Foundations of Data Driven Algorithm Design

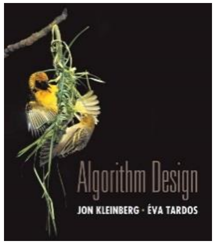
Maria-Florina (Nina) Balcan

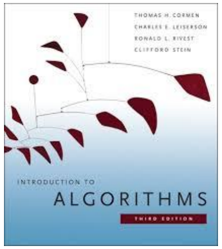
Carnegie Mellon University

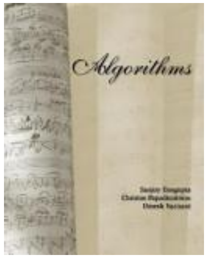
Data Driven Algorithm Selection

Some domains we have polynomial time optimal algorithms:

- E.g., sorting, searching, shortest paths…





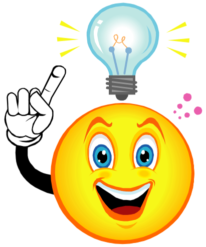


Some domains we don't:

- Different methods work better in different settings.

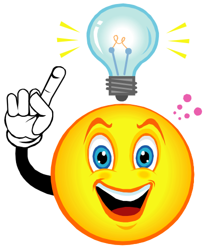
- Large family of methods – what's best in our application?

- E.g., data clustering, partitioning problems, auction design, …



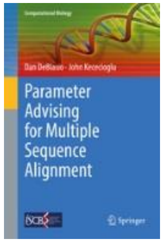
Use ML to automate algo design in difficult domains.

Data Driven Algorithm Selection



Use ML to automate algo design in difficult domains.

- **Large body of empirical work.**
  - AI community: E.g., [Xu-Hutter-Hoos-LeytonBrown, JAIR 2008]
  - Computational Biology: E.g., [DeBlasio-Kececioglu, 2018]
  - Game Theory: E.g., [Likhodedov and Sandholm, 2004]



- **This talk: formal guarantees for this approach.**

Algorithm Selection as a Learning Problem

Goal: given large family of algos, sample of typical instances from domain, find an algo that performs well on new instances from same domain.

Large family F of algorithms

MST + Dynamic Programming

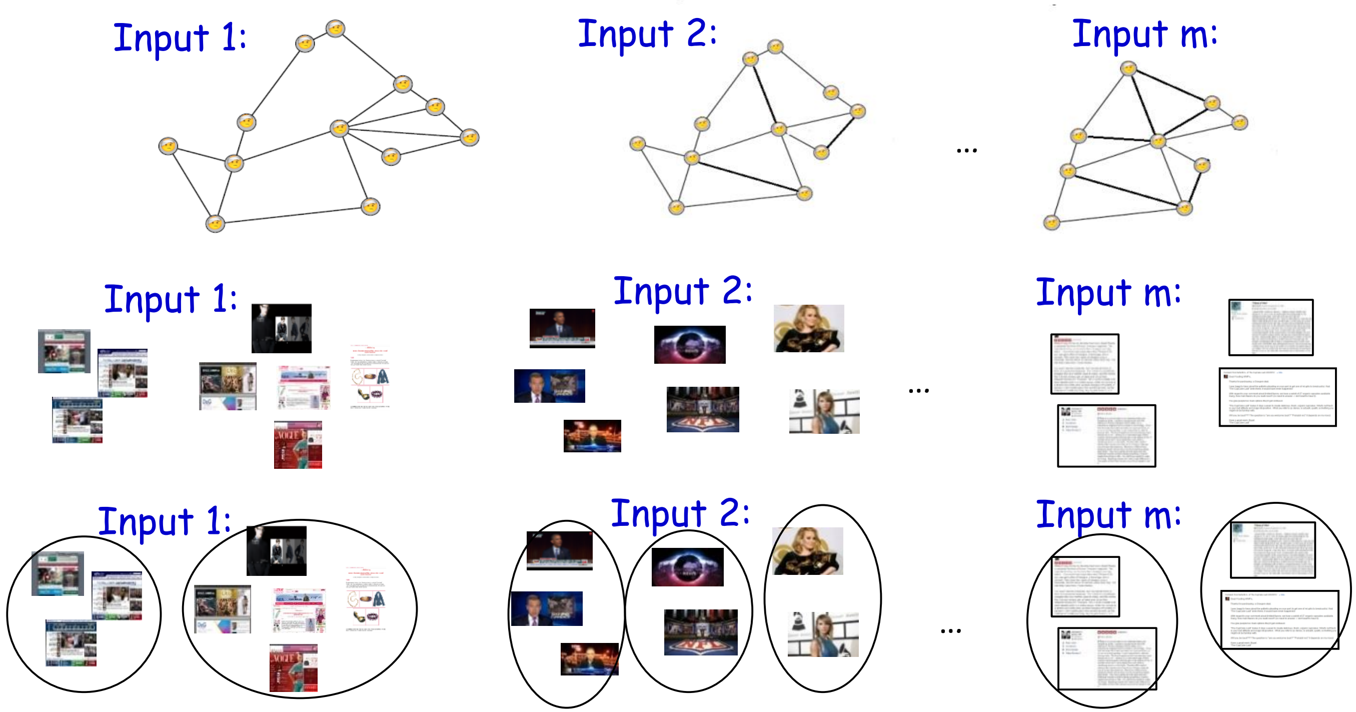
Greedy + Farthest Location

…

Sample of typical inputs

Facility location:

Clustering:

