Foundations of Application-Specific Algorithm Configuration

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Clustering is a general technique applied in diverse settings.

We can cluster web pages by topic.
Clustering is a general technique applied in diverse settings.

We can cluster images by subject.
Clustering is a general technique applied in diverse settings.

We can cluster residences in towns to determine optimal locations for fire stations.
Like many real-world problems, clustering is NP-hard.
There are many approximation and heuristic algorithms that work well for some problems and poorly for others.
For a given application domain, how do we know which algorithm to use?
We could compare worst-case guarantees, but this won’t help if worst-case instances don’t appear in the application domain.
Given a set of typical problem instances from our application domain, we can **learn** the best algorithm for that domain.
How can I use the set of samples to find an algorithm that’s best for my application domain?
This model has been studied in applied communities (e.g. [Hutter et al. ‘09]).

How can I use the set of samples to find an algorithm that’s best for my application domain?
This model has been studied from a theoretical perspective [Gupta and Roughgarden ‘16].

How can I use the set of samples to find an algorithm that’s best for my application domain?
Several works beyond Gupta and Roughgarden’s work have explored algorithm configuration with theoretical guarantees [Li et al. ‘16, Garg and Kalai ‘17, Kleinberg, Leyton-Brown, and Lucier ’17, Cohen-Addad and Kanade ’17]
How can I use the set of samples to find an algorithm that’s best for my application domain?
1. Fix a class of (clustering) algorithms $\mathcal{A}$
2. Receive a sample of (clustering) problem instances from an unknown distribution $\mathcal{D}$
3. Find the algorithm $A^*$ in $\mathcal{A}$ that does best on the sample

“Best” could mean closest to ground truth, smallest k-means objective, etc.
1. What should the class $\mathcal{A}$ of clustering algorithms be?

2. How do we find the empirically optimal algorithm $A^*$ in $\mathcal{A}$?

3. Will the performance of $A^*$ generalize to the distribution?
1. What should the class $\mathcal{A}$ of clustering algorithms be?

2. How do we find the empirically optimal algorithm $A^*$ in $\mathcal{A}$?

3. $A^*$ has high performance over the sample, but will it have high performance in expectation over $\mathcal{D}$?
1. Clustering algorithm configuration
   a. What should the class of clustering algorithms be?
   b. How do we find the empirically optimal algorithm $A^*$?
   c. Will the performance of $A^*$ generalize to the distribution?

2. Integer quadratic programming algorithm configuration

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

2. Perform dynamic programming over this tree to identify a pruning corresponding to the best clustering.
Dynamic programming

Output clustering
Data

Dynamic programming

Output clustering

Average linkage
Single linkage
Complete linkage

\( \alpha \) linkage
\( \alpha \)-linkage: Merge \( \mathcal{N}_i \) and \( \mathcal{N}_j \) if they minimize

\[
\min_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^\alpha + \max_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^{1-\alpha}
\]

Varying \( \alpha \) interpolates between complete and single linkage.
What clustering algorithm is best for my application domain?
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**Key challenge:** Neighboring $\alpha$ values could result in different trees, and therefore very different performance costs.
We explicitly break the real line into a small number of intervals such that **on each sample:**

Two $\alpha$’s from one interval result in the same tree.
\( \alpha \in \mathbb{R} \)
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Two $\alpha$’s from one interval result in the same tree. And therefore the same clustering. And therefore the same performance cost.

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<table>
<thead>
<tr>
<th>Theorem</th>
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<tbody>
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<td>For a clustering instance of $n$ points, there are $O(n^8)$ intervals such that any two $\alpha$’s from one interval result in the same tree.</td>
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</table>
**α-linkage**: Merge $\mathcal{N}_i$ and $\mathcal{N}_j$ if they minimize

$$
\min_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^\alpha + \max_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^{1-\alpha}
$$

**Main idea:**
Over any $\alpha$ interval, so long as the order in which all pairs of nodes are merged is fixed, then the resulting tree will be invariant.
**α-linkage:** Merge $\mathcal{N}_i$ and $\mathcal{N}_j$ if they minimize

$$\min_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^\alpha + \max_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^{1-\alpha}$$

Which will merge first, $\mathcal{N}_1$ and $\mathcal{N}_2$, or $\mathcal{N}_3$ and $\mathcal{N}_4$?

