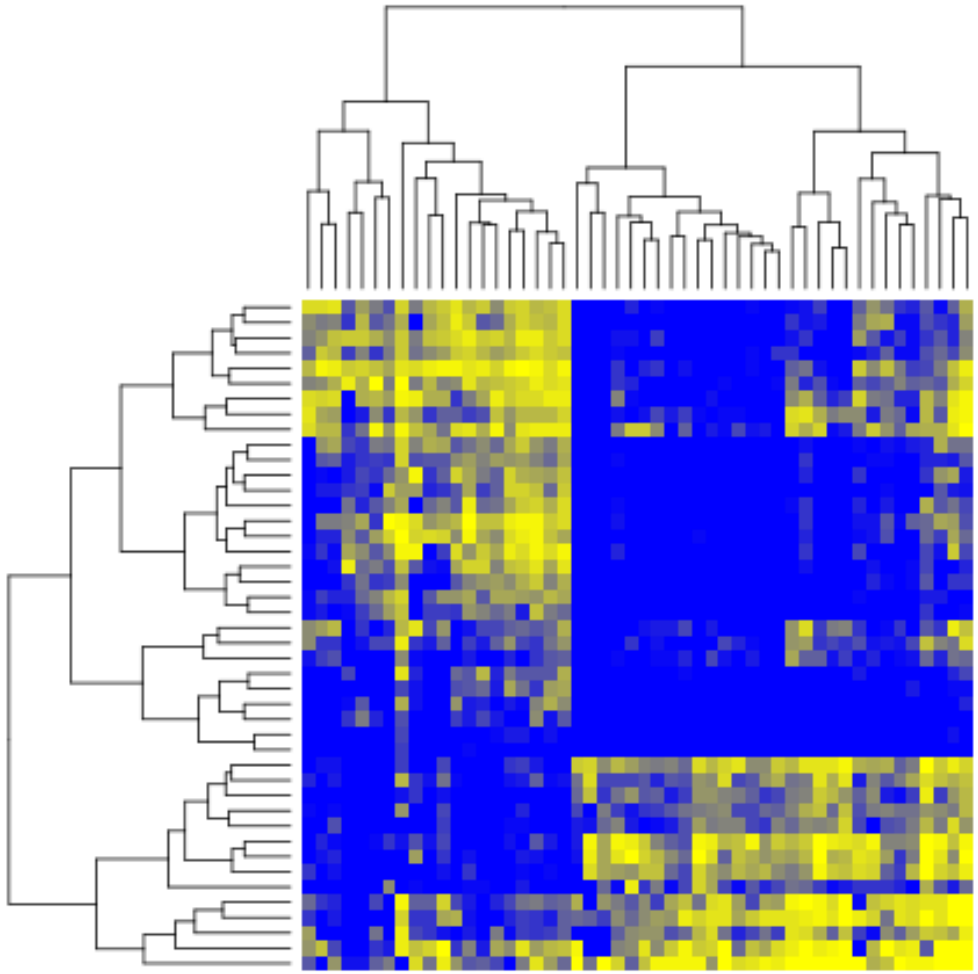
Clustering

Find groups of objects which are similar to each other.

Biclustering

Simultaneously find groups of features & observations.

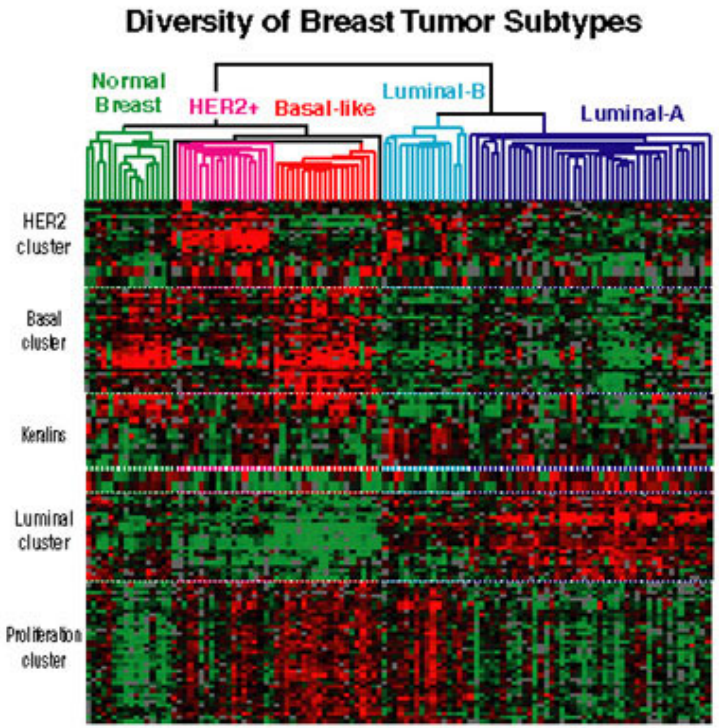
- Cluster rows & columns of data matrix.



Motivation: Clustering & Biclustering

Cancer Subtypes:
Groups of patients that share distinct genomic signatures and exhibit differing clinical outcomes.

- Major Success Story:
  Breast Cancer.
- Significance:
  Precision medicine!



Motivation: Clustering & Biclustering

Text Mining:

	data	R	big	cluster	shiny	fast	plot
doc 1	57	1	43	2	0	22	4
doc 2	17	29	2	3	35	6	44
doc 3	47	33	0	0	24	3	19
doc 4	23	0	0	31	0	7	2
doc 5	40	5	28	9	0	21	6
doc 6	8	10	7	46	12	17	9

Motivation: Clustering & Biclustering

Recommender Systems:

2			4	5	
5		4			1
		5		2	
	1		5		4
		4			2
4	5		1		

Clustering Approaches

The Good:

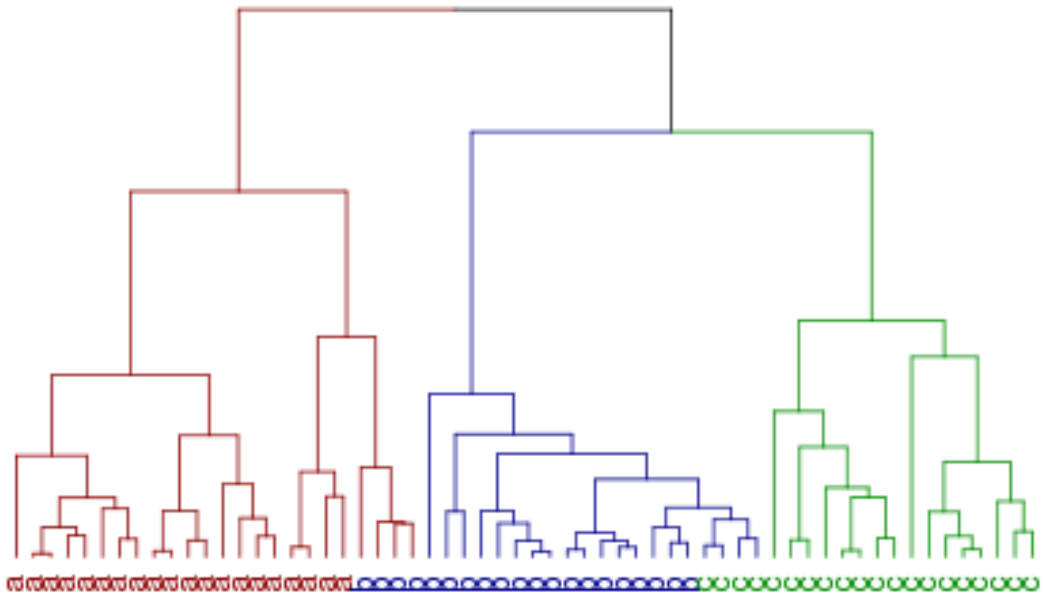
- Simple & Fast.
- Appealing Visualizations.
- Easy Interpretation.

The Bad:

- Local solutions.
- Instability.
- Tuning parameters.

The Ugly:

- How many clusters?
- Inference.



Hierarchical

Convex Clustering & Biclustering

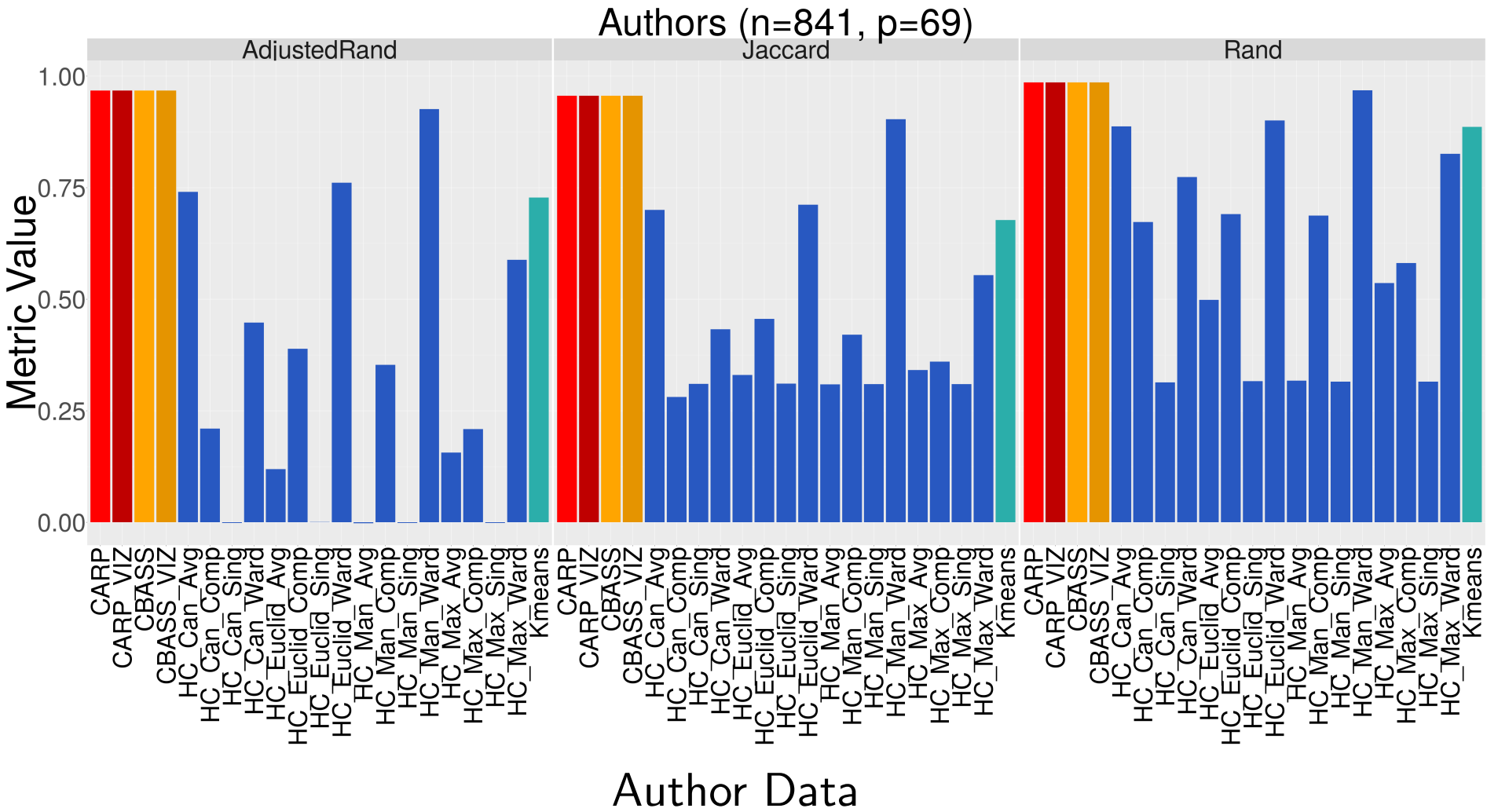
Solution: Convex Clustering & Biclustering

Why Convex?