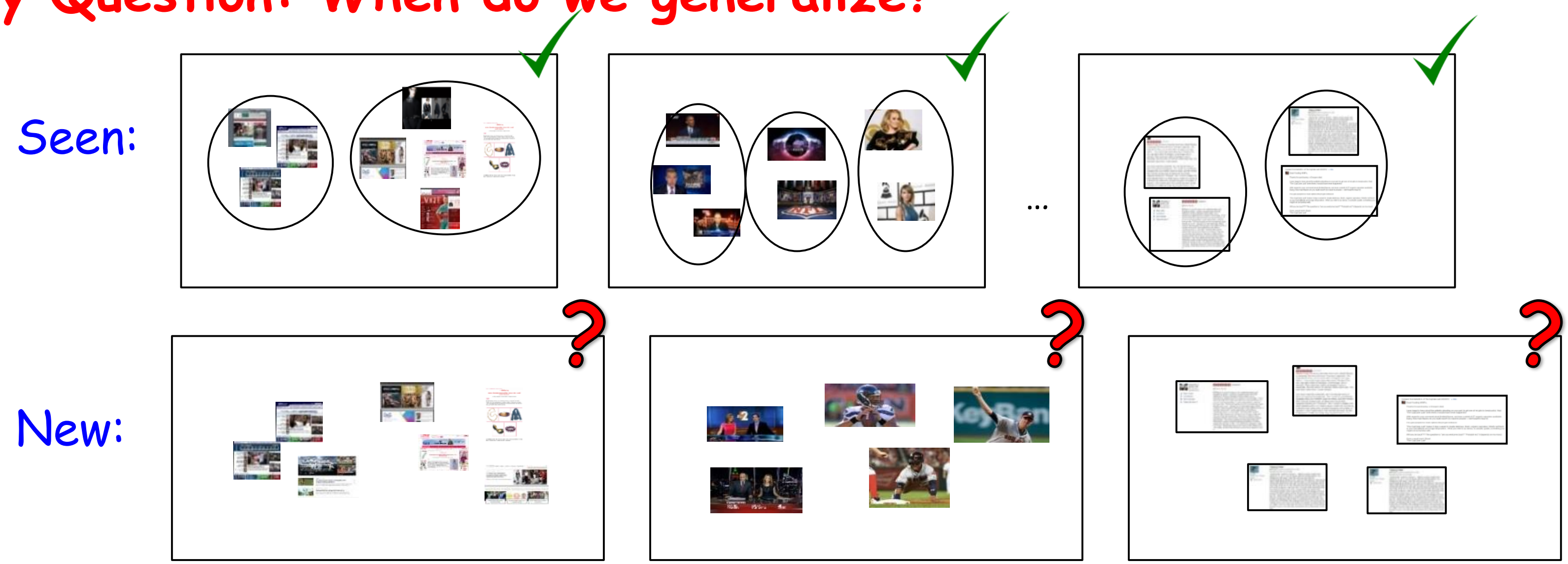


Sample Complexity of Algorithm Selection

Goal: given large family of algos, sample of typical instances from domain, find an algo that performs well on new instances from same domain.

Approach: ERM, find the algo that performs best over our sample.

Key Question: When do we generalize?



Sample Complexity: How large should our sample of typical instances be in order to guarantee good performance on new instances?

Data Driven Algorithm Selection

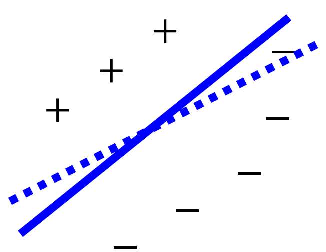
Goal: widely applicable techniques for analyzing the intrinsic complexity of families of algos and ensuring good generalizability.

Also design an efficient meta-algorithm.

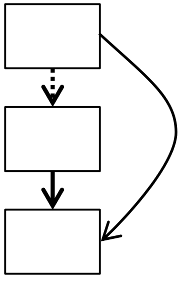
Natural Idea: apply tools from learning theory.

$m = O(\dim(F)/\epsilon^2)$ instances suffice to ensure generalizability

Challenge: analyze dim(F), due to combinatorial & modular nature, "nearby" programs/algos can have drastically different behavior.



Classic machine learning



Our work

Formal Guarantees for Algorithm Selection

Prior Work:

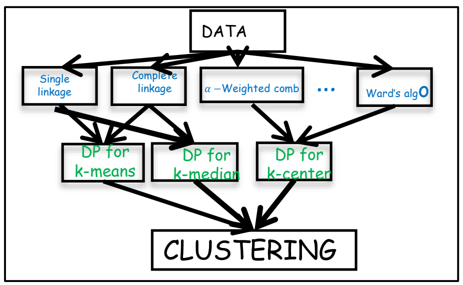
[Gupta-Roughgarden, ITCS 2016 & SICOMP 2017]: proposed learning theoretic model for analyzing algorithm selection; analyzed greedy procedures for subset selection problems (knapsack & independent set).

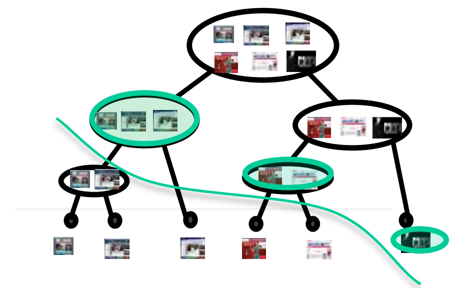
Formal Guarantees for Algorithm Selection

- Our Work: Distributional settings, new algo classes applicable for a wide range of problems.

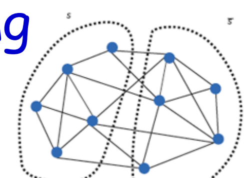
[Balcan-Nagarajan-Vitercik-White, COLT 2017]

- Clustering: Linkage + Dynamic Programming



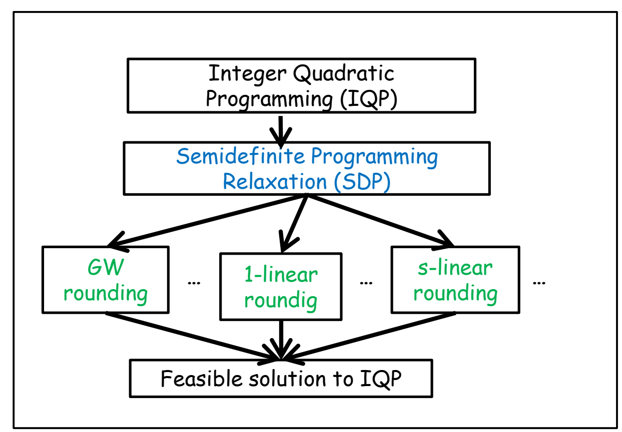


- Partitioning pbs via IQPs: SDP + Rounding



E.g., Max-Cut,

Max-2SAT, Correlation Clustering



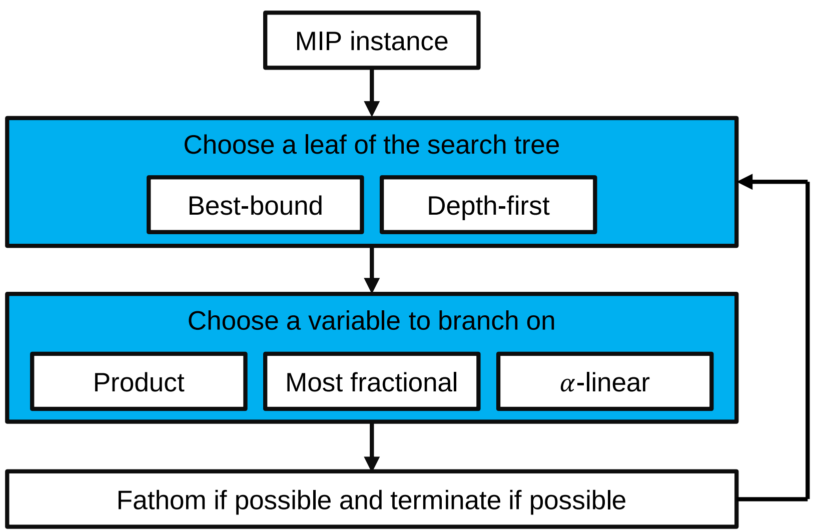
Formal Guarantees for Algorithm Selection