Depends on whether

$$d(p, q)^{1-\alpha} + d(p', q')^\alpha \geq d(r, s)^{1-\alpha} + d(r', s')^\alpha$$
\( \alpha \)-linkage: Merge \( \mathcal{N}_i \) and \( \mathcal{N}_j \) if they minimize

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\min_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^{\alpha} + \max_{p \in \mathcal{N}_i, q \in \mathcal{N}_j} (d(p, q))^{1-\alpha}
\]

Which will merge first, \( \mathcal{N}_1 \) and \( \mathcal{N}_2 \), or \( \mathcal{N}_3 \) and \( \mathcal{N}_4 \)?

Depends on the sign of

\[
d(p, q)^{1-\alpha} + d(p', q')^{\alpha} - d(r, s)^{1-\alpha} - d(r', s')^{\alpha}
\]
The expression
\[ d(p, q)^{1-\alpha} + d(p', q')^\alpha - d(r, s)^{1-\alpha} - d(r', s')^\alpha \]
has \( \leq 4 \) zeros. We call these 4 zeros **critical \( \alpha \) values**.

Sort all \( 4n^8 \) critical \( \alpha \) values for all \( n^8 \) 8-tuples of points.

\[ \alpha \in \mathbb{R} \]

**For all 8-tuples**, the sign of
\[ d(p, q)^{1-\alpha} + d(p', q')^\alpha - d(r, s)^{1-\alpha} - d(r', s')^\alpha \]
is **fixed** between any two critical \( \alpha \) values.

Therefore, the **order of all merges is fixed** between any two critical \( \alpha \) values.
Since on a single interval, the order of all merges is fixed, the resulting tree will also be fixed.

**Theorem**

For a clustering instance of $n$ points, there are $O(n^8)$ intervals such that any two $\alpha$'s from one interval result in the same tree.
### Algorithm (high level)

1. Solve for all $\alpha$ intervals over the sample
2. Find the $\alpha$ interval with the smallest empirical cost

(We prove that any $\alpha$ from that interval will have approximately smallest expected cost)
1. Clustering algorithm configuration
   a. What should the class of clustering algorithms be?
   b. How do we find the empirically optimal algorithm $A^*$?
   c. Will the performance of $A^*$ generalize to the distribution?

2. Integer quadratic programming algorithm configuration

3. Ongoing work
We’ve shown that over any set of samples, there are only a small number of significantly different algorithms.

This implies low complexity (think VC dimension)
Theorem

Given a sample of $\tilde{O}(1/\epsilon^2)$ clustering problems, with high probability, the expected performance cost of the best $\alpha$ over the sample is $\epsilon$-close to optimal over the distribution.
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3. Ongoing work
Many classic problems can be formulated as IQPs, including max-cut, max-2sat, and correlation clustering. These problems have applications in computational biology, circuit design, and statistical physics.
We focus on IQPs of the form:

$$\text{maximize } x^T A x \text{ subject to } x \in \{-1,1\}^n$$
Transform SDP output to a feasible solution
Out of infinitely many ways to perform ③ how do we choose the best?

NP-hard problem → Integer-quadratic programing formulation → Semidefinite programing (SDP) relaxation

Transform SDP output to a feasible solution
How can I use the set of samples to find an SDP rounding algorithm that’s best for my application domain?
NP-hard problem \rightarrow Integer-quadratic programing formulation \rightarrow Semidefinite programing (SDP) relaxation

Transform SDP output to a feasible solution
2. SDP relaxation

**IQP formulation**

| maximize $x^T A x = \sum_{i,j} a_{i,j} x_i x_j$ subject to $x \in \{-1,1\}^n$ |

Associate each binary variable $x_i$ with a vector $u_i$.