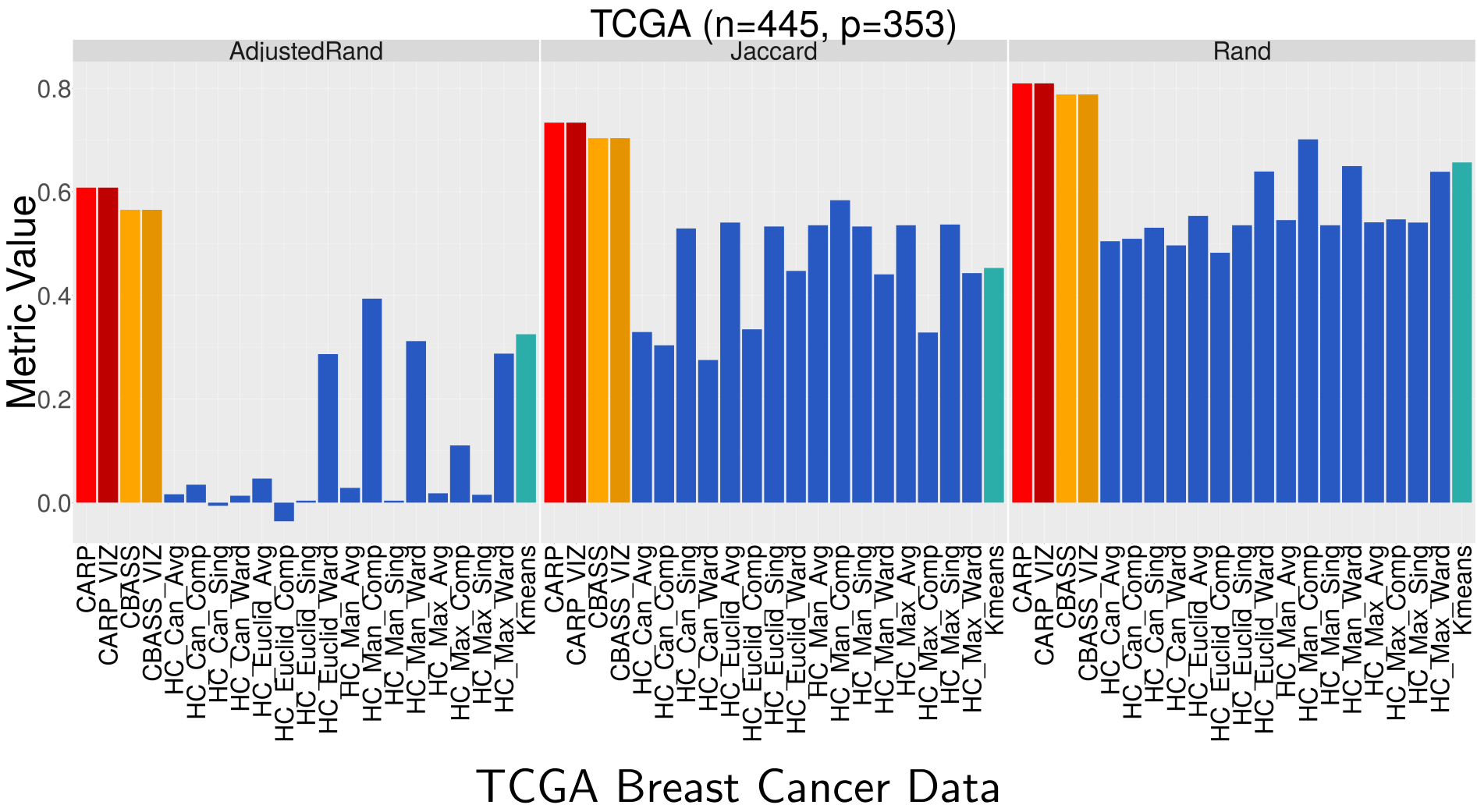
- Global solution!
- Superior mathematical and statistical properties:
  - Consistency.
  - Stability.
  - Improved clustering performance.
- Data-driven selection of # of clusters.

Pelckmans et al. 2005; Lindsten et al. 2011; Hocking et al. 2011; Chi & Lange 2013; Tan & Witten 2015; Chi, Allen & Baraniuk, 2017; Radchenko & Mukherjee, 2017

Clustering Accuracy



Clustering Accuracy



Convex Clustering

$$\underset{\mathbf{u}}{\text{minimize}} \quad \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \lambda \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

- $\mathbf{x}_i$ - each observation (p-vector).
- $\mathbf{u}_i$ - cluster centroid for each observation.

Convex fusion penalty shrinks centroids together!

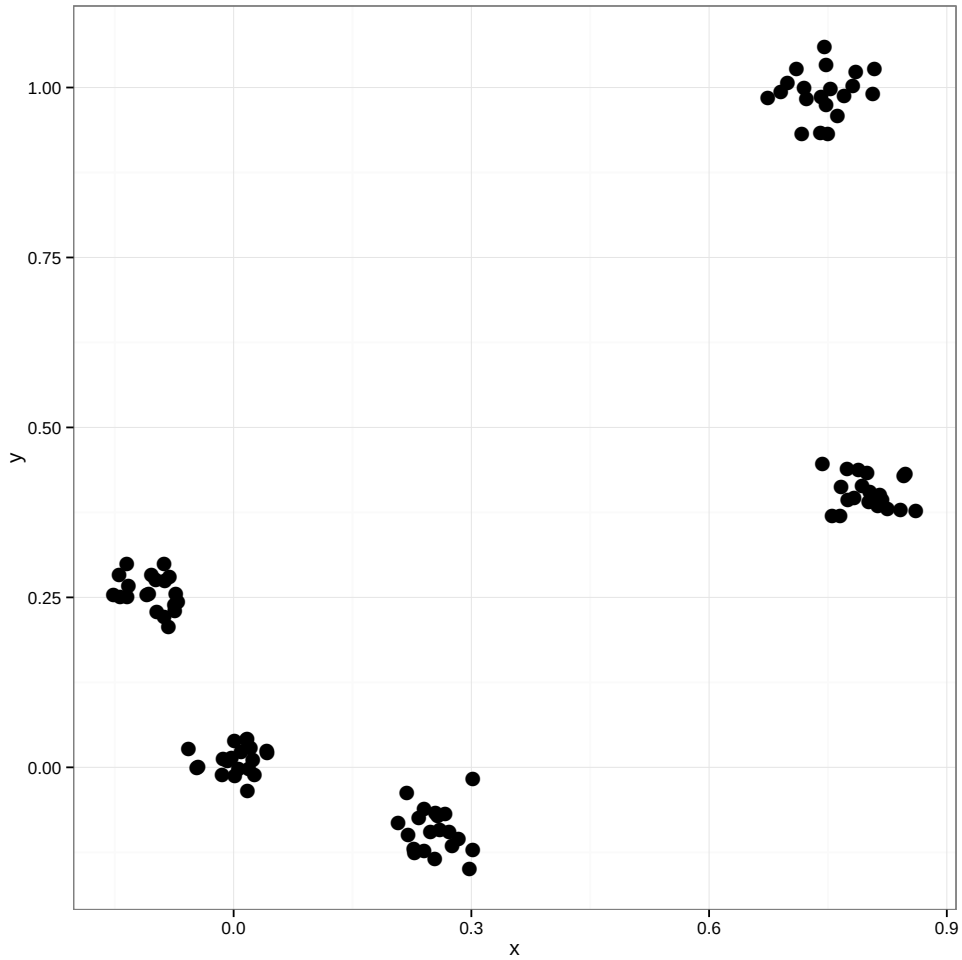
Pelckmans et al. 2005; Lindsten et al. 2011; Hocking et al. 2011; Chi & Lange 2013; Tan & Witten 2015.

Convex Clustering

$$\underset{\mathbf{u}}{\text{minimize}} \quad \frac{1}{2}\sum_{i=1}^{n}\|\mathbf{x}_i - \mathbf{u}_i\|_2^2 + \lambda \sum_{i<j} w_{ij}\|\mathbf{u}_i - \mathbf{u}_j\|_2$$

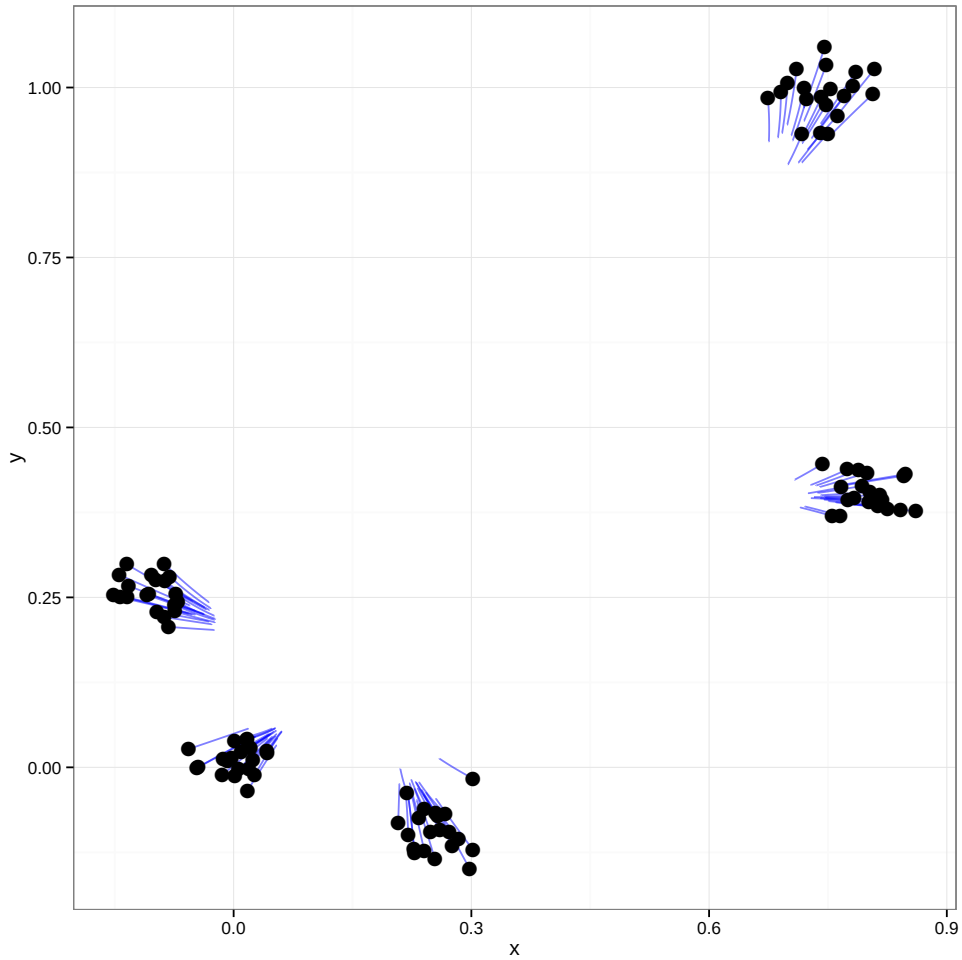
- λ controls BOTH cluster assignments & number of clusters.
  - $\lambda = 0$ - each observation is its own cluster.
  - λ larger - column means begin to coalesce together into clusters.
  - λ very large - all observations fused into one cluster.
- Algorithm: Alternating Minimization Algorithm.
- In R: `cvxclustr`.

