Foundations of Data Driven Combinatorial Algorithm Selection

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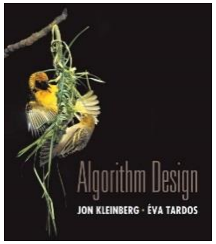
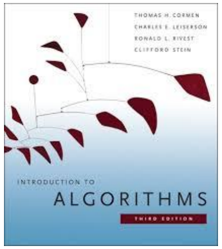
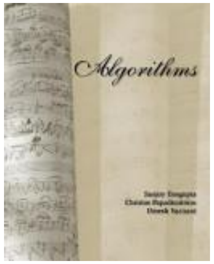
Data Driven Algorithm Selection

Some domains we have polynomial time optimal algorithms:

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





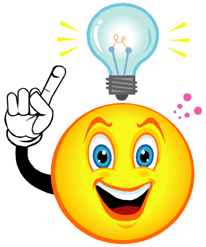


Some domains we don't:

- Different methods work better in different settings.

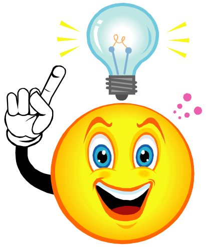
- Large family of methods – what's best in our application?

- 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.

- **Long history in the AI community.**
  - E.g., [Xu-Hutter-Hoos-LeytonBrown, JAIR 2008]
- **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

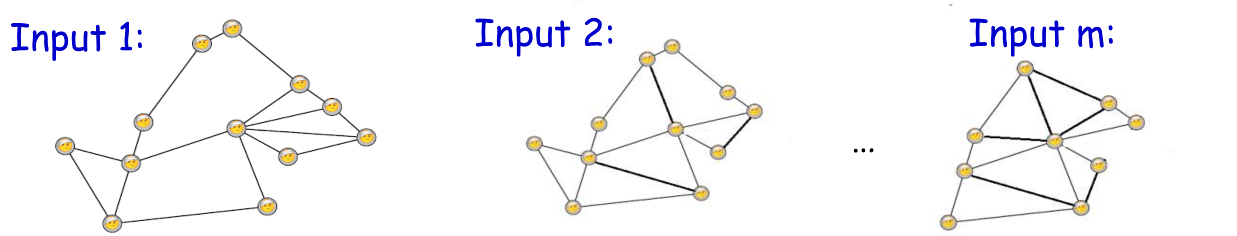
MST + Dynamic Programming

Greedy + Farthest Location

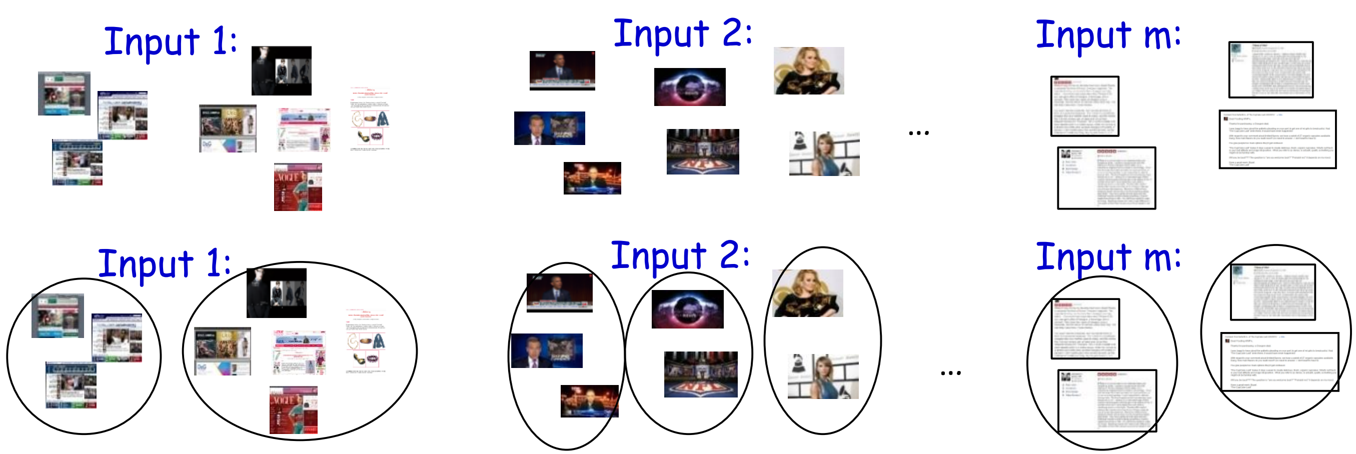
...

Sample of typical inputs

Facility location:



Clustering:



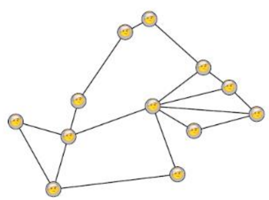
Algorithm Selection as a Learning Problem

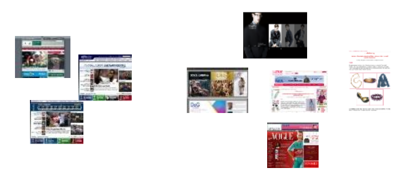
Goal: given large family of algos, sample of typical instances from domain, find an algo that performs well on new instances from same domain.

Why is it important?

- For some problems we don't know **any** algos that do well in the worst case, but we hope some algo in our family will do well in our domain.