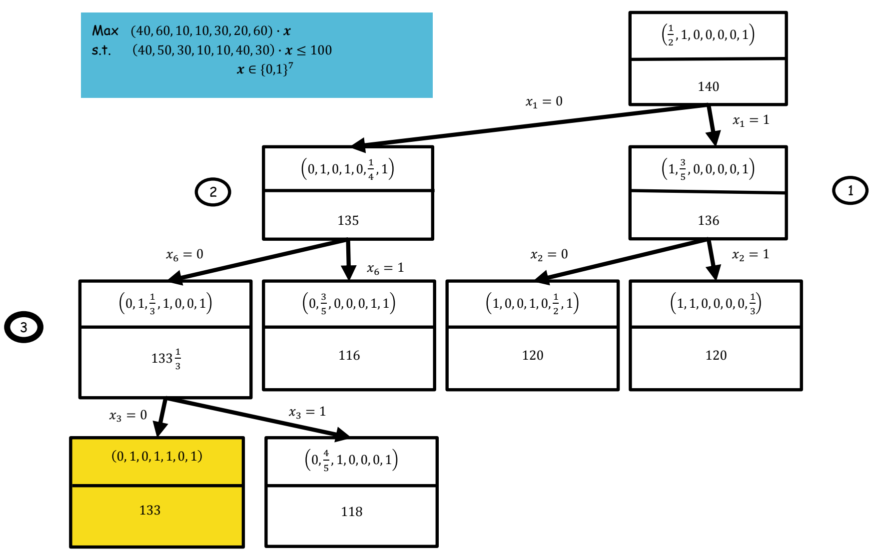
- <u>Our Work</u>: Distributional settings, new algo classes applicable for a wide range of problems.

[Balcan-Dick-Sandholm-Vitercik, ICML 2018]

- Branch and Bound Techniques for solving MIPs

Max $\boldsymbol{c} \cdot \boldsymbol{x}$
s.t. $\quad A\boldsymbol{x} = \boldsymbol{b}$
$\quad\quad x_i \in \{0,1\}, \forall i \in I$





Formal Guarantees for Algorithm Selection

- <u>Our Work</u>: Distributional settings, new algo classes applicable for a wide range of problems.

  [Balcan-Nagarajan-Vitercik-White, COLT 2017]

  [Balcan-Dick-Sandholm-Vitercik, ICML 2018]

- Related Work: guarantees for automated mechanism design in distributional settings. [Balcan-Sandholm-Vitercik, EC 2018]

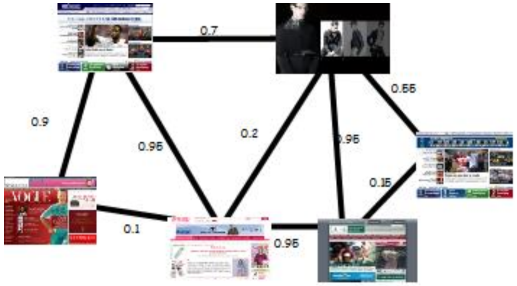
  [Balcan-Sandholm-Vitercik, Tutorial ICML 2018]

- <u>Recent Work</u>: General results for private and online algorithm selection.

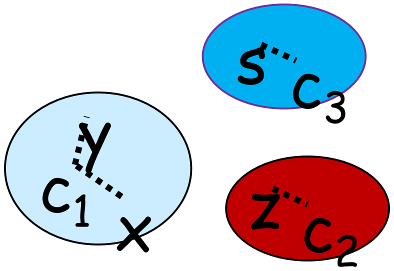
  [Balcan-Dick-Vitercik, FOCS 2018]

Clustering

Problem: Given a S set of n objects (news articles, customer surveys, web pages, …), organize into natural groups.



- E.g., objective based clustering
  - k-median: find centers $\{c_1, c_2, \ldots, c_k\}$ to min $\sum_p \min d(p, c_i)$
  - k-means: find centers $\{c_1, c_2, \ldots, c_k\}$ to min $\sum_p \min d^2(p, c_i)$
  - k-center: find centers to minimize the maximum radius.

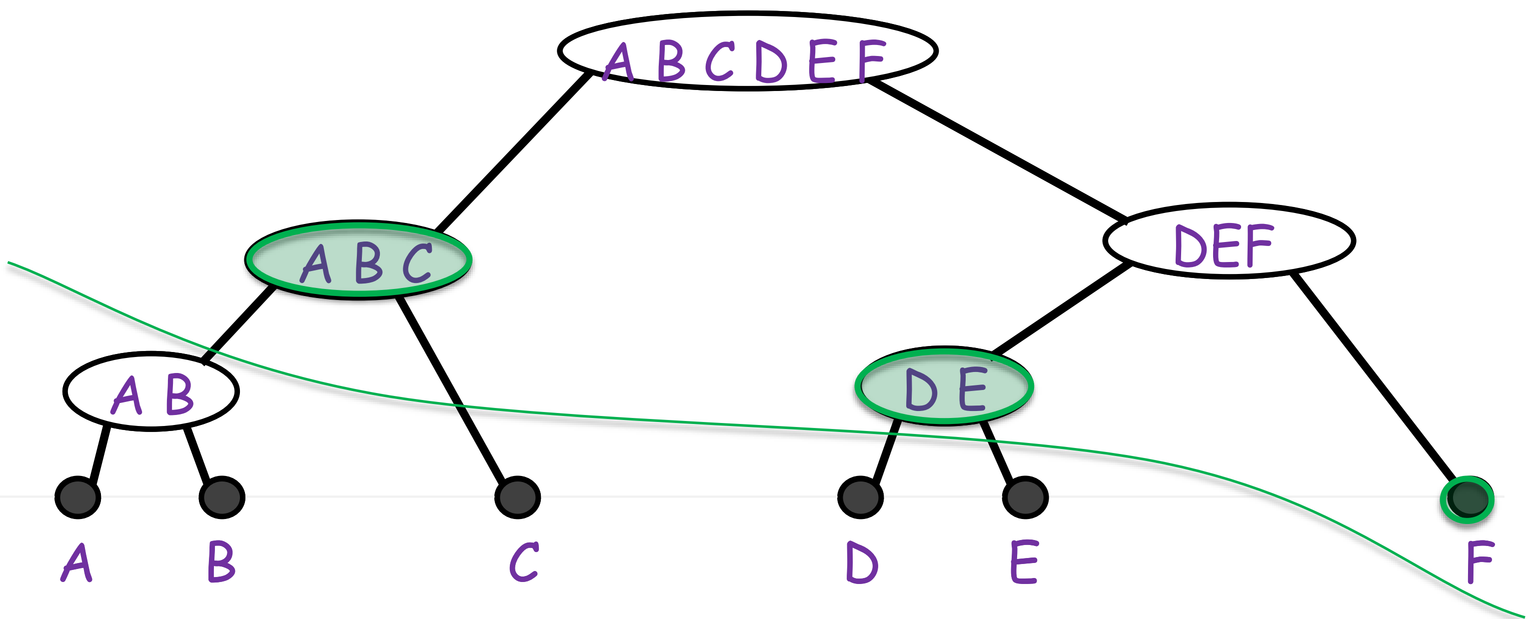


- Finding OPT is NP-hard, so no universal efficient algo that works on all domains.