**SDP relaxation**

| maximize $\sum_{i,j} a_{i,j} \langle u_i, u_j \rangle$ subject to $\|u_i\| = 1$ |

The SDP yields an optimal embedding... but **how does it indicate a feasible solution $x$ to the IQP?**
Transform SDP output to a feasible solution
<table>
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<td>1. Choose a random hyperplane</td>
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![Diagram](image)
Rounding procedure [Goemans and Williamson ‘95]

1. Choose a random hyperplane

2. (Deterministic thresholding.) Set $x_i$ to -1 or 1 based on which side of the hyperplane the vector $u_i$ falls on

Zwick ['99] and Feige and Langberg ['06] showed that randomized thresholding works even better in some cases.

1 or $-1$?

Definitely 1.
Feige and Langberg ['06] proposed a parameterized algorithm family. The parameter controls the level of randomness in the final vertex assignment.
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This parameterized family is defined by \textit{s-linear rounding} functions: 
\[ \varphi_s(x) = -1_{x<-s} + \frac{x}{s} \cdot 1_{x\in[-s,s]} + 1_{x>s} \]

\begin{center}
\begin{tikzpicture}
  \draw[->] (-4,0) -- (4,0) node[right] {$\varphi_s(x)$};
  \draw[->] (0,-3) -- (0,3) node[above] {$x$};
  \draw (-2,0) -- (-2,1);
  \draw (2,0) -- (2,1);
  \draw (0,-2) -- (0,2);
  \draw (0,0) -- (0,0) node[above] {$s$};
\end{tikzpicture}
\end{center}

**Rounding procedure** [Feige and Langberg ‘06]

1. Draw a random hyperplane $Z$
2. Set $x_i$ to 1 with probability $\frac{1}{2} + \frac{1}{2} \varphi_s(\langle u_i, Z \rangle)$ and
   -1 with probability $\frac{1}{2} - \frac{1}{2} \varphi_s(\langle u_i, Z \rangle)$
The expected IQP objective value is \textit{piecewise quadratic} in \( \frac{1}{s} \) with a \textbf{small} number of pieces.
### Rounding procedure [Feige and Langberg ‘06]

1. Draw a random hyperplane \( Z \)
2. Set \( x_i \) to 1 with probability \( \frac{1}{2} + \frac{1}{2} \varphi_s(\langle u_i, Z \rangle) \) and
   -1 with probability \( \frac{1}{2} - \frac{1}{2} \varphi_s(\langle u_i, Z \rangle) \)

Notice that \( \mathbb{E}[x_i] = \varphi_s(\langle u_i, Z \rangle) \).
Given a hyperplane $Z$, the expected value of the solution produced by this $s$-linear rounding scheme is

$$\mathbb{E} \left[ \sum_{i,j} a_{i,j} x_i x_j \right] = \sum_{i,j} a_{i,j} \varphi_s(\langle u_i, Z \rangle) \varphi_s(\langle u_j, Z \rangle)$$

$\varphi_s(\langle u_i, Z \rangle)$ is $-1, +1$ or $\frac{\langle u_i, Z \rangle}{s}$ depending on whether $\langle u_i, Z \rangle < -s$, $\langle u_i, Z \rangle \in [-s, s]$, or $\langle u_i, Z \rangle > s$

The expected IQP value is piecewise quadratic in $\frac{1}{s}$ with boundaries at the points $|\langle u_i, Z \rangle|$. 
**Algorithm** *(high level)*

1. Solve for all intervals over the sample where the objective function is piecewise quadratic.
2. Find the best parameter over each interval.
3. Output the best parameter overall.

(We prove that this parameter is approximately optimal over the unknown distribution)
We give an **efficient** algorithm for determining a nearly **optimal randomized rounding function** from Feige and Langberg’s infinite class. It requires $\tilde{O}(1/\epsilon^2)$ samples.

**Diagram:**

1. NP-hard problem
2. Integer-quadratic programming formulation
3. Semidefinite programming (SDP) relaxation
4. Transform SDP output to a feasible solution
1. Clustering algorithm configuration
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2. Integer quadratic programming algorithm configuration

3. Ongoing work
In recently submitted work, we extract structure shared among many configuration problems.

We show how to use this structure to design both online and private configuration algorithms.

Thanks!

Questions?