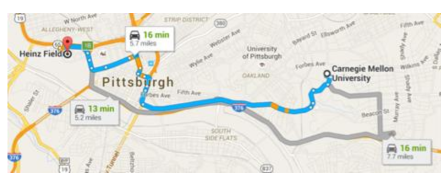
Facility location and clustering:





- For others, we do have good worst-case algorithms, but still, some do better than others on different domains.

Shortest paths:



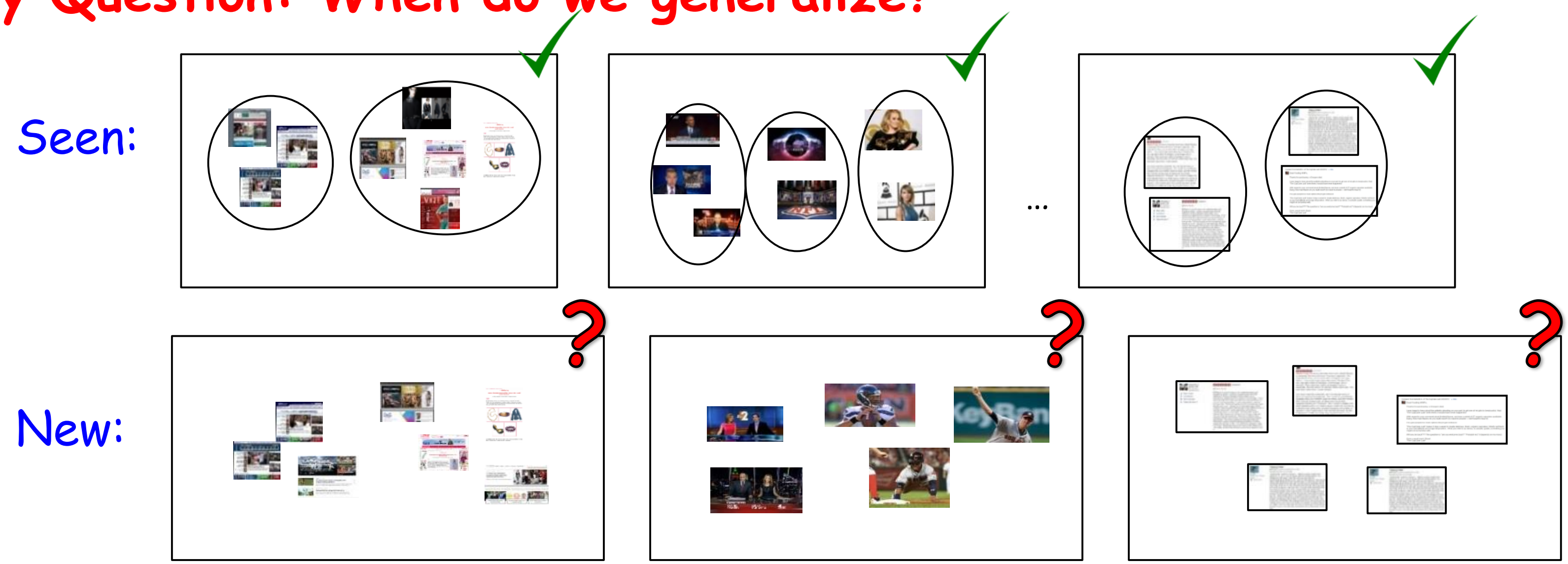
Adaptive algorithms have better performance!

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: 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

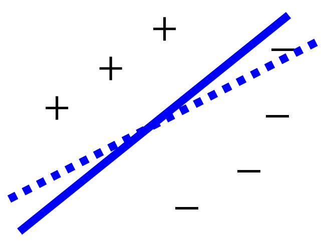
Goal: widely applicable techniques for analyzing the intrinsic complexity of families of algos and ensuring good generalizability.

Idea: apply tools from learning theory to analyze intrinsic complexity/dimension of families of algos.

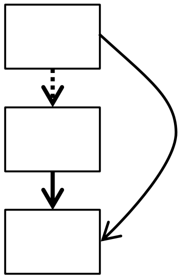
$m = O(\dim(F)/\epsilon)$ instances suffice to ensure generalizability

- Use this to design an efficient meta-algorithm

Challenge: due to combinatorial and modular nature, "nearby" programs/algos can have drastically different behavior.



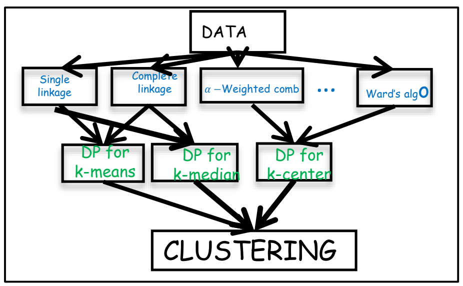
Classic machine learning

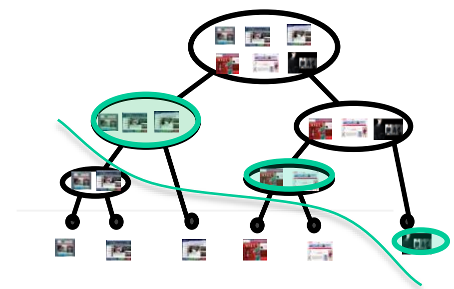


Our work

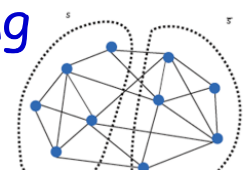
Sample Complexity of Algorithm Selection