Clustering: Linkage + Dynamic Programming

Family of poly time 2-stage algorithms:

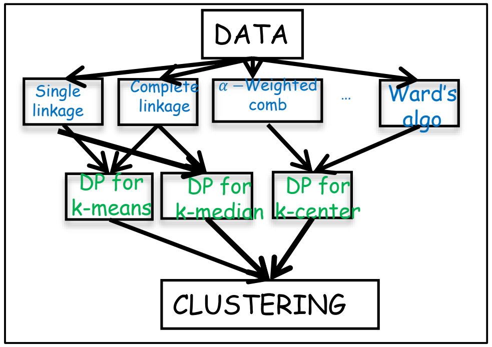
1. Use a greedy linkage-based algorithm to organize data into a hierarchy (tree) of clusters.
2. Dynamic programming over this tree to identify pruning of tree corresponding to the best clustering.

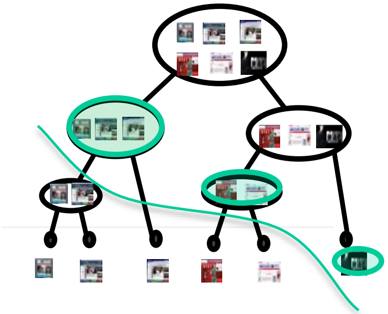


Clustering: Linkage + Dynamic Programming

1. Use a linkage-based algorithm to get a hierarchy.
2. Dynamic programming to the best prunning.

Both steps can be done efficiently.

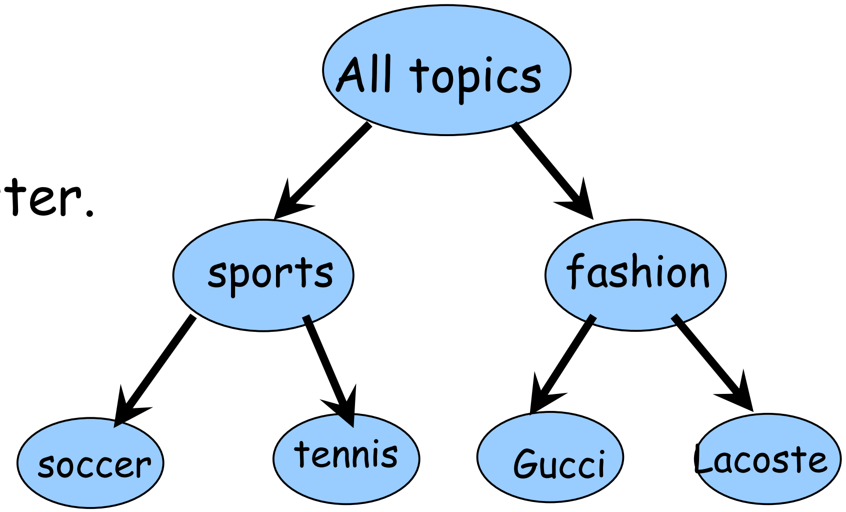




Linkage Procedures for Hierarchical Clustering

Bottom-Up (agglomerative)

- Start with every point in its own cluster.
- Repeatedly merge the "closest" two clusters.



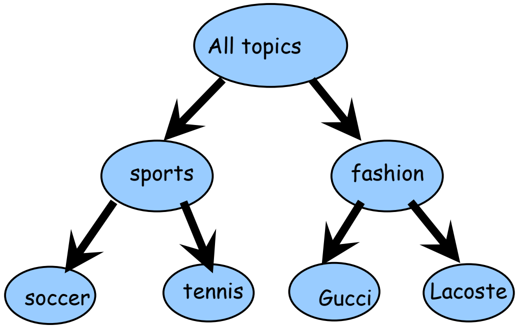
Different defs of "closest" give different algorithms.

Linkage Procedures for Hierarchical Clustering

Have a distance measure on pairs of objects.

$d(x,y)$ – distance between x and y

E.g., # keywords in common, edit distance, etc



- Single linkage: $\mathrm{dist}(A, B) = \min_{x \in A, x' \in B'} \mathrm{dist}(x, x')$

- Complete linkage: $\mathrm{dist}(A, B) = \max_{x \in A, x' \in B'} \mathrm{dist}(x, x')$

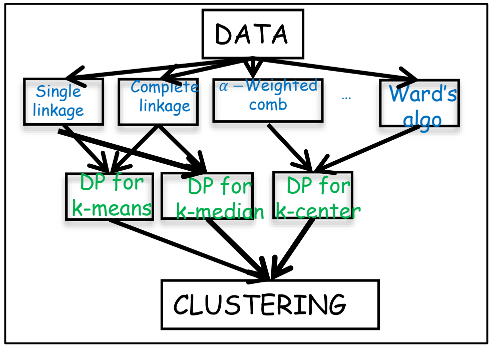
- Average linkage: $\mathrm{dist}(A, B) = \operatorname{avg}_{x \in A, x' \in B'} \mathrm{dist}(x, x')$

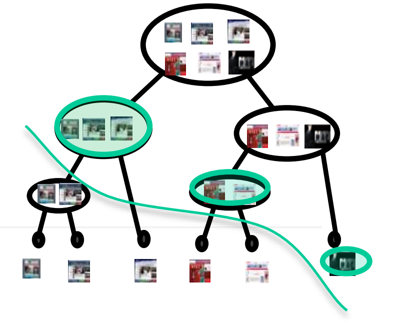
- α-weighted linkage:

$$\mathrm{dist}(A, B) = \alpha \min_{x \in A, x' \in B'} \mathrm{dist}(x, x') + (1 - \alpha) \max_{x \in A, x' \in B'} \mathrm{dist}(x, x')$$

Clustering: Linkage + Dynamic Programming

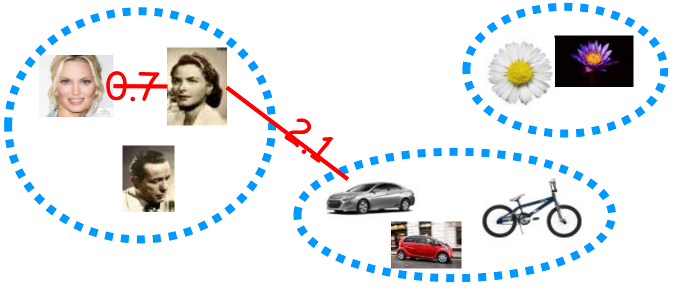
1. Use a linkage-based algorithm to get a hierarchy.
2. Dynamic programming to the best prunning.





