Machine Learning for Optimization

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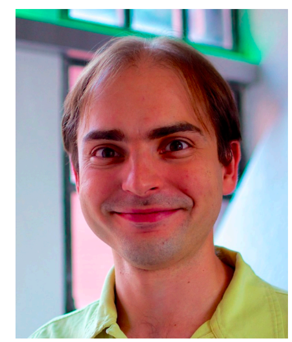


S.Vassilvitskii

Online Scheduling via Learned Weights. SODA 2020.

Learnable and Instance-Robust Predictions for Matchings, Flows and Load Balancing. ESA 2021

Using Predicted Weights for Ad Delivery. ACDA 2021

Faster Matching via Learned Duals. NeurIPS 2021 (oral)