- [Gupta-Roughgarden, SICOMP 2017]: greedy procedures for subset selection problems: knapsack, independent set.
- Our Work: [Balcan-Nagarajan-Vitercik-White, COLT 2017]
  - Clustering: Linkage + Dynamic Programming



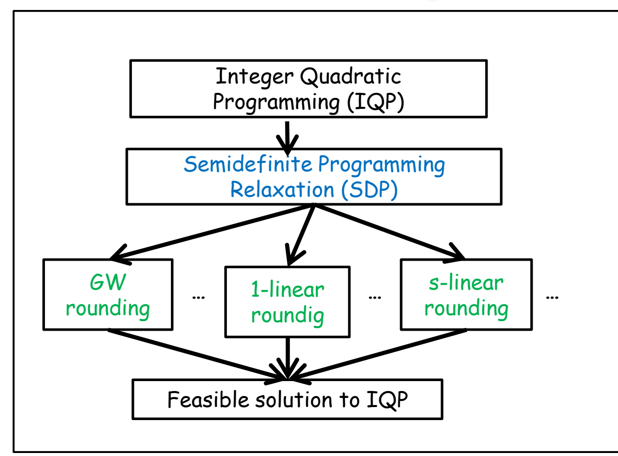


  - Partitioning pbs via IQPs: SDP + Rounding



E.g., Max-Cut,

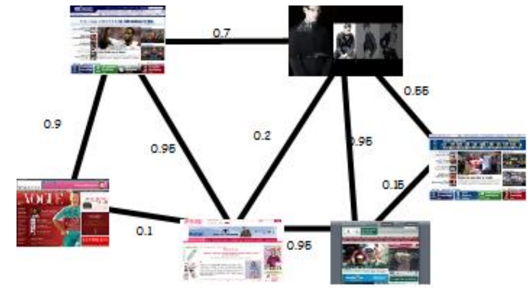
Max-2SAT, Correlation Clustering



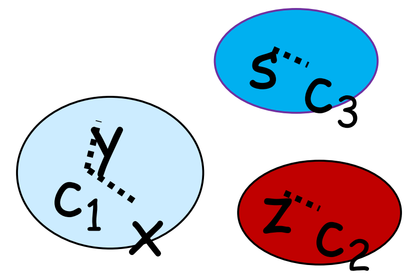
- Recent Work: [Balcan-Dick-Vitercik, 2017]
  - Private and online algorithm selection

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.



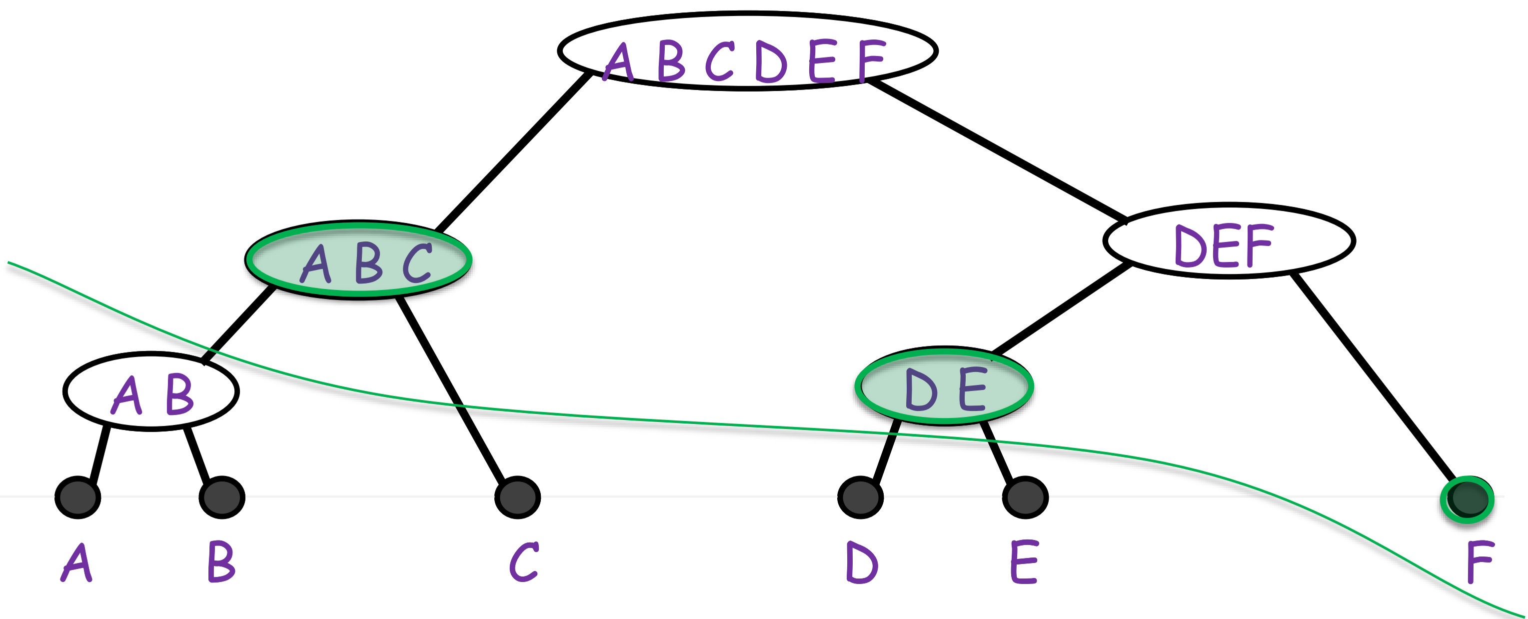
- Finding OPT is NP-hard, so no universal efficient algo that works on all domains.