- Used in practice.

E.g., [Filippova-Gadani-Kingsford, BMC Informatics]



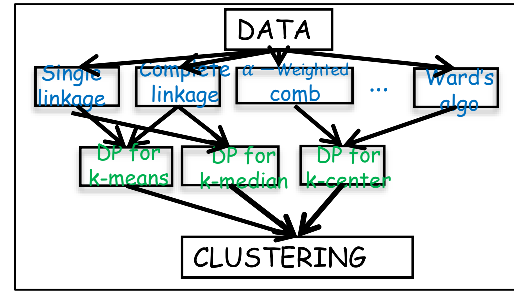
- Strong properties.

E.g., best known algos for perturbation resilient instances for k-median, k-means, k-center.

[Balcan-Liang, SICOMP 2016] [Awasthi-Blum-Sheffet, IPL 2011]
[Angelidakis-Makarychev-Makarychev, STOC 2017]

PR: small changes to input distances shouldn't move optimal solution by much.

Clustering: Linkage + Dynamic Programming

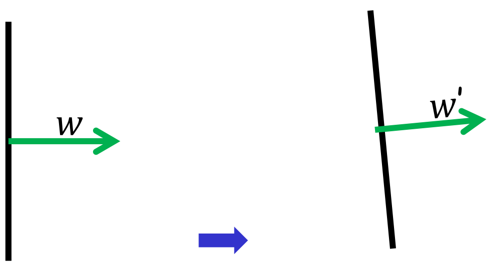


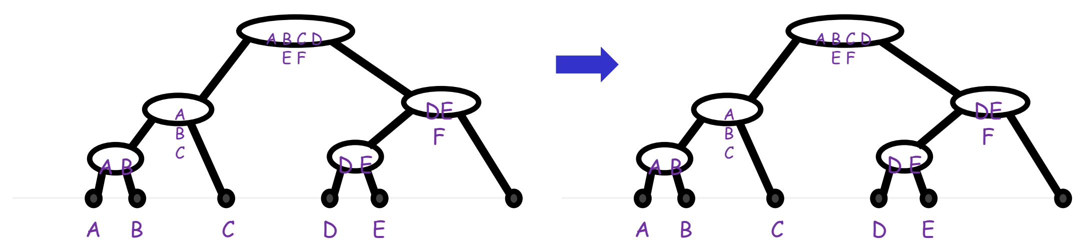
Our Results: α-weighted linkage+DP

- Pseudo-dimension is O(log n), so small sample complexity.

- Given sample S, find best algo from this family in poly time.

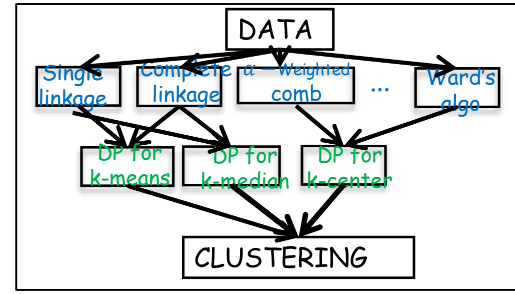
Key Technical Challenge: small changes to the parameters of the algo can lead to radical changes in the tree or clustering produced.





Problem: a single change to an early decision by the linkage algorithm can snowball and produce large changes later on.

Clustering: Linkage + Dynamic Programming

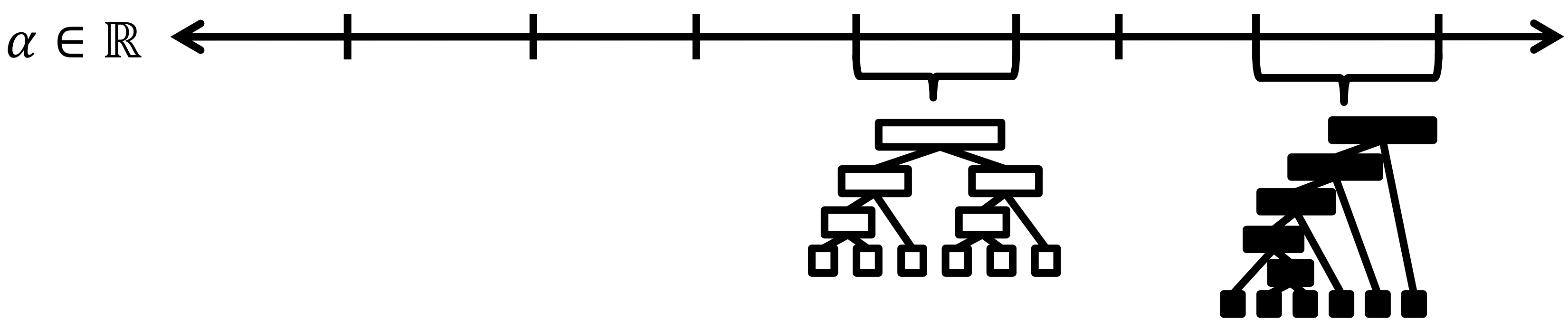


Our Results: α-weighted linkage+DP

- Pseudo-dimension is O(log n), so small sample complexity.

Key idea:

- Break real line into a small number of intervals s.t. **on each instance**:



- Two α's from one interval result in the same tree.
- And therefore the same clustering.
- And therefore the same performance cost.

Clustering: Linkage + Dynamic Programming

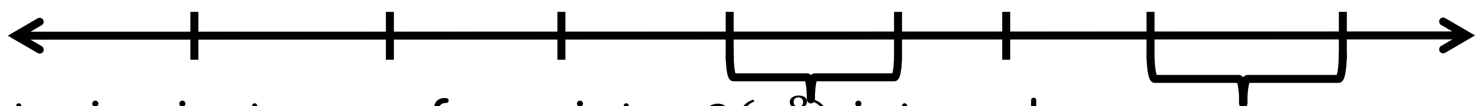
Our Results: α-weighted linkage+DP

Pseudo-dimension is O(log n), so small sample complexity.

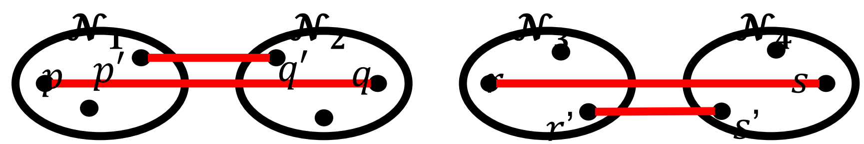
Key idea:

- Break real line into intervals s.t. **on each instance** same performance.

$\alpha \in \mathbb{R}$



- For a clustering instance of n points, $O(n^8)$ intervals.
  - Over any α interval, so long as order in which all pairs of nodes are merged is fixed, then resulting tree is invariant.
  - Which will merge first, $\mathcal{N}_1$ and $\mathcal{N}_2$, or $\mathcal{N}_3$ and $\mathcal{N}_4$?