Convex Clustering Solution Path



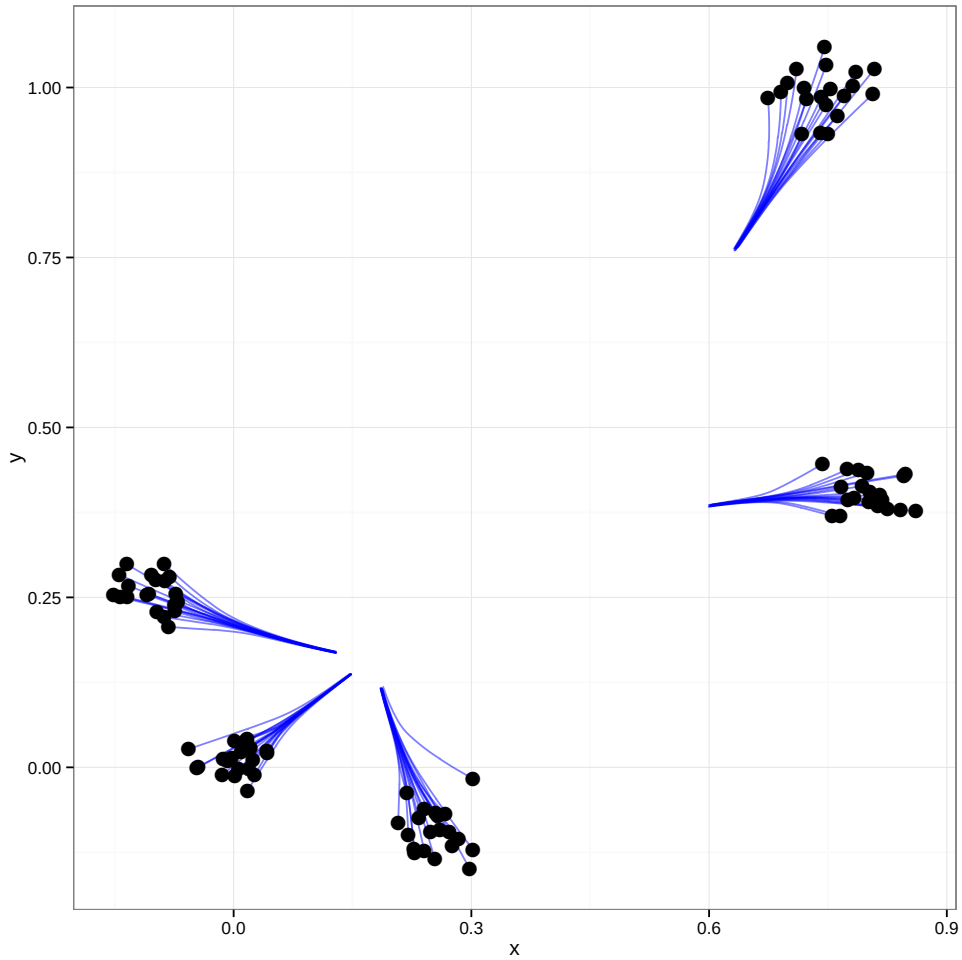
$\lambda = 0$

Convex Clustering Solution Path



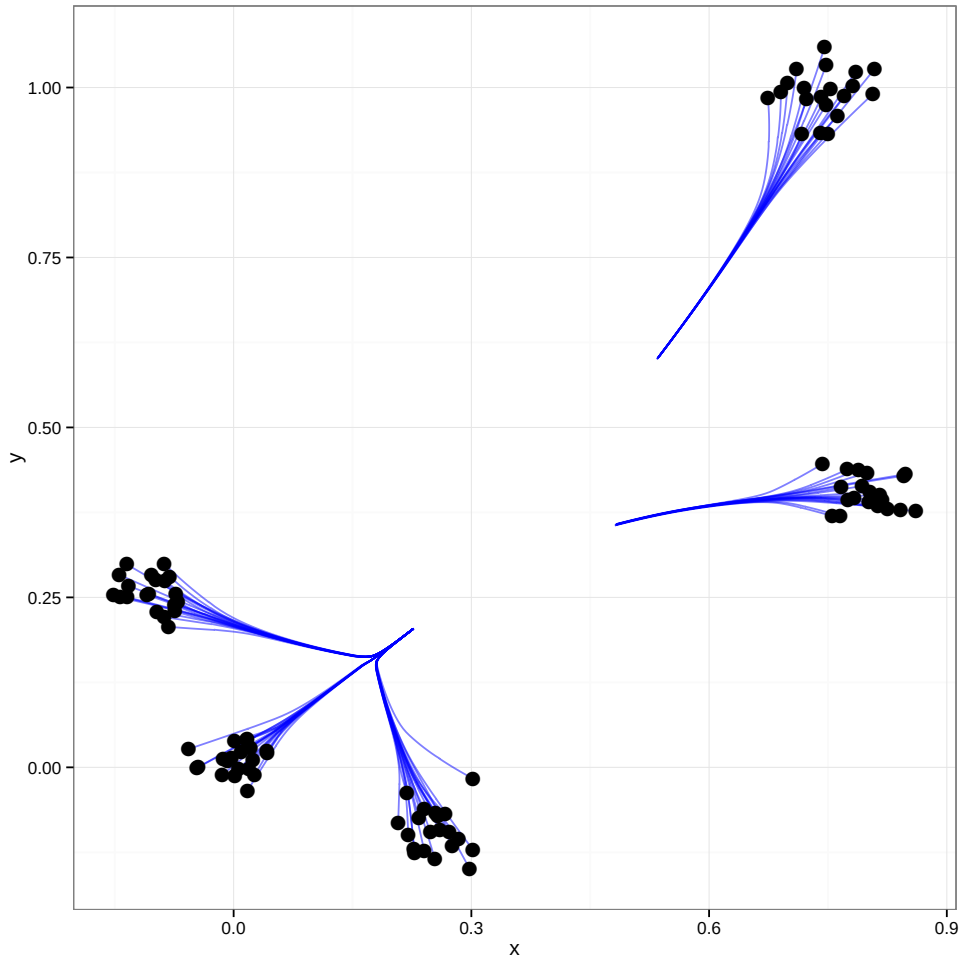
λ

Convex Clustering Solution Path



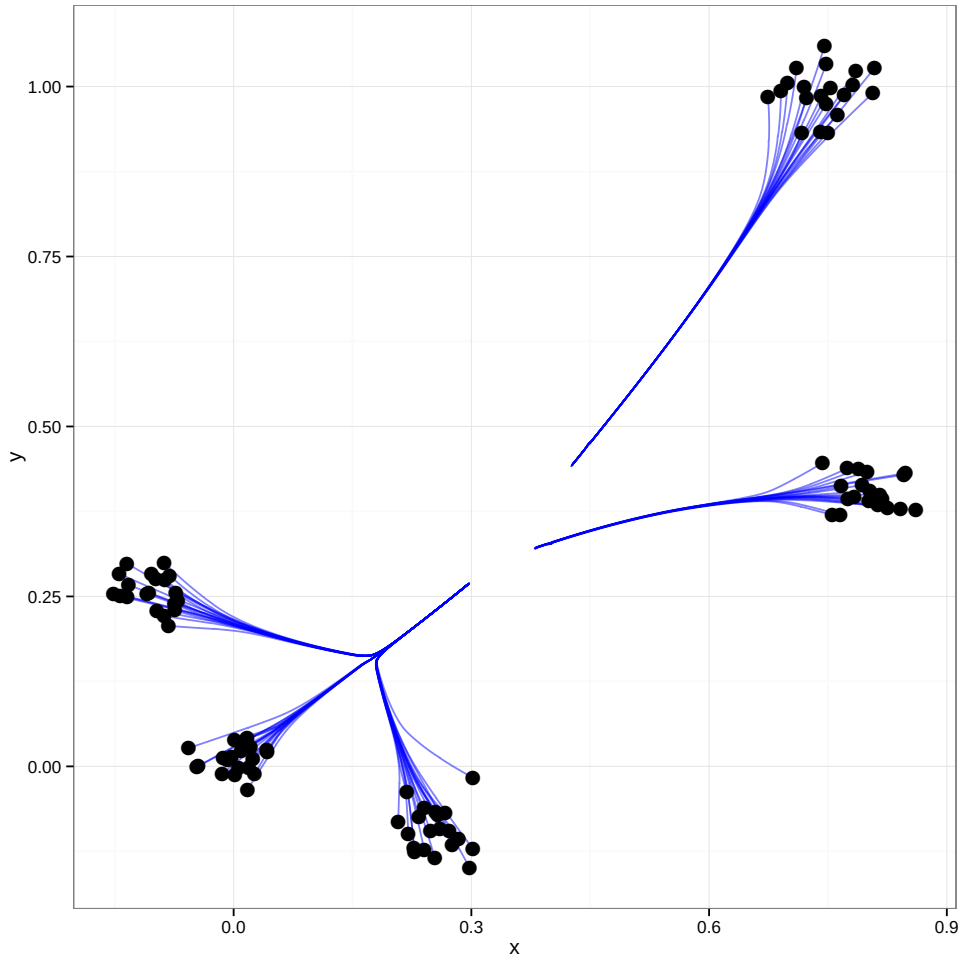
λ

Convex Clustering Solution Path

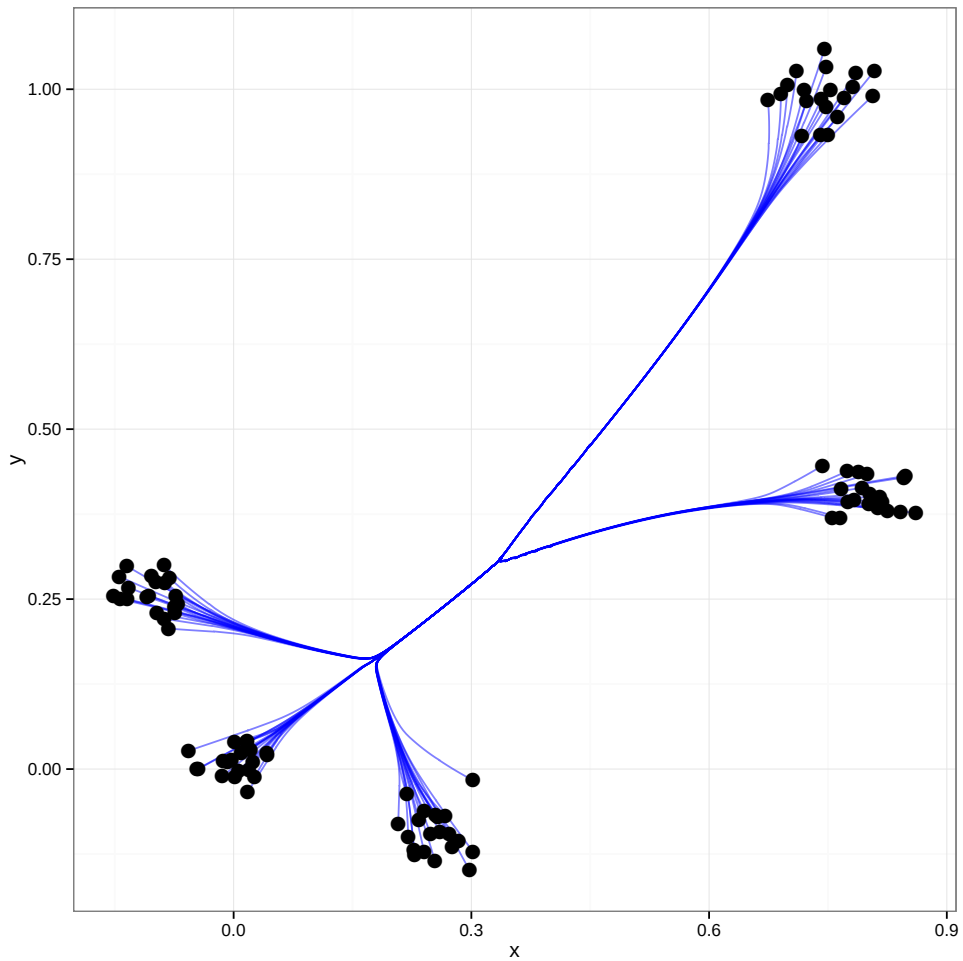


λ

Convex Clustering Solution Path

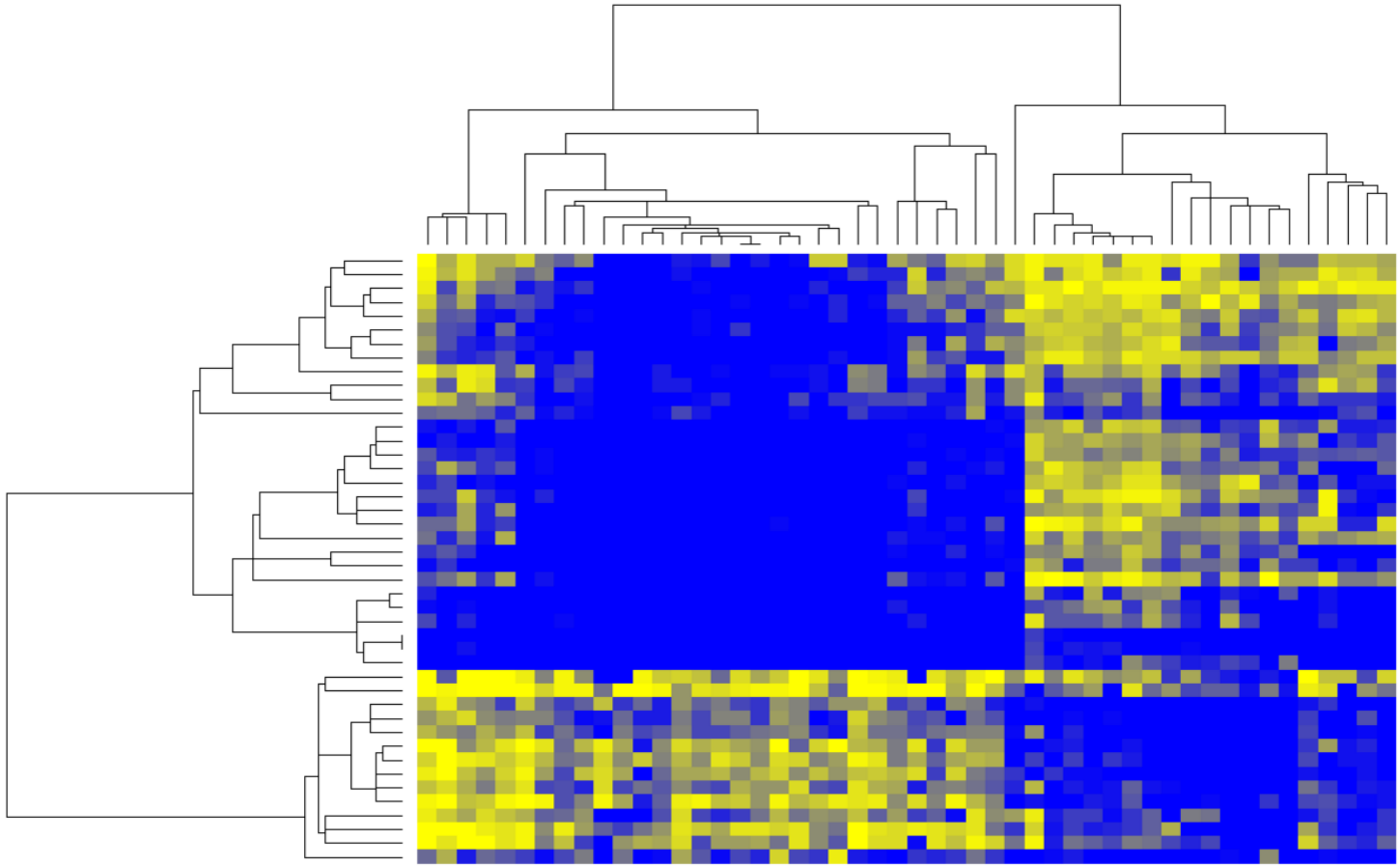


Convex Clustering Solution Path



λ

Convex Biclustering



Convex Biclustering

$$\underset{\mathbf{U}}{\text{minimize}} \quad \frac{1}{2}\|\mathbf{X}-\mathbf{U}\|_F^2 + \lambda\Big(\sum_{i<j} w_{ij}\|\mathbf{U}_{i\cdot}-\mathbf{U}_{j\cdot}\|_2 + \sum_{l<k} \tilde{w}_{lk}\|\mathbf{U}_{\cdot l}-\mathbf{U}_{\cdot k}\|_2\Big)$$