- Exhaustive search is too expensive, and efficient heuristics sometimes work and sometimes don't.

Clustering: Linkage + Dynamic Programming

Family of poly time 2-stage algorithms:

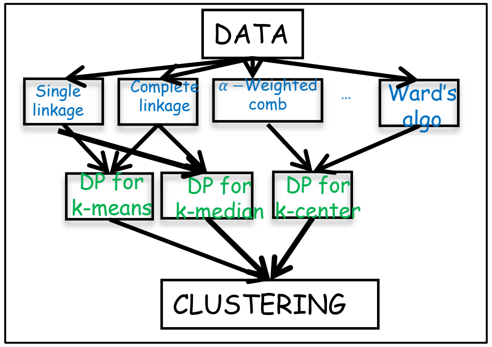
1. Use a linkage-based algorithm to organize data into a hierarchy (tree) of clusters.
2. Dynamic programming over this tree to identify pruning of tree corresponding to the best clustering.

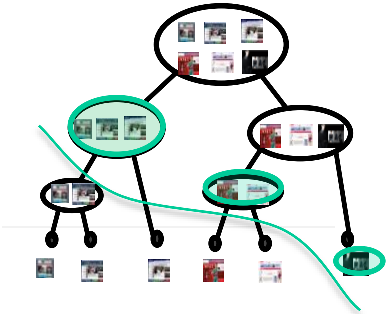


Clustering: Linkage + Dynamic Programming

1. Use a linkage-based algorithm to get a hierarchy.

2. Dynamic programming to the best prunning.

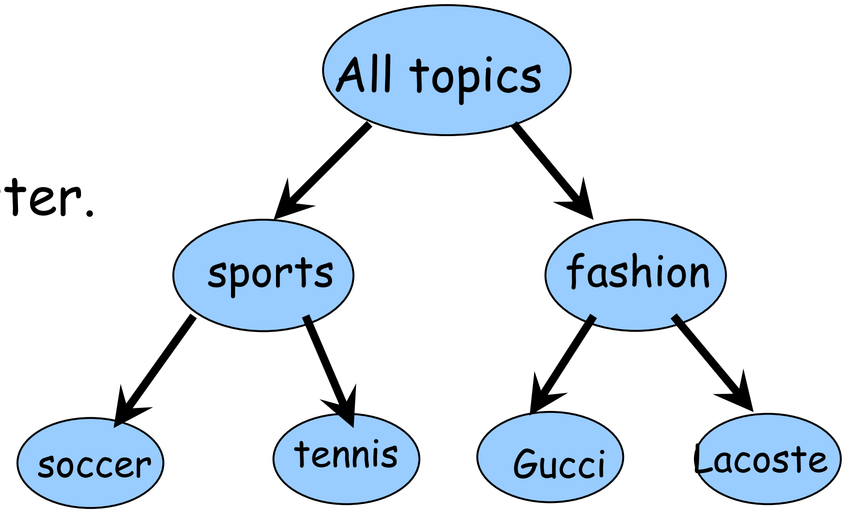




Linkage Procedures for Hierarchical Clustering

Bottom-Up (agglomerative)

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



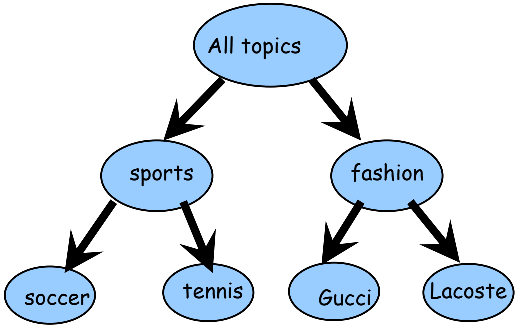
Different defs of "closest" give different algorithms.

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: $$\text{dist}(A,B) = \min_{x \in A, x' \in B} \text{dist}(x,x')$$

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

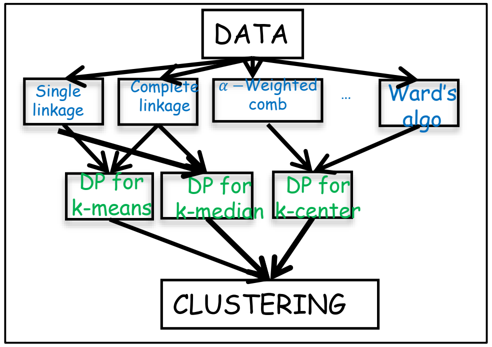
- Average linkage: $$\text{dist}(A,B) = \operatorname{avg}_{x \in A, x' \in B} \text{dist}(x,x')$$

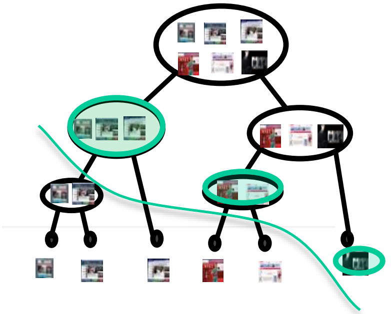
- α-weighted linkage:

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

Clustering: Linkage + Dynamic Programming

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



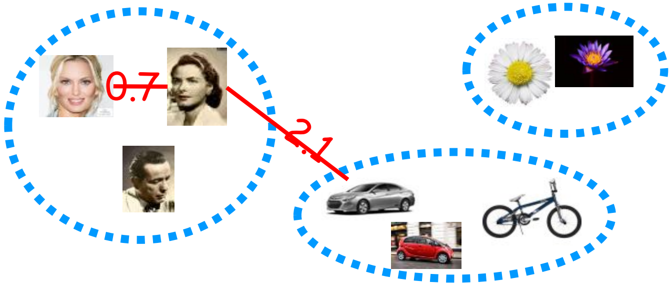


- Used in practice.