  - Depends on which of $(1-\alpha)d(p,q) + \alpha d(p',q')$ or $(1-\alpha)d(r,s) + \alpha d(r',s')$ is smaller.
  - Any interval boundary must be an equality for some such set of 8 points, so $O(n^8)$ interval boundaries. Order of merges is fixed between any two adjacent interval boundaries.

Clustering: Linkage + Dynamic Programming

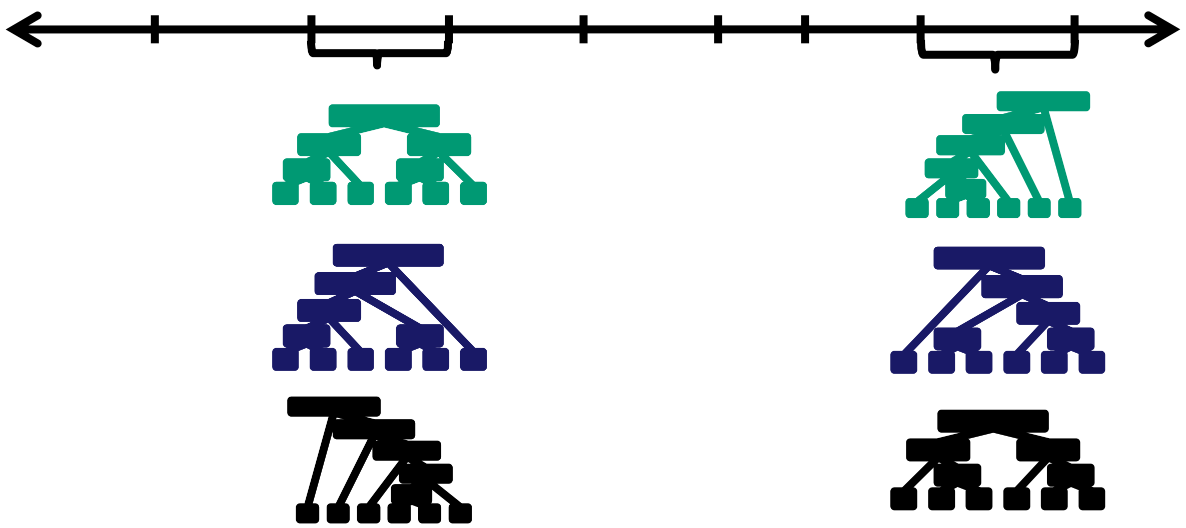
Our Results: α-weighted linkage+DP

Pseudo-dimension is O(log n), so small sample complexity.

Key idea:

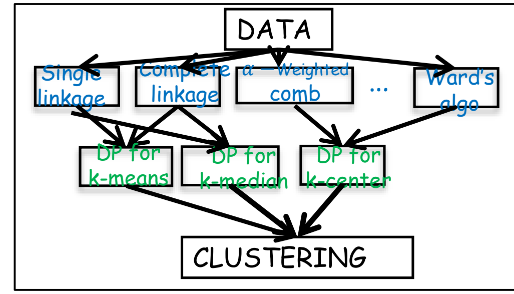
- Break real line into intervals s.t. **on each instance** same performance.
- For m clustering instances of n points, $O(mn^8)$ intervals.

$\alpha \in \mathbb{R}$



So, pseudo-dim is O(log n).

Clustering: Linkage + Dynamic Programming



Our Results: α-weighted linkage+DP

- Pseudo-dimension is O(log n).

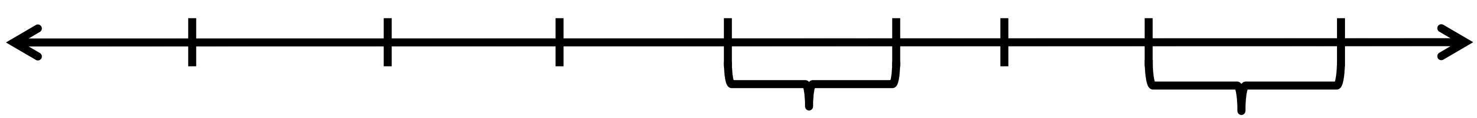
For $m = \tilde{O}(\log n / \epsilon^2)$, w.h.p. expected performance cost of best α over the sample is ϵ-close to optimal over the distribution

- Given sample S, can find best algo from this family in poly time.

Algorithm (high level)

- Solve for all α intervals over the sample

$\alpha \in \mathbb{R}$



- Find the α interval with the smallest empirical cost

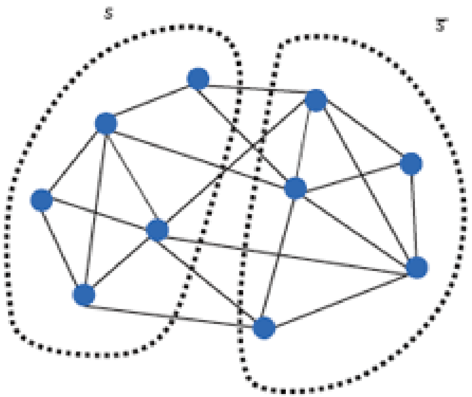
Partitioning Problems via IQPs

IQP formulation

$$\text{Max } \boldsymbol{x}^T A \boldsymbol{x} = \sum_{i,j} a_{i,j} x_i x_j$$
$$\text{s.t. } \boldsymbol{x} \in \{-1,1\}^n$$

E.g., max-cut

$$\text{Max } \sum_{(i,j)\in E} w_{ij} \left(\frac{1 - v_i v_j}{2}\right)$$
$$\text{s.t. } \quad v_i \in \{-1,1\}$$



Many of these problems are NP-hard.

Partitioning Problems via IQPs

IQP formulation

Max $\boldsymbol{x}^T A \boldsymbol{x} = \sum_{i,j} a_{i,j} x_i x_j$

s.t. $\boldsymbol{x} \in \{-1,1\}^n$

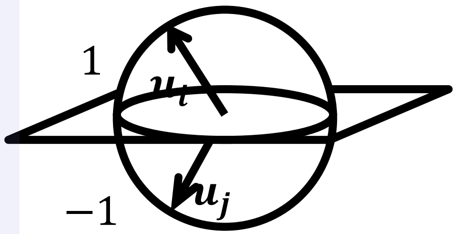
Algorithmic Approach: SDP + Rounding

1. SDP relaxation:

Associate each binary variable x_i with a vector $\boldsymbol{u}_i$.

Max $\sum_{i,j} a_{i,j} \langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle$

subject to $\|\boldsymbol{u}_i\| = 1$



2. Rounding procedure [Goemans and Williamson '95]

- Choose a random hyperplane.
- (Deterministic thresholding.) Set x_i to -1 or 1 based on which side of the hyperplane the vector $\boldsymbol{u}_i$ falls on.