- Checkerboard-like pattern: every data point X_{ij} has its own bicluster centroid U_{ij}.
- Simultaneously fuses row centroids AND column centroids to yield biclusters!

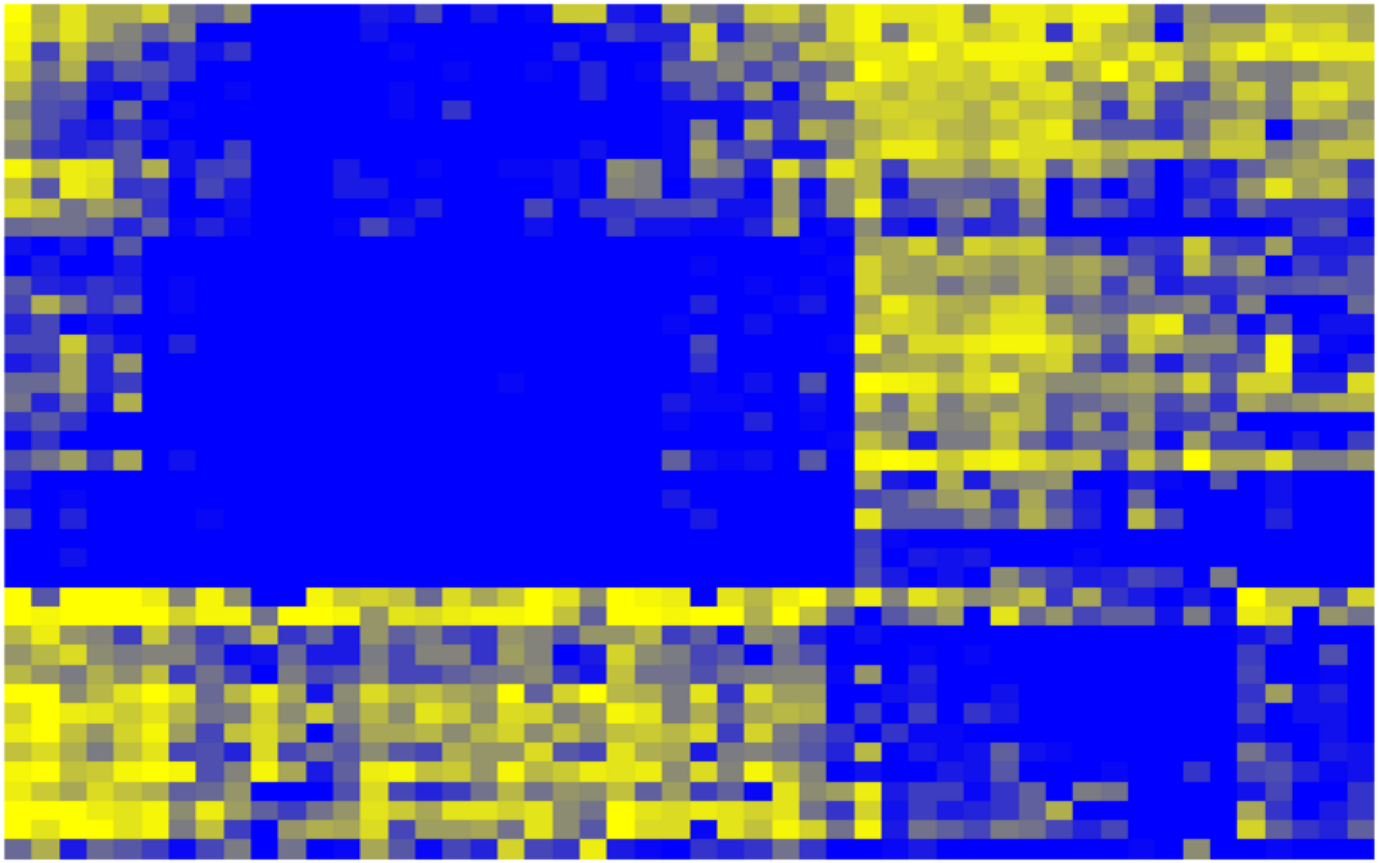
Chi, Allen, and Baraniuk, 2017

Convex Biclustering

$$\underset{\mathbf{U}}{\text{minimize}} \quad \frac{1}{2}\|\mathbf{X}-\mathbf{U}\|_F^2 + \lambda\Bigg(\sum_{i<j} w_{ij}\|\mathbf{U}_{i\cdot}-\mathbf{U}_{j\cdot}\|_2 + \sum_{l<k}\tilde{w}_{lk}\|\mathbf{U}_{\cdot l}-\mathbf{U}_{\cdot k}\|_2\Bigg)$$

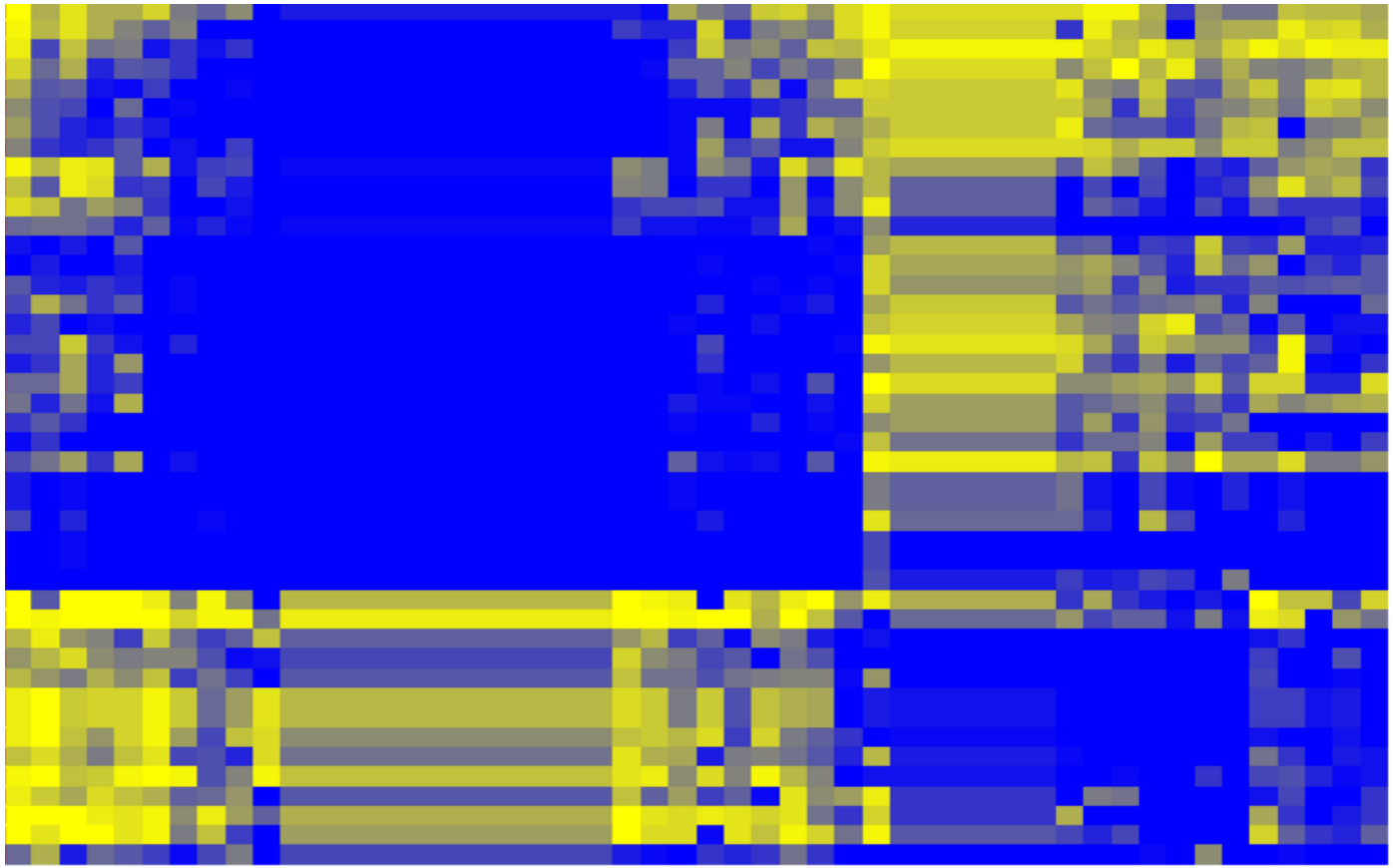
- λ controls BOTH bicluster assignments and # of biclusters.
- Weights similar to convex clustering.
  - Must sum to $1/\sqrt{p}$ and $1/\sqrt{n}$ to ensure the same fusion rate.
- Algorithm: Dystra-like Proximal Algorithm + AMA.
- In R: `cvxbiclustr`.