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

- Strong properties.

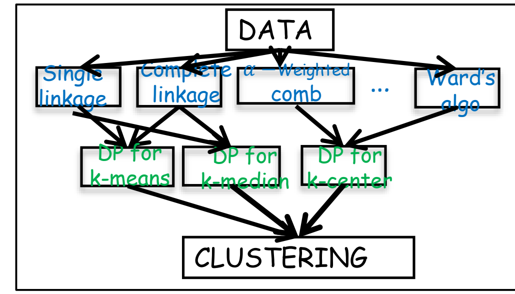
E.g., best known algos for perturbation resilient instances for k-median, k-means, k-center.



[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

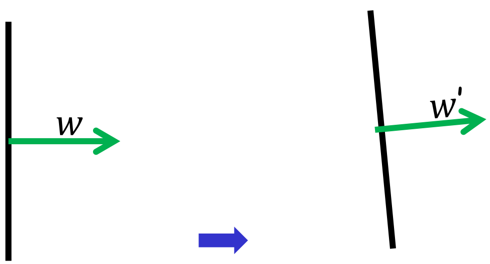


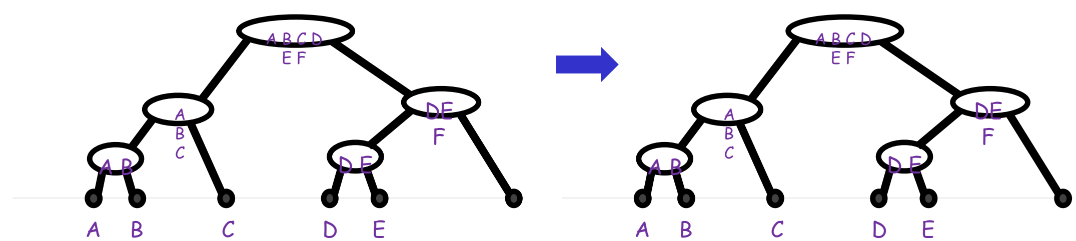
Our Results: α-weighted linkage+DP

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

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

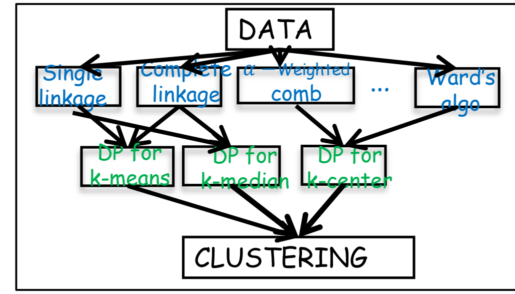
Key Technical Challenge: small changes to the parameters of the algo can lead to radical changes in the tree or clustering produced.