Parametrized family of rounding procedures

IQP formulation

Max $\boldsymbol{x}^T A \boldsymbol{x} = \sum_{i,j} a_{i,j} x_i x_j$

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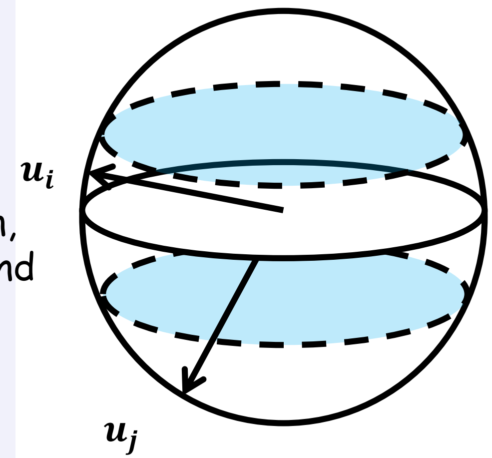
subject to $\|\boldsymbol{u}_i\| = 1$

2. s-Linear Rounding [Feige&Landberg'06]

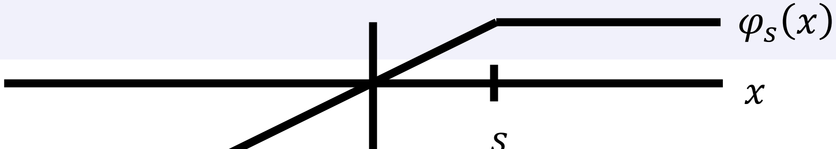
- Choose a random hyperplane.
- Random thresholding

Set x_i to 1 w.p $\frac{1}{2} + \frac{1}{2}\varphi_s(\langle \boldsymbol{u}_i, \boldsymbol{Z} \rangle)$ and -1 w.p $\frac{1}{2} - \frac{1}{2}\varphi_s(\langle \boldsymbol{u}_i, \boldsymbol{Z} \rangle)$



Inside margin, randomly round

outside margin, round to -1.



$\varphi_s(x) = -\mathbf{1}_{x<-s} + \frac{x}{s} \cdot \mathbf{1}_{x\in[-s,s]} + \mathbf{1}_{x>s}$

Parametrized family of rounding procedures

IQP formulation

$\text{Max } \boldsymbol{x}^T A \boldsymbol{x} = \sum_{i,j} a_{i,j} x_i x_j$

$\text{s.t. } \boldsymbol{x} \in \{-1,1\}^n$

Algorithmic Approach: SDP + Rounding

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$$\text{subject to} \|\boldsymbol{u}_i\| = 1$$

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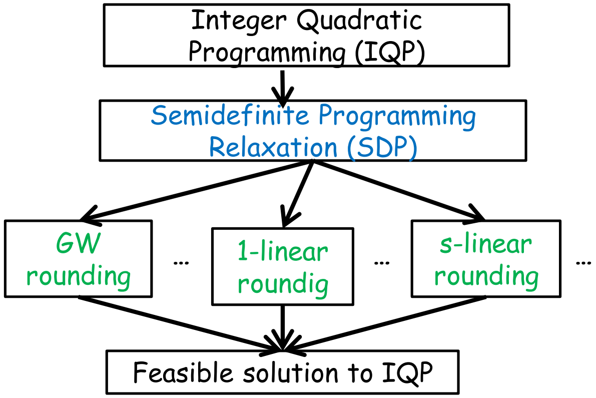
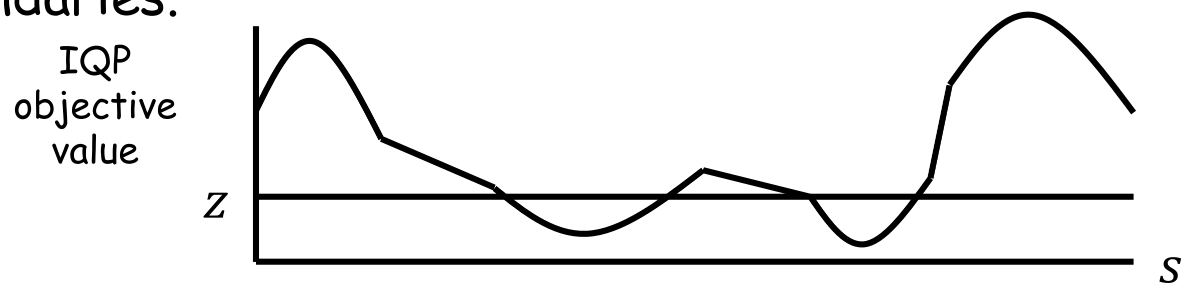


Partitioning Problems via IQPs

Our Results: SDP + s-linear rounding

Pseudo-dimension is O(log n), so small sample complexity.

Key idea: expected IQP objective value is piecewise quadratic in $\frac{1}{s}$ with n boundaries.

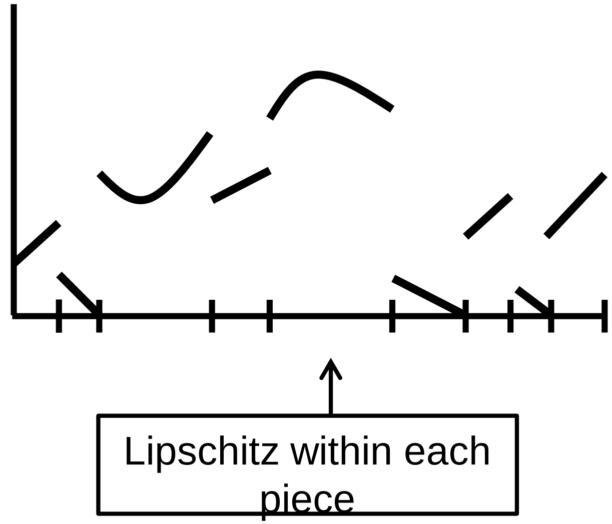


Given sample S, can find best algo from this family in poly time.

- Solve for all α intervals over the sample, find best parameter over each interval, output the best parameter overall.

Online Algorithm Selection

- So far, batch setting: collection of typical instances given upfront.
- [Balcan-Dick-Vitercik, FOCS 2018] online and private alg. selection.
- Scoring functions non-convex, with lots of discontinuities, cannot use known techniques. They are piecewise Lipschitz.
- Online optimization with Piecewise Lipschitz functions.
- Identify a general structural property called dispersion that allows us to get good regret bounds and show this property holds for many alg. selection problems.



Recent Work: Online Algorithm Selection

Recent Work: [Balcan-Dick-Vitercik, FOCS 2018]

Online optimization

On each round $t \in \{1, \ldots, T\}$:

1. The online learning algorithm chooses a parameter $\boldsymbol{\rho}_{\mathbf{t}}$
2. The adversary chooses a piecewise Lipschitz function $u_t : \mathcal{C} \to [0, H]$
   (corresponds to some problem instance and its induced scoring function)
   Receive the score of the parameter we selected $u_t(\rho_t)$.
3. **Full information:** Algorithm observes the function $u_t(\cdot)$
4. **Bandit feedback:** Algorithm only receives payout $u_t(\boldsymbol{\rho}_{\mathbf{t}})$.