Convex Biclustering Solution Path



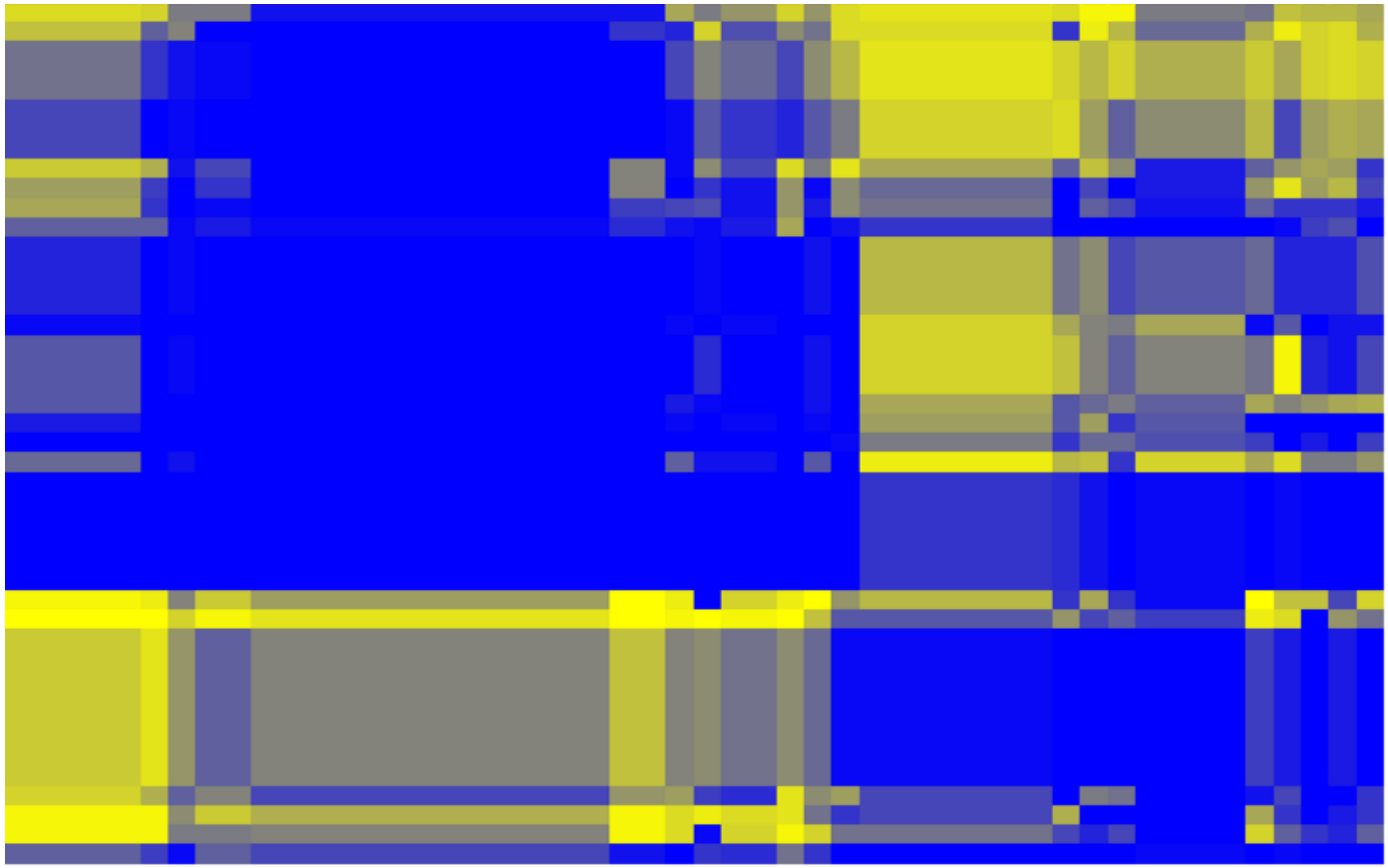
$\lambda = 0$

Convex Biclustering Solution Path



λ

Convex Biclustering Solution Path



λ

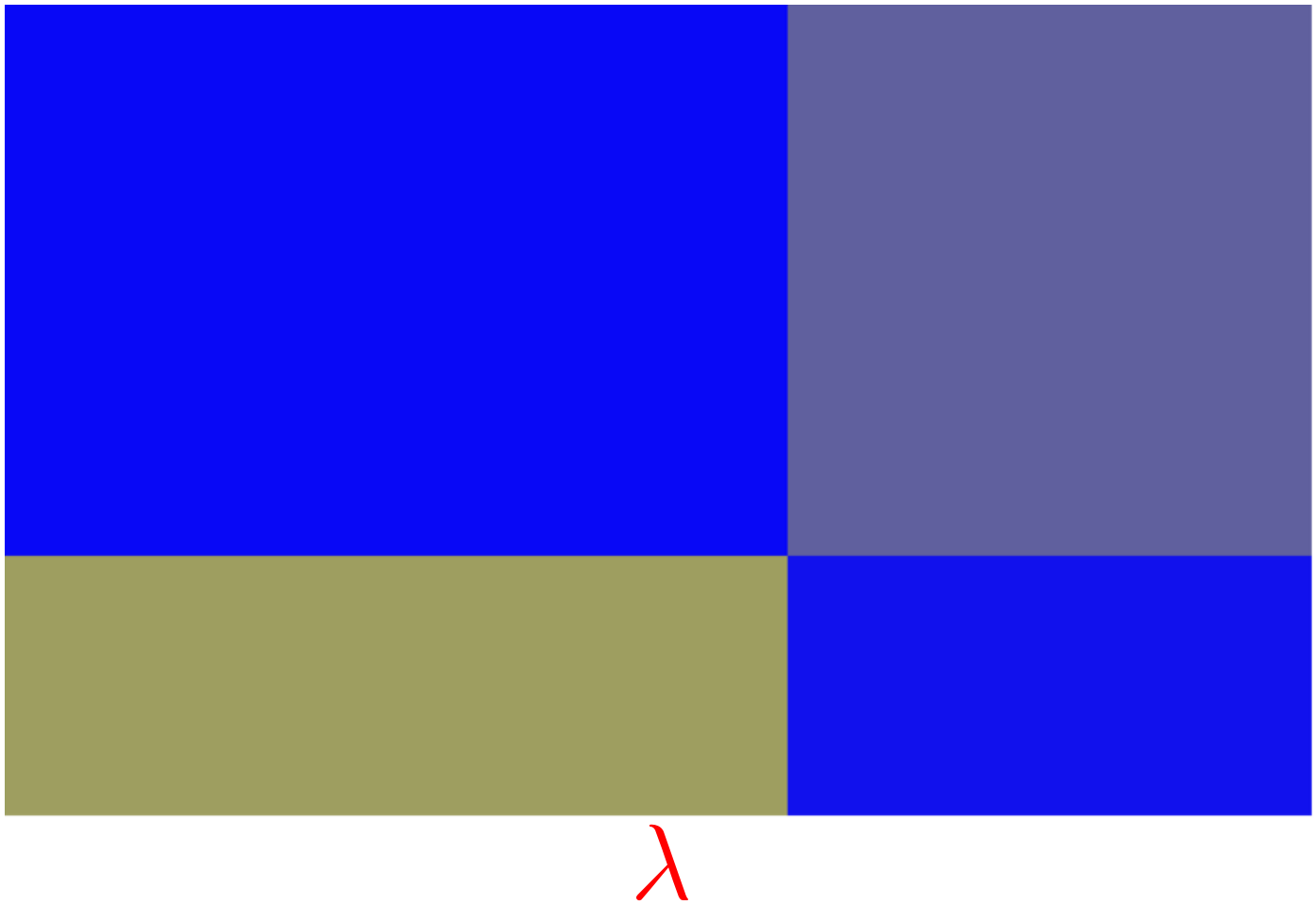
Convex Biclustering Solution Path

λ

Convex Biclustering Solution Path

λ

Convex Biclustering Solution Path



Convex Biclustering Solution Path

λ

Advantages

The Good:

- Global solution!
  - Stable, reproducible results.
- One tuning parameter.
  - λ controls BOTH # of clusters & cluster assignments.
  - Can select in data-driven manner - **Cross Validation**!
- Statistical Consistency.

The Bad:

- Nested family of clustering solutions?
- Slower iterative algorithms to find solution.
- Inference.

Chi, Allen, and Baraniuk, 2017; Tan & Witten 2015; Radchenko & Mukherjee, 2017

Our Objective

Watch your data form clusters & biclusters!

Goal

- Dendograms & Clusterheatmaps.
- Convex clustering & biclustering solution paths.

Our Objective

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Watch your data form clusters & biclusters!

Goal

- Dendograms & Clusterheatmaps.
- Convex clustering & biclustering solution paths.

Problems:

- Potential fissions.
  - *Hocking et al. 2011; Tan & Witten 2015*
- Need exact λ where all fusions occur.
  - Existing algorithms solve for one λ at a time.
  - LAR / Path algorithm for Generalized Lasso doesn't work for convex clustering problem.

Computationally way too slow!

Our Objective

Watch your data form clusters & biclusters!

Goal

- Dendograms & Clusterheatmaps.
- Convex clustering & biclustering solution paths.

Our Approach: **Algorithmic Regularization Paths**

- Quickly approximate clustering solution path at a very fine resolution.
  - *Hu, Allen, & Chi, 2017*

Algorithmic Regularization Paths for Clustering

Classical Regularization Paths

Start: Each observation is its own cluster & no regularization.

Do: Increase the regularization level (λ) by a tiny amount.

Do: Solve the optimization problem at λ.

Iterate the AMA updates until convergence.

Stop: All observations fused to one cluster.

Output: Solution at each λ as the Clustering Path.

Algorithmic Regularization Paths for Clustering

Idea

Start: Each observation is its own cluster & no regularization.

Do: Perform one iterate of the AMA.

Do: Increase the regularization level by a tiny amount.

Stop: All observations fused to one cluster.

Output: Iterates as the Algorithmic Clustering Path.

Algorithmic Regularization Paths for Clustering

Idea

Start: Each observation is its own cluster & no regularization.

Do: Perform one iterate of the AMA.

Do: Increase the regularization level by a tiny amount.

Stop: All observations fused to one cluster.

Output: Iterates as the Algorithmic Clustering Path.

CARP

Convex clustering via Algorithmic Regularization Paths

Algorithmic Regularization Paths for Clustering

Idea

Start: Each observation is its own cluster & no regularization.

Do: Perform one iterate of the AMA.

Do: Increase the regularization level by a tiny amount.

Stop: All observations fused to one cluster.