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

Clustering: Linkage + Dynamic Programming

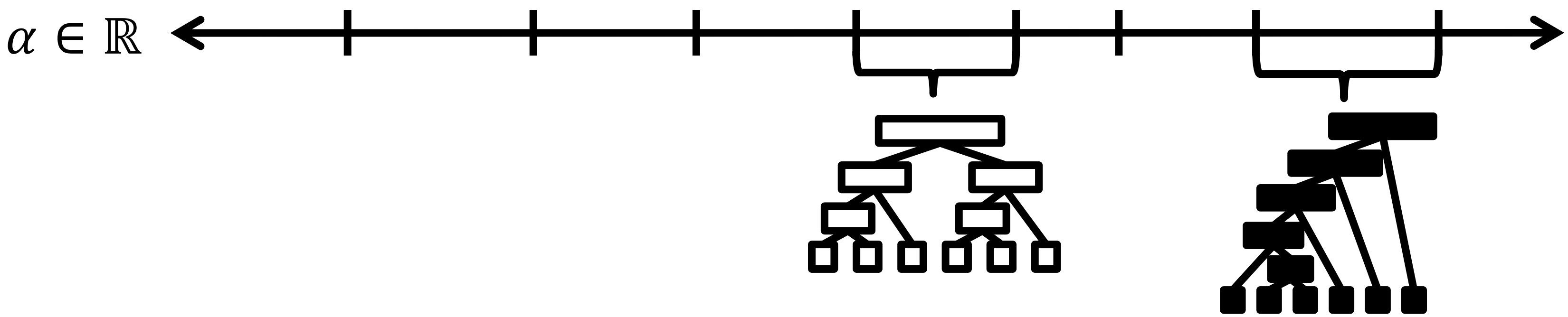


Our Results: α-weighted linkage+DP

- 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

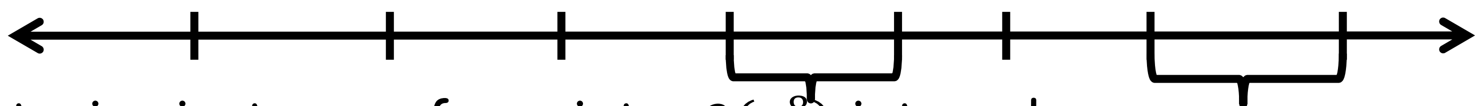
Our Results: α-weighted linkage+DP

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

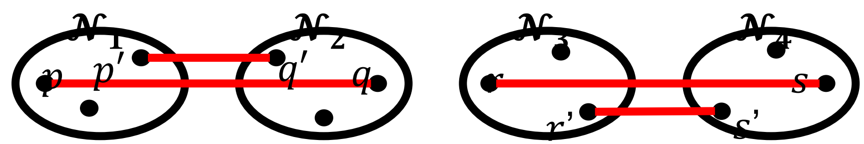
Key idea:

- 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.

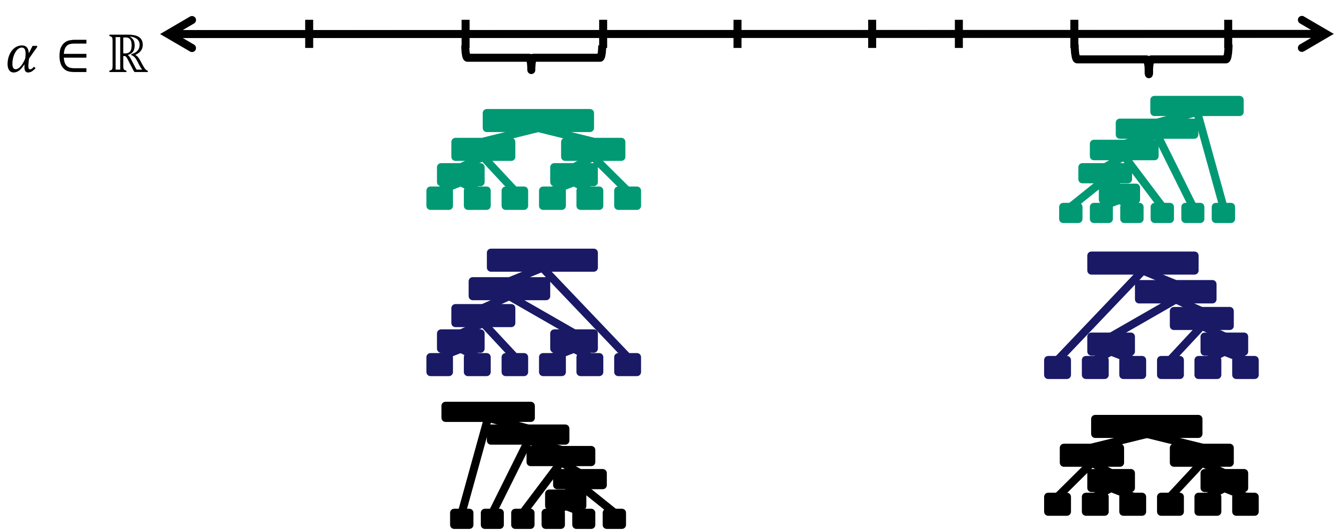
Clustering: Linkage + Dynamic Programming

Our Results: α-weighted linkage+DP

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

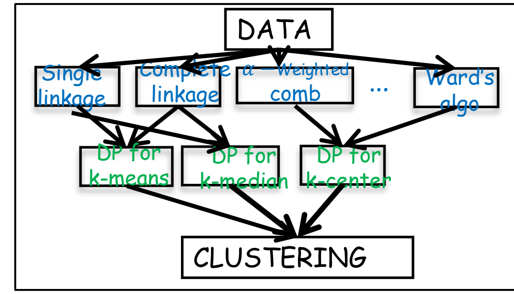
Key idea:

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



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

Clustering: Linkage + Dynamic Programming



Our Results: α-weighted linkage+DP

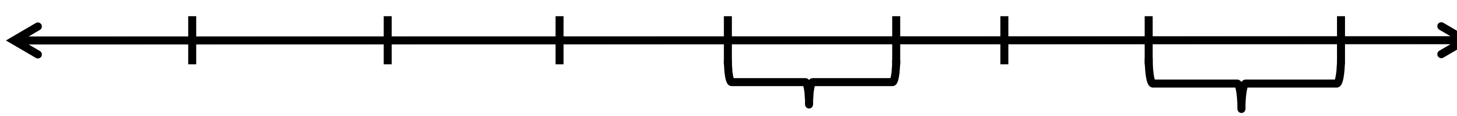
- Pseudo-dimension is O(log n).