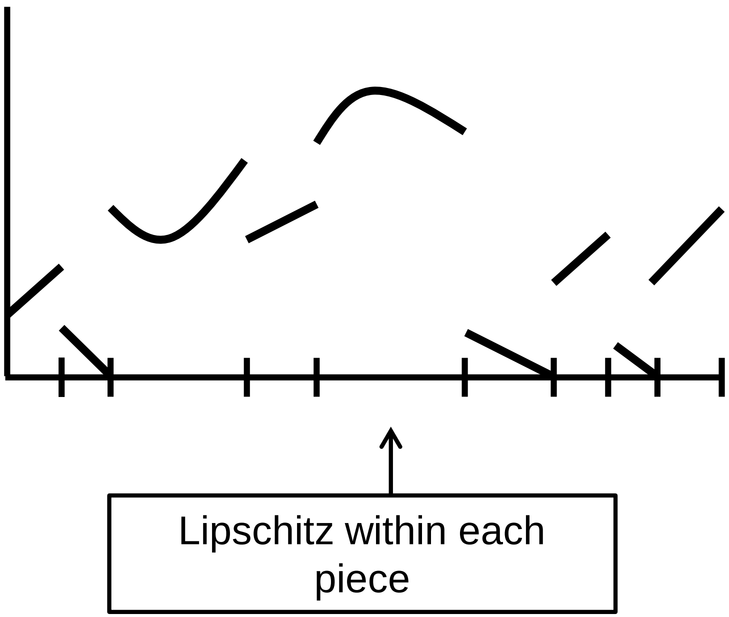
Goal: minimize regret: $\max_{\boldsymbol{\rho} \in \mathcal{C}} \sum_{t=1}^{T} u_t(\boldsymbol{\rho}) - \mathbb{E}\left[\sum_{t=1}^{T} u_t(\boldsymbol{\rho}_{\mathbf{t}})\right]$

↑ Performance of best parameter in hindsight

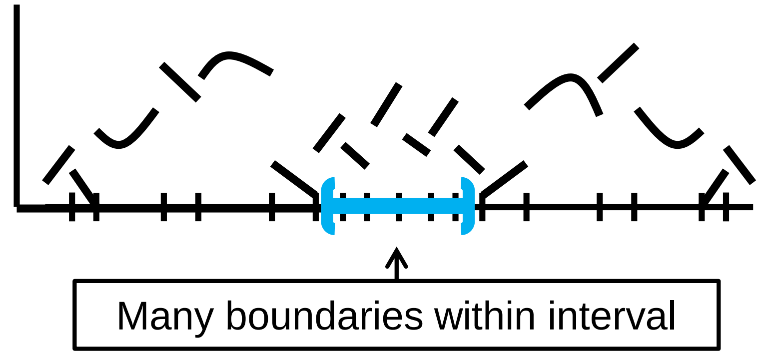
↑ Our cumulative performance

Dispersion, Sufficient Condition for No-Regret

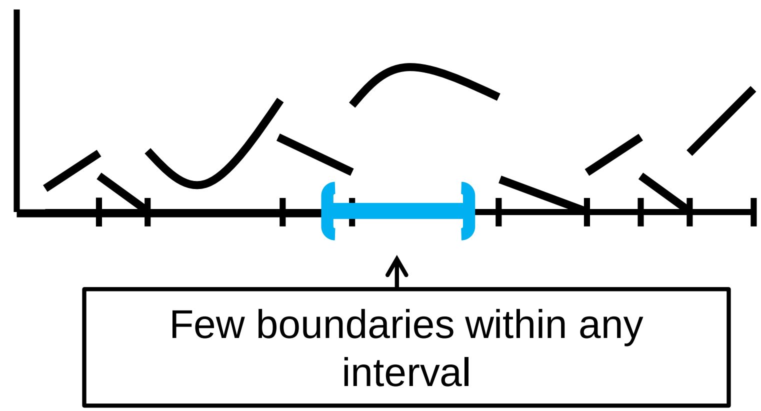
Piecewise Lipschitz function



Not disperse



Disperse



$\{u_1(\cdot), \ldots, u_T(\cdot)\}$ is $(\mathbf{w}, \mathbf{k})$-dispersed if any ball of radius $\mathbf{w}$ contains boundaries for at most $\mathbf{k}$ of the u_i.

Full information: exponentially weighted forecaster

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On each round $t \in \{1, \dots, T\}$:

- Sample a vector $\boldsymbol{\rho}_t$ from a distribution p_t where

$$p_t(\boldsymbol{\rho}) \propto \exp\left(\lambda \sum_{s=1}^{t-1} u_s(\boldsymbol{\rho})\right)$$

Our Results:

If $\sum_{t=1}^{T} u_t(\cdot)$ piecewise L-Lipschitz, $\{u_1(\cdot), \dots, u_T(\cdot)\}$ is $(\mathbf{w}, \mathbf{k})$-dispersed.

The expected regret is $O\left(H\left(\sqrt{Td\log\frac{1}{\mathbf{w}}} + \mathbf{k}\right) + TL\mathbf{w}\right)$.

Usual $\sqrt{T}$ bound, but lose a log(1/w) multiplicative term, and an additive kH term [for the k discontinuities that might be inside a ball of radius w around the optimal solution] and an additive TLw for the Lipschitz constant.

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For most problems:

- Set $\mathbf{w} \approx 1/\sqrt{T}$
- Get $\mathbf{k} = \sqrt{T} \times (\text{some function of problem})$
- Overall, get regret $\tilde{O}(H\sqrt{Td})$.

Example: rounding of SDP relaxation of IQP

Idea:

- Exploit **randomness of algorithm** to give a guarantee on dispersion.

- Prove that whp, for any $\alpha \geq \frac{1}{2}$, the set of u_i are

$$\left(\mathrm{T}^{\alpha-1}, \mathrm{O}\left(\mathrm{n}\mathrm{T}^{\alpha}\sqrt{\log \mathrm{n}}\right)\right)\text{-dispersed}$$

- Lipschitz value depends on which class of rounding schemes.

- Setting $\alpha = \frac{1}{2}$ leads to regret of $\tilde{\mathrm{O}}(\mathrm{Hn}\sqrt{\mathrm{T}})$.

Discussion

- Strong performance guarantees for data driven algorithm selection for combinatorial problems.
- Exploit structure to provide good sample complexity and regret bounds. Also privacy guarantees.
- From a learning theory point of view, techniques of independent interest beyond algorithm configuration.

- Related in spirit to Hyperparameter tuning, AutoML, MetaLearning.
- **Future Work**: use our insights to analyze problems commonly studied in these settings (e.g., tuning hyper-parameters in deep nets)