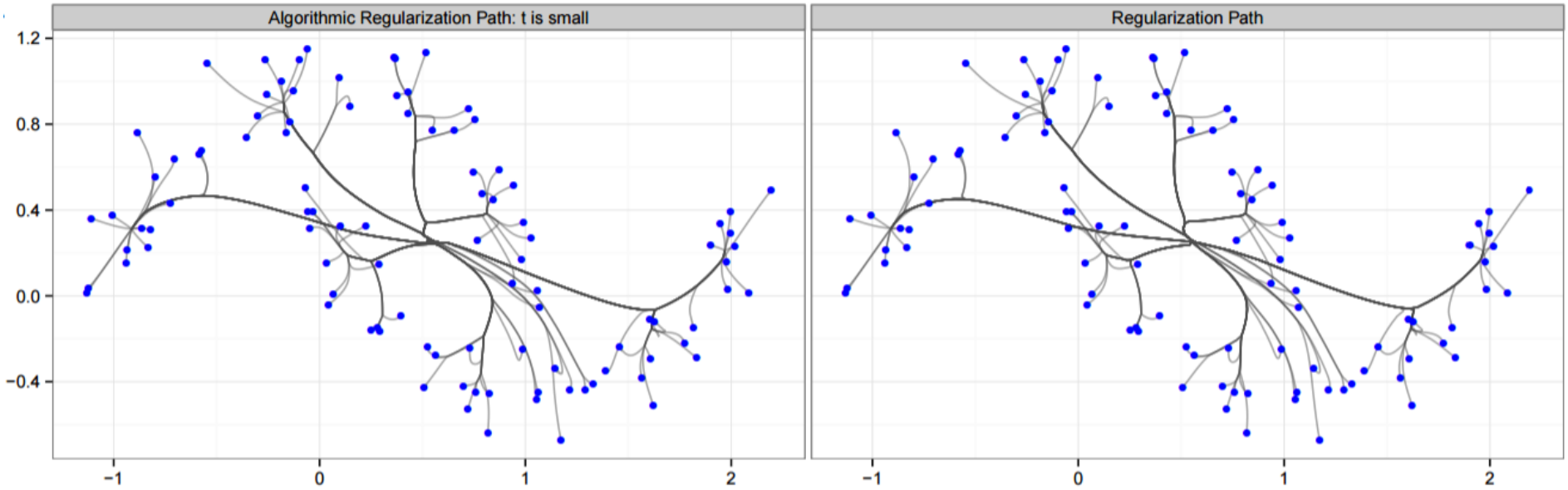
Output: Iterates as the Algorithmic Clustering Path.

CBASS

Convex Biclustering via Algorithmic Regularization with Small Steps

Clustering Path Equivalence

Clustering Path Equivalence for small t:



Very Fast!

Clustering Path Equivalence

Theorem

The algorithmic convex clustering path, $\tilde{\mathbf{U}}_t(k)$, is equivalent to the convex clustering path, $\hat{\mathbf{U}}(\lambda)$, as the step size $t \longrightarrow 1$:

$$d_H(\hat{\mathbf{U}}(\lambda), \tilde{\mathbf{U}}_t(k)) \longrightarrow 0.$$

where $d_H(\hat{\mathbf{U}}(\lambda), \tilde{\mathbf{U}}_t(k))$ is the Hausdorff distance:

$$d_H(\hat{\mathbf{U}}(\lambda), \tilde{\mathbf{U}}_t(k)) = \max\Big\{ \max_k \min_\lambda ||\mathbf{U}(\lambda) - \tilde{\mathbf{U}}_t(k)||_F^2, \max_\lambda \min_k ||\mathbf{U}(\lambda) - \tilde{\mathbf{U}}_t(k)||_F^2 \Big\}.$$

Visualization Algorithm

CARP-VIZ

Convex clustering via Algorithmic Regularization Paths

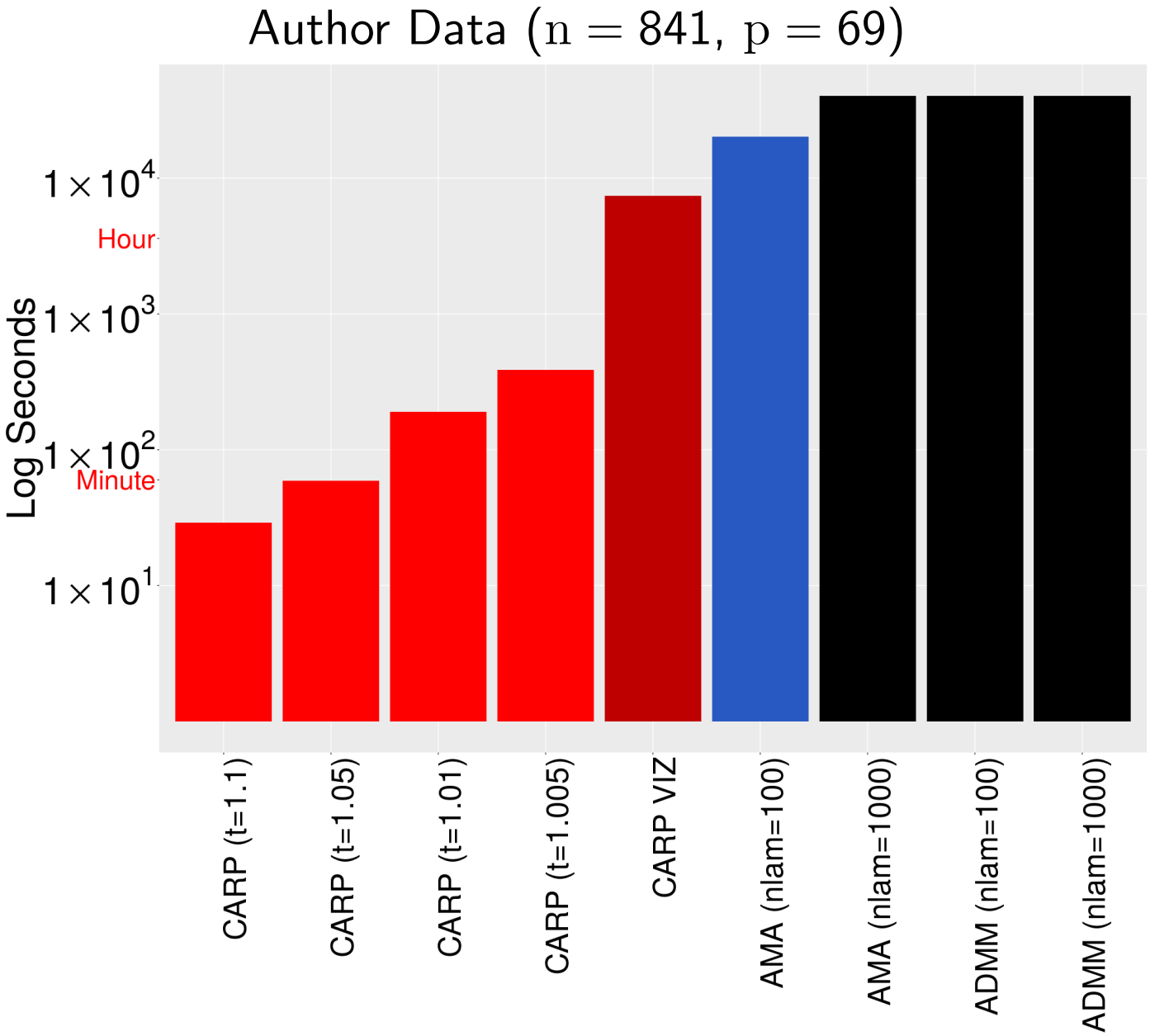
CBASS-VIZ

Convex Biclustering via Algorithmic Regularization with Small Steps

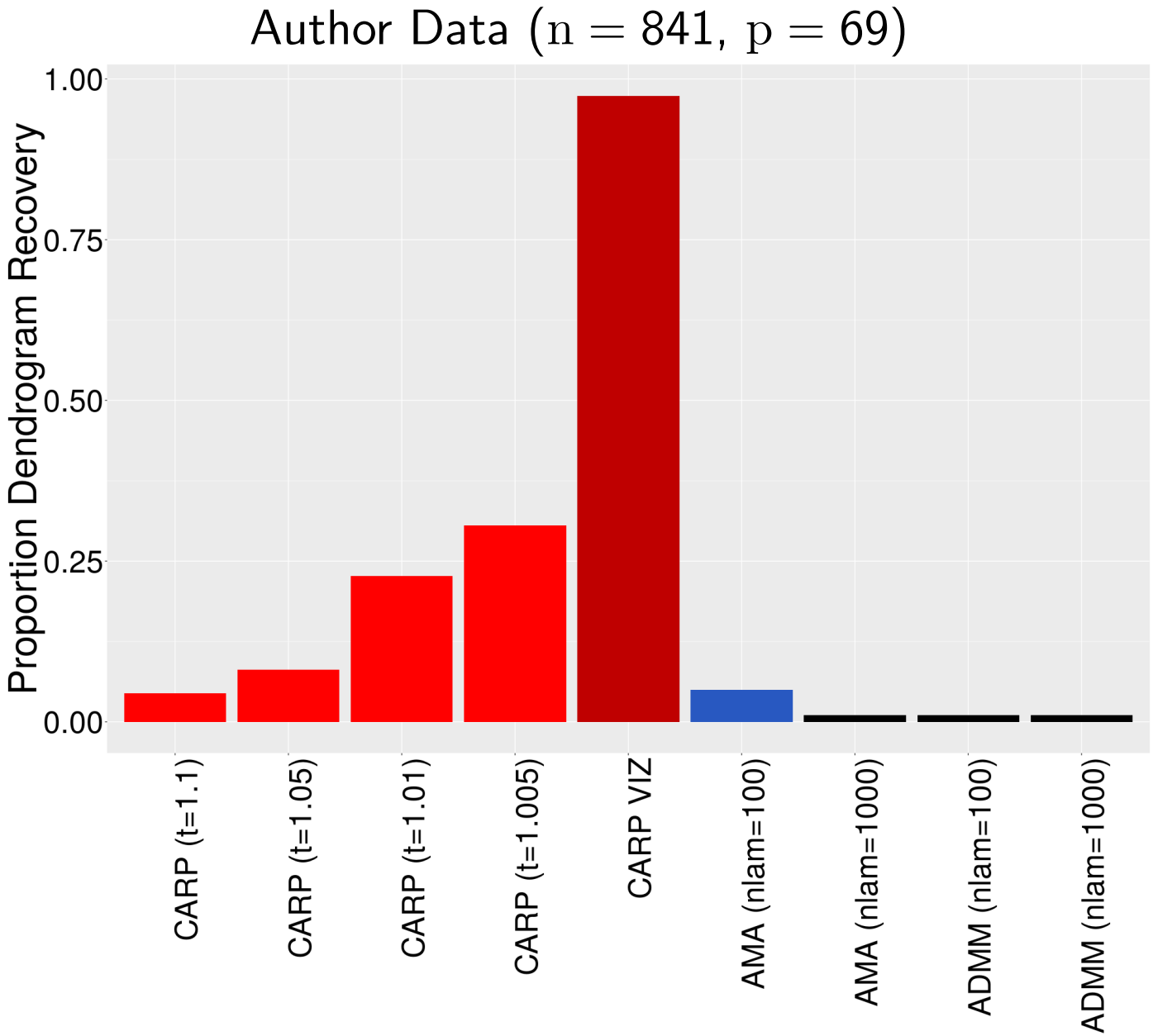
Algorithm to approximate the dendogram:

- Altered proximal operator to prevent fissions.
- Adaptively increase the amount of regularization to find each fusion.