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

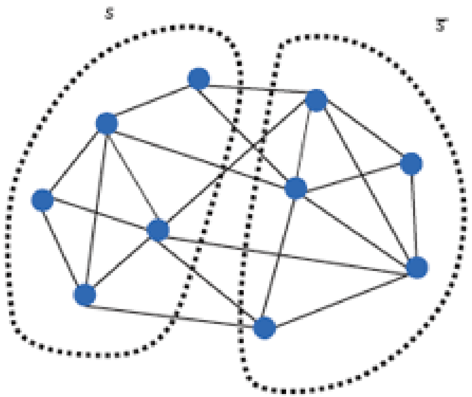
Partitioning Problems via IQPs

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

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



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

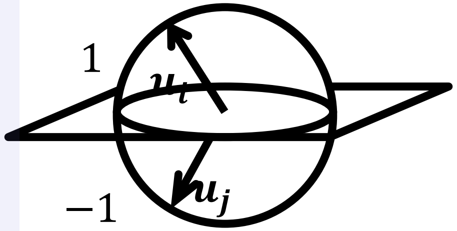
Algorithmic Approach: SDP + Rounding

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

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

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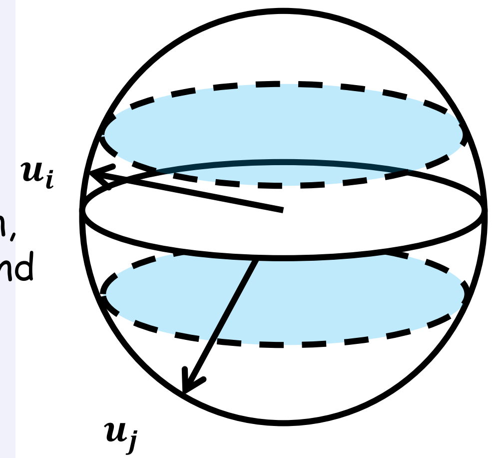


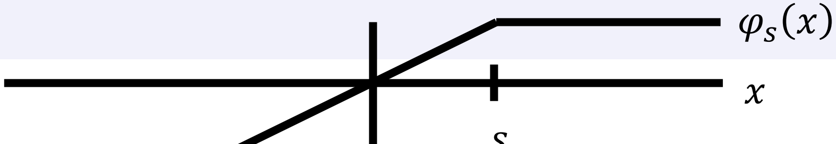
Inside margin, randomly round

outside margin, round to -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 $\frac{1}{2} - \frac{1}{2}\varphi_s(\langle \boldsymbol{u}_i, \boldsymbol{Z} \rangle)$



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

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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- Choose a random hyperplane.
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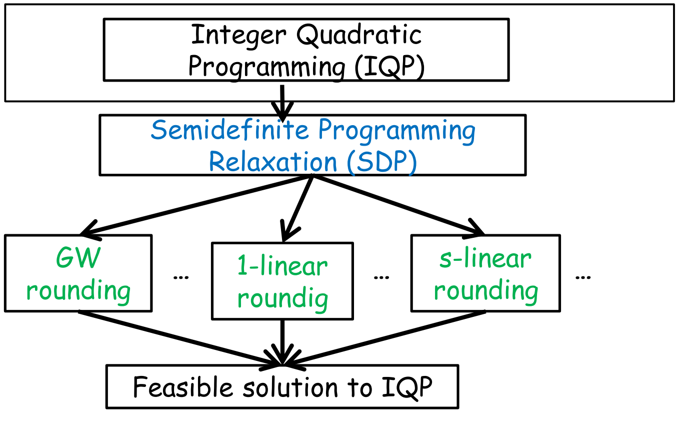
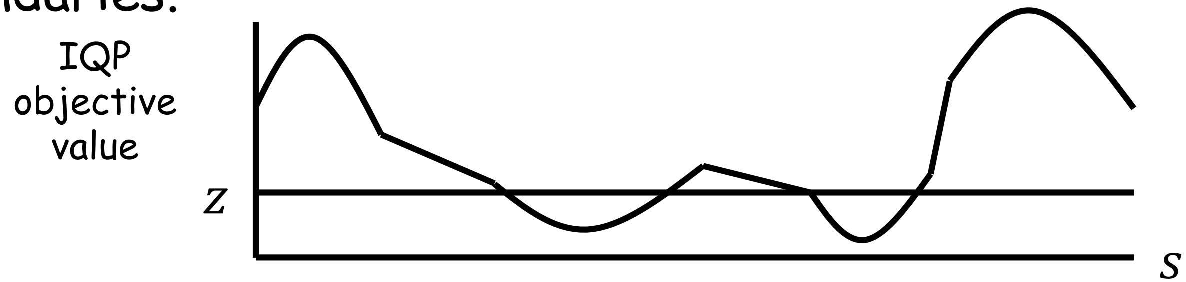


Partitioning Problems via IQPs

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.

Recent Work: Online Private Alg. Selection

Recent Work: [Balcan, Dick, Vitercik'17]