Timing Comparisons



Timing Comparisons



Text Mining Example

US Presidential Speeches Data Set:

Text Mining Example

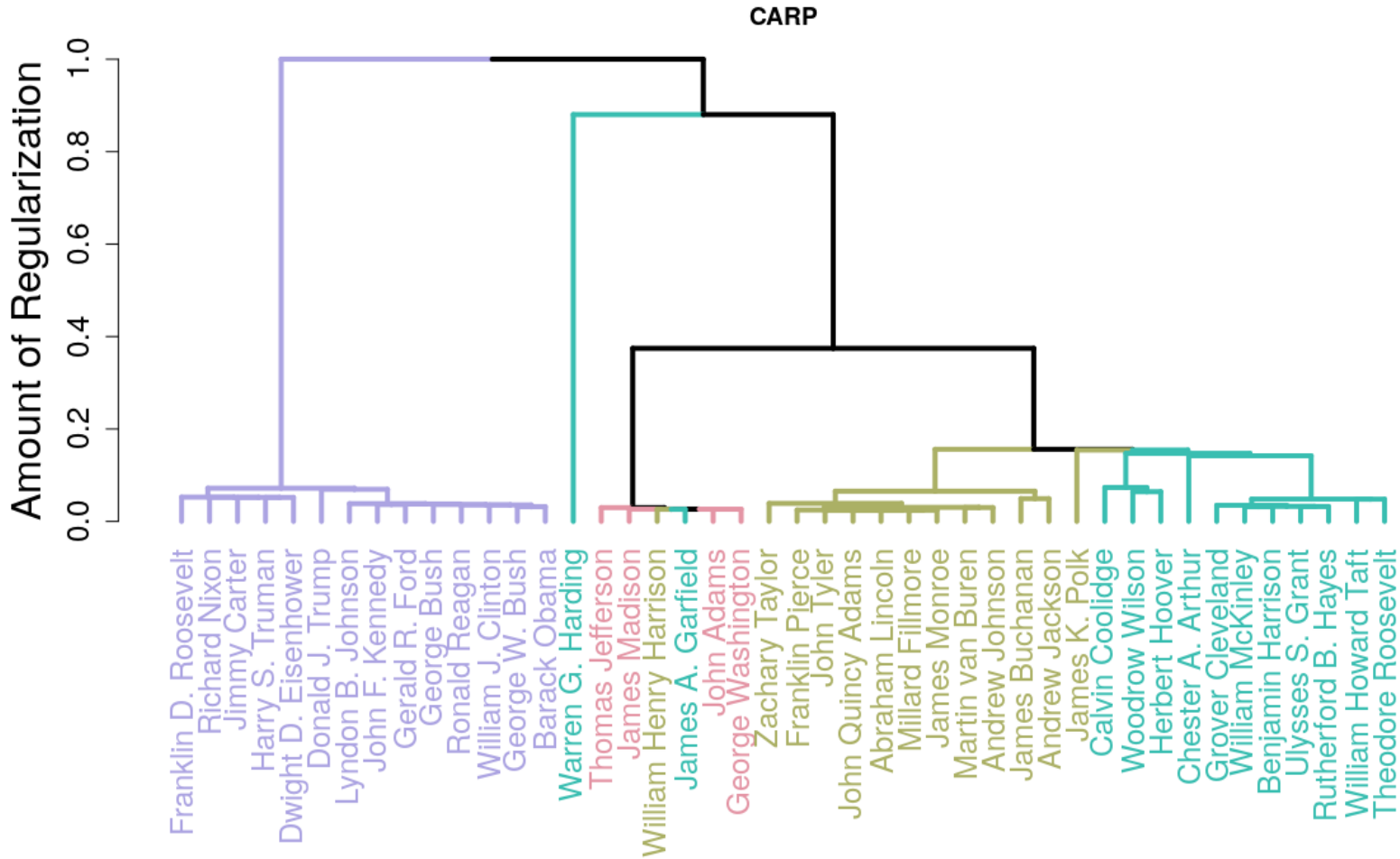
US Presidential Speeches Data Set:

- Text of Inauguration and State of the Union speeches scraped from web: `http://www.presidency.ucsb.edu`.

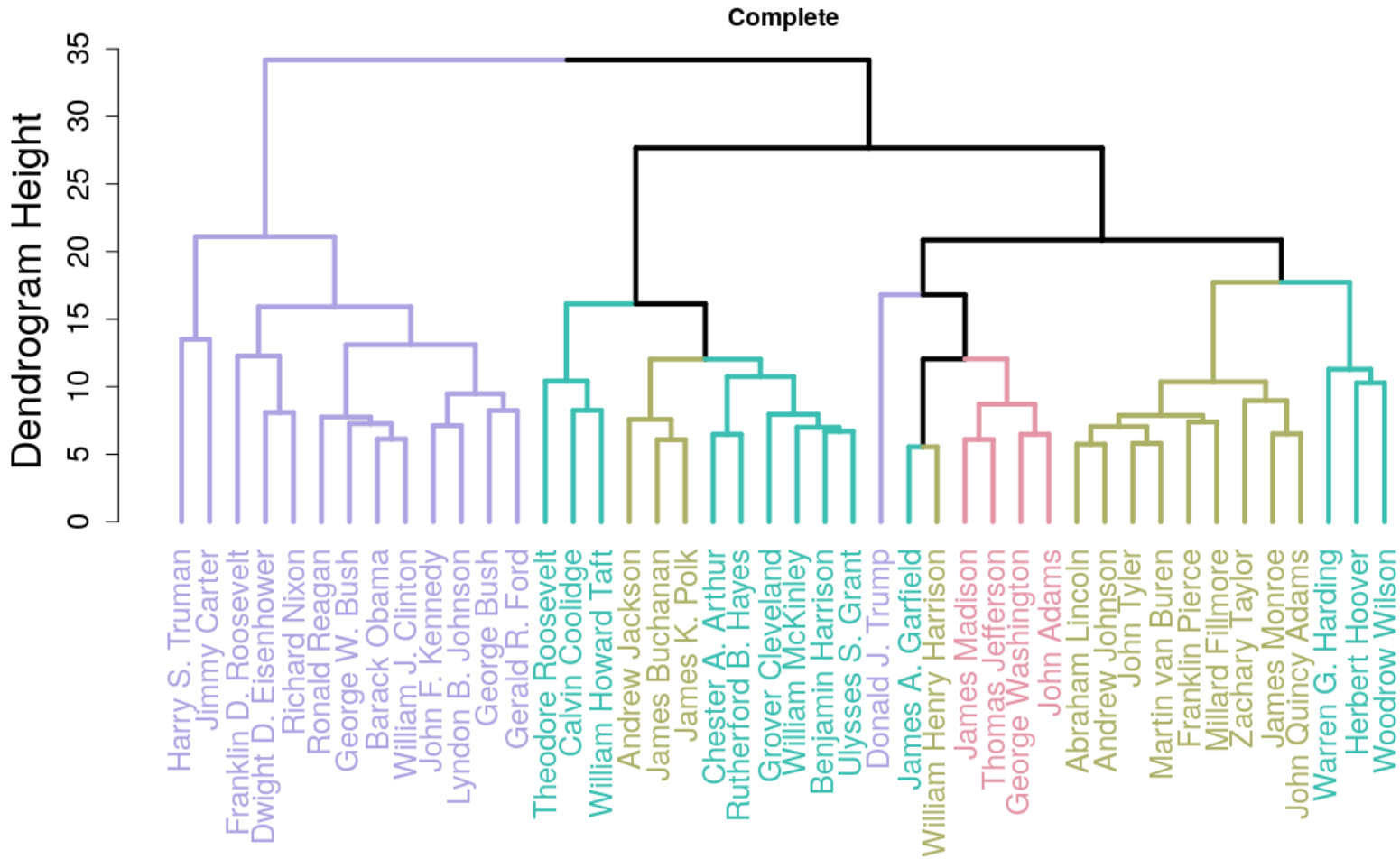
- Processed into a document-word count matrix using the `tm`, ‘‘`Text Mining`’’, `R` package.
  - Lower case; remove white space, stop words, symbols; stem words (remove prefixes and suffixes), etc.

- Filter to top 75 most variable words.
- Log-transform & center and scale whole matrix.

CARP Results - Presidents Data



CARP Results - Presidents Data



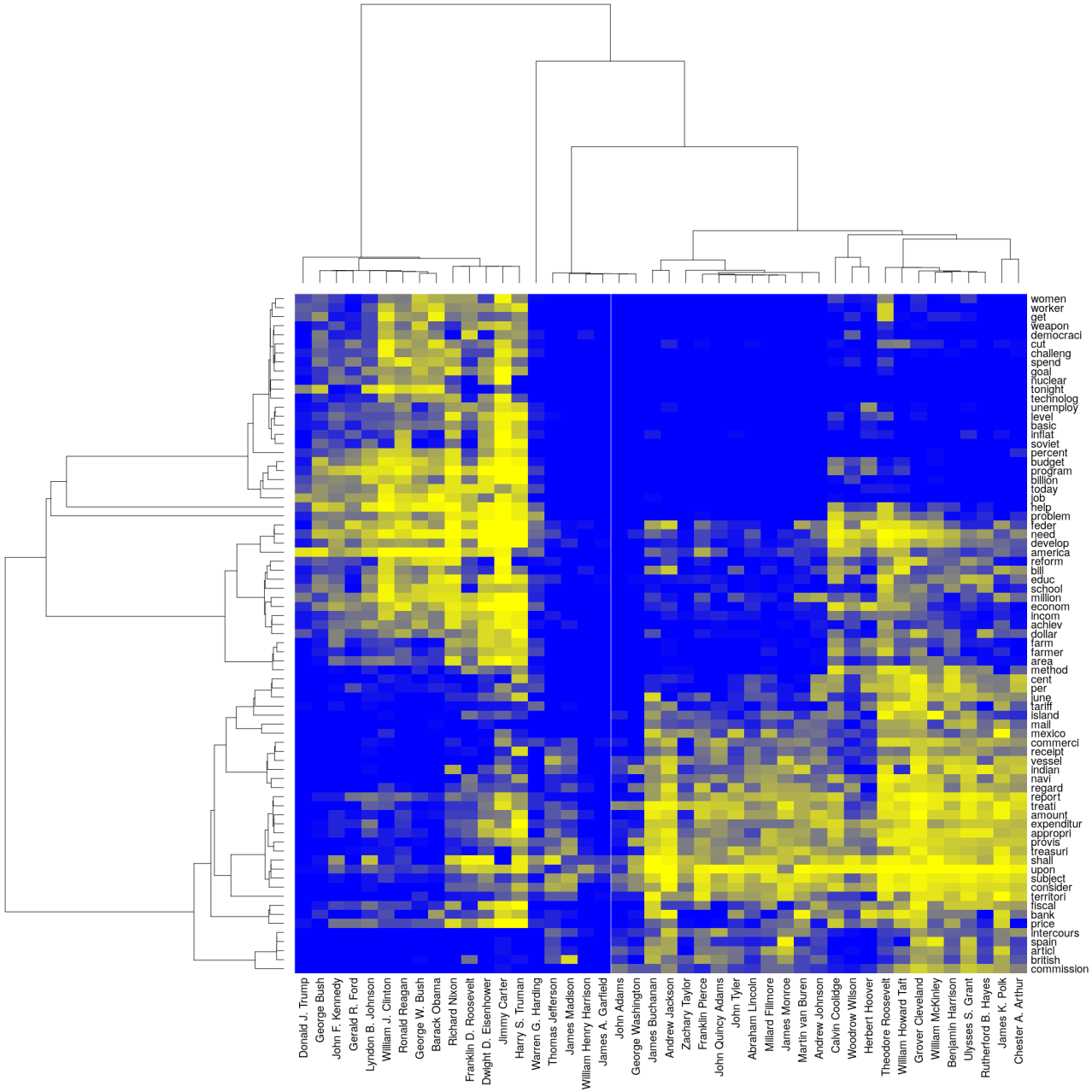
Hierarchical Clustering - Complete Linkage

CARP Results - Presidents Data

CARP Results - Presidents Data

CBASS Results - Presidents Data

CBASS Results - Presidents Data



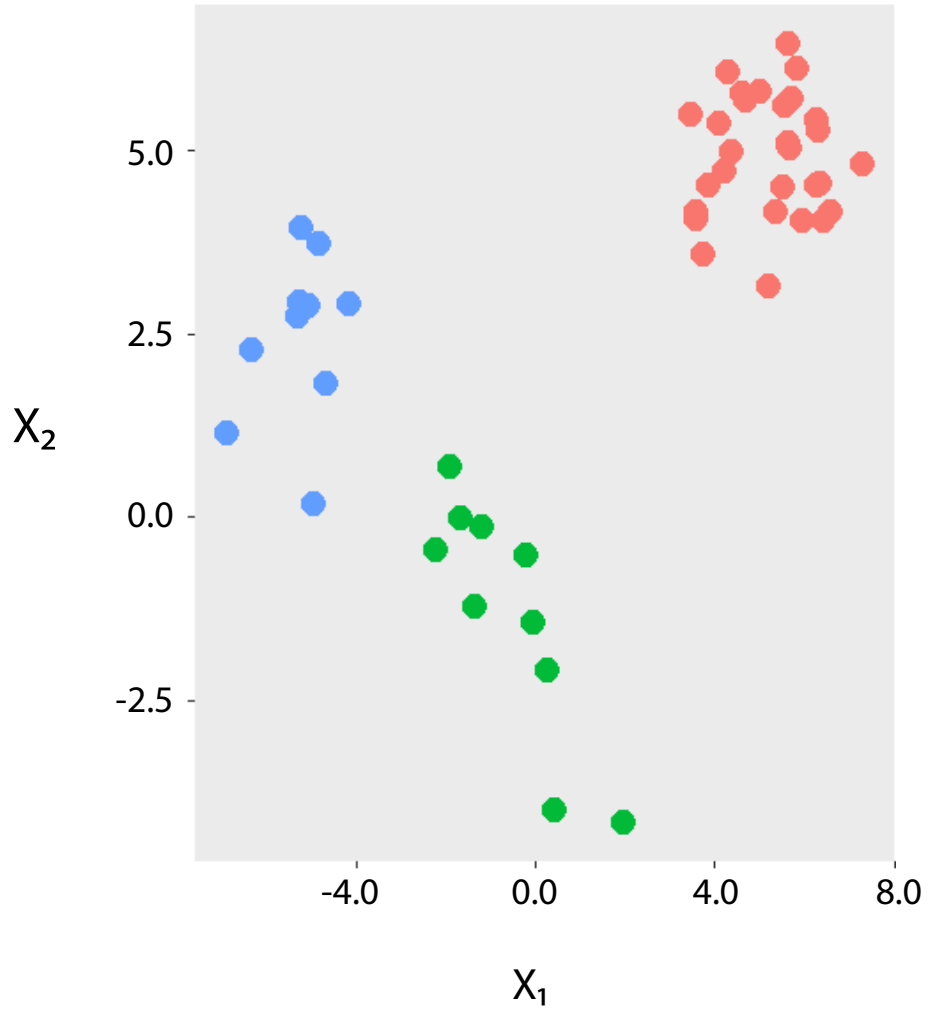
Software

clustRviz

Coming soon!

Inference for Clustering

- Are there true clusters in my data?
- How many clusters?



Heller and Ghahramani (2005); Liu et al. (2008); Kimes et al. (2017); Huang et al. (2015); Hyun et al. (2016)

Our Work

We derive exact null distributions for the following tests:

- One-Sample Test. Conditional on the estimated convex clustering solution, test cluster $\mathrm{g_k}$'s mean:

$$\mathrm{H_0}: \quad \boldsymbol{\mu}_\mathrm{k} = \boldsymbol{\mu}_0 \quad \text{vs.} \quad \mathrm{H_A}: \boldsymbol{\mu}_\mathrm{k} \neq \boldsymbol{\mu}_0 \;\Big|\; \text{Convex Clustering Solution}$$

$\Longrightarrow$ Confidence regions for cluster means.

- Two-Sample Test. Conditional on the estimated convex clustering solution, test whether cluster $\mathrm{g_k}$ and $\mathrm{g_j}$ have equal means:

$$\mathrm{H_0}: \quad \boldsymbol{\mu}_\mathrm{k} = \boldsymbol{\mu}_\mathrm{j} \quad \text{vs.} \quad \mathrm{H_A}: \boldsymbol{\mu}_\mathrm{k} \neq \boldsymbol{\mu}_\mathrm{j} \;\Big|\; \text{Convex Clustering Solution}$$

$\Longrightarrow$ Test whether two clusters are truly separate.

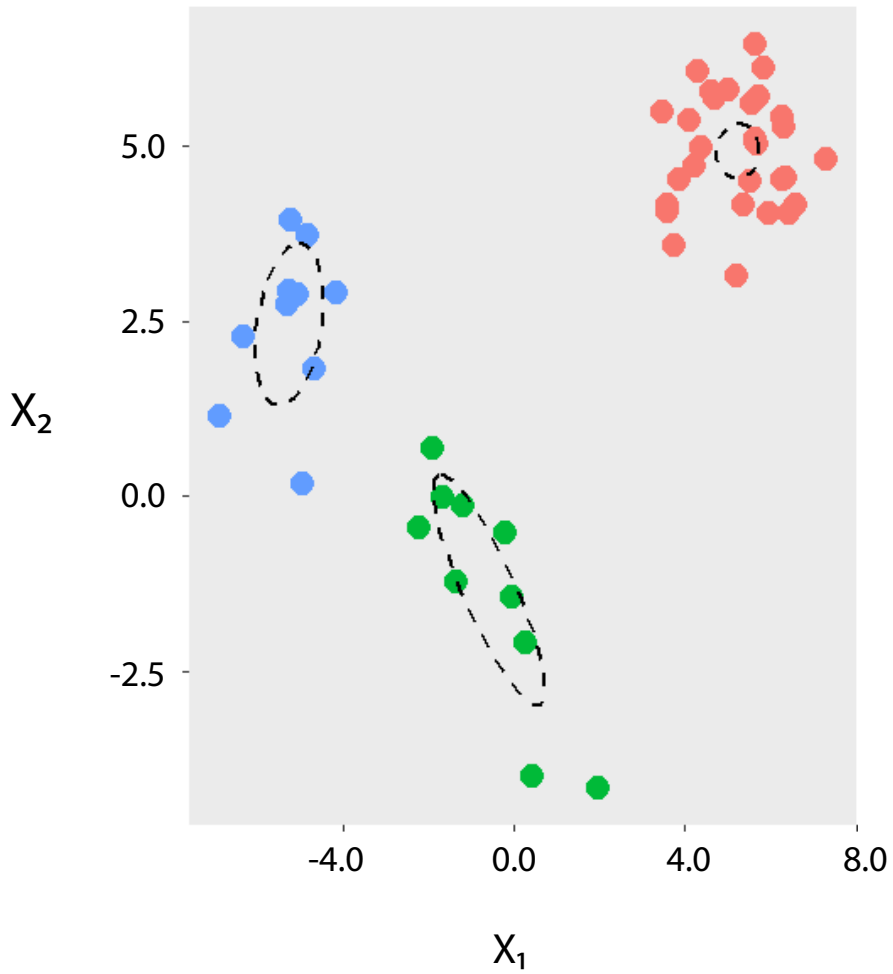
Our Work

- Derive novel representations of one-sample & two-sample Hotelling's T^2 statistic in terms of principal angles.
- Derive novel data decompositions as a function of principal angles.
- Selective inference framework to derive exact null distributions.
  - Post Selection Inference.

Skipping the math ...

Inference for Convex Clustering: Example

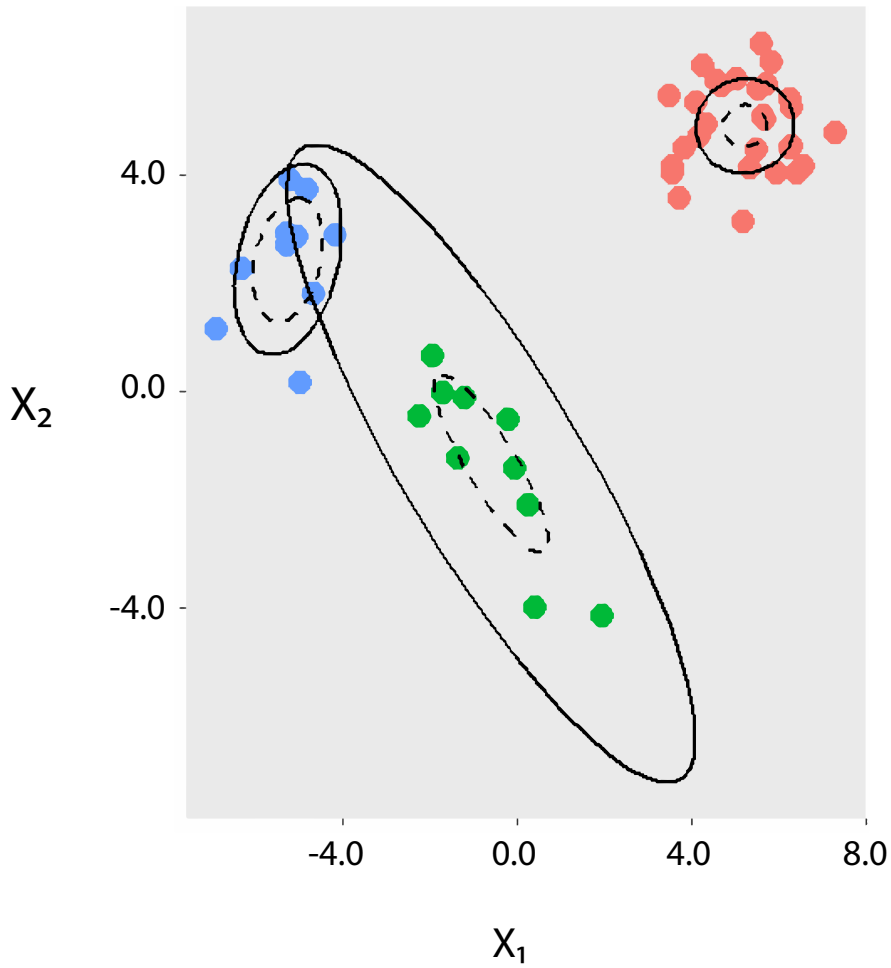
- Confidence ellipsoids for cluster means.
  - Naive: dashed lines.
- Two sample test for equality of cluster green and blue means.
  - Naive:
    p-value $=$ 1.683517e-07



Inference for Convex Clustering: Example

- Confidence ellipsoids for cluster means.
  - Naive: dashed lines.
  - Ours: solid lines.

- Two sample test for equality of cluster green and blue means.
  - Naive:
    p-value $=$ 1.683517e-07
  - Ours:
    p-value $=$ 0.1598832



Summary

Summary

1. Convex Clustering & Biclustering have many advantages!
2. Developed a fast algorithm to compute cluster solution path & approximate cluster dendogram.
   - Novel approach: Algorithmic Regularization Paths.
3. Developed interactive & dynamic visualizations for clustering and biclustering.
4. Developed valid inference procedures for convex clustering.
   - Novel representations of data in terms of principal angles.

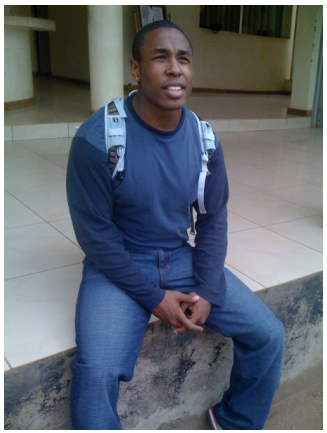
clustRviz

Coming soon!

Acknowledgments & References

John Nagorski,
PhD, Statistics, Rice University

Frederick Campbell,
PhD, Statistics, Rice University



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Thank You!