Online optimization

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

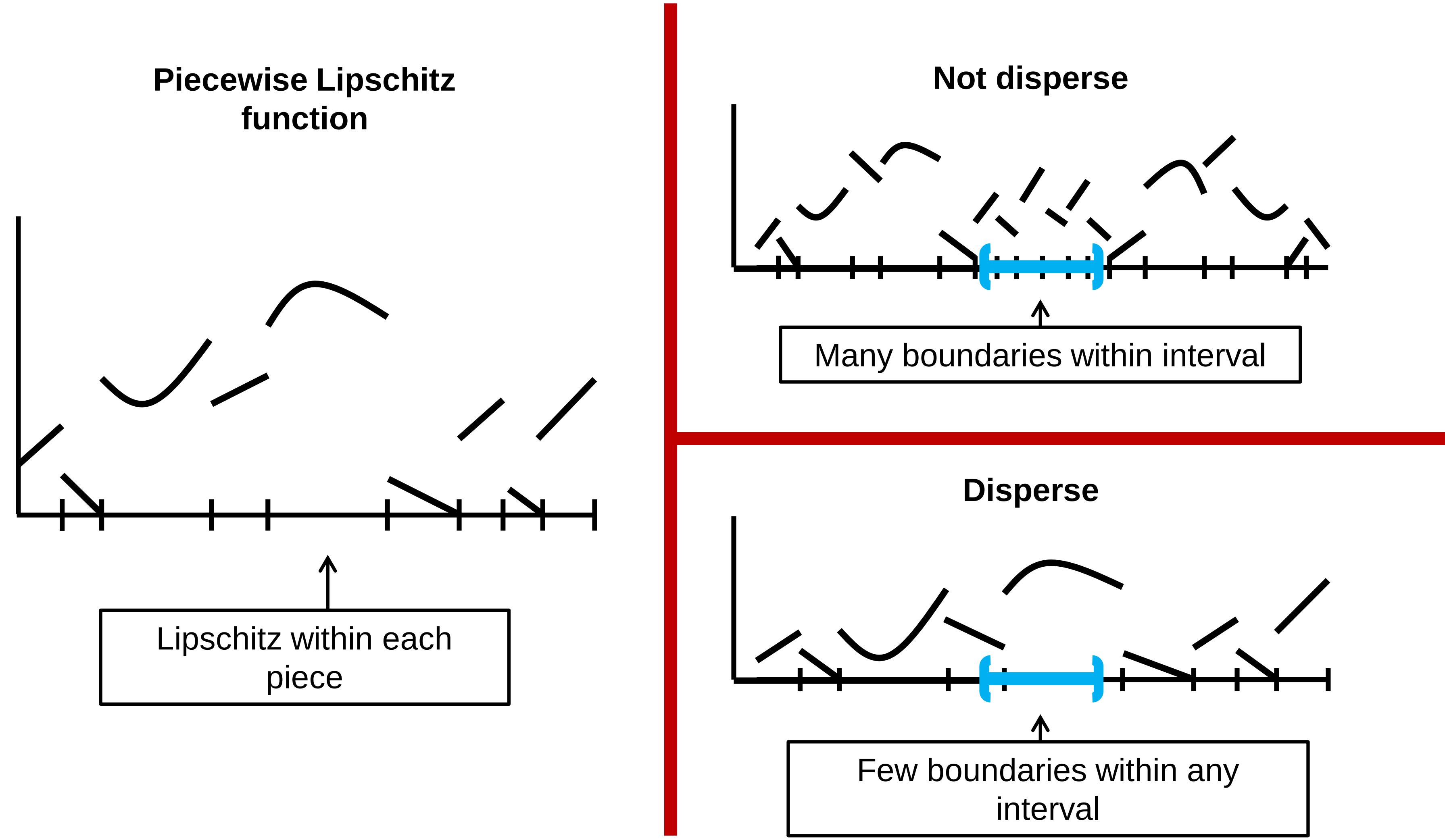
1. The online learning algorithm chooses a parameter $\boldsymbol{\rho_t}$
2. The adversary chooses a piecewise Lipschitz function $u_t: \mathcal{C} \to [0, H]$

   (Equivalently, the adversary can choose a problem instance x_t and sets $u_t(\boldsymbol{\rho_t}) = u(x_t, \boldsymbol{\rho_t})$.)
3. **Full information:** Algorithm observes the function $u_t(\cdot)$ and receives payout $u_t(\boldsymbol{\rho_t})$.

   Bandit feedback: Algorithm only receives payout $u_t(\boldsymbol{\rho_t})$.

We want to minimize regret: $\max_{\boldsymbol{\rho} \in \mathcal{C}} \sum_{t=1}^{T} u_t(\boldsymbol{\rho}) - \mathbb{E}[\sum_{t=1}^{T} u_t(\boldsymbol{\rho_t})]$

Dispersion, Sufficient Condition for No-Regret



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

Full information: exponentially weighted forecaster

Full information: exponentially weighted forecaster [Cesa-Bianchi and Lugosi 2006]

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 $(\boldsymbol{w}, \boldsymbol{k})$-dispersed.

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

Example: rounding of SDP relaxation of IQP

We consider s-linear rounding and "outward rotation" rounding.

Idea:

- Exploit randomness of algor to give a guarantee on dispersion.
- View random hyperplane Z as part of problem instance.
- Prove that whp, for any $\alpha \geq \frac{1}{2}$, the set of u_i are

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

- Lipschitz value depends on which class of rounding schemes.

Example: Knapsack

A problem instance is collection of items i, each with a value v_i and a size s_i, along with a knapsack capacity C.

Goal: select most valuable subset of items that fits. Find subset T to maximize $\sum_{i\in T} v_i$ subject to $\sum_{i\in T} s_i \leq C$.

Natural family of algorithms: given ρ, select the better of:

- Greedily pack items in order of value (highest value first) subject to feasibility.
- Greedily pack items in order of v_i/s_i^{ρ} subject to feasibility.

We show: under natural conditions on items (every pair of items has a bounded joint value distribution), can get $\boldsymbol{\tilde{O}(n^2\sqrt{T})}$ regret.

Summary

- Strong performance guarantees for data driven algorithm selection.
  - Exploit structure to overcome in-stability.

- Related work: sample complexity of automated mechanism design.

  [Balcan-Sandholm-Vitercik, NIPS'16]

Auction Design

Future Work: analyze other problems (e.g., tuning parameters in deep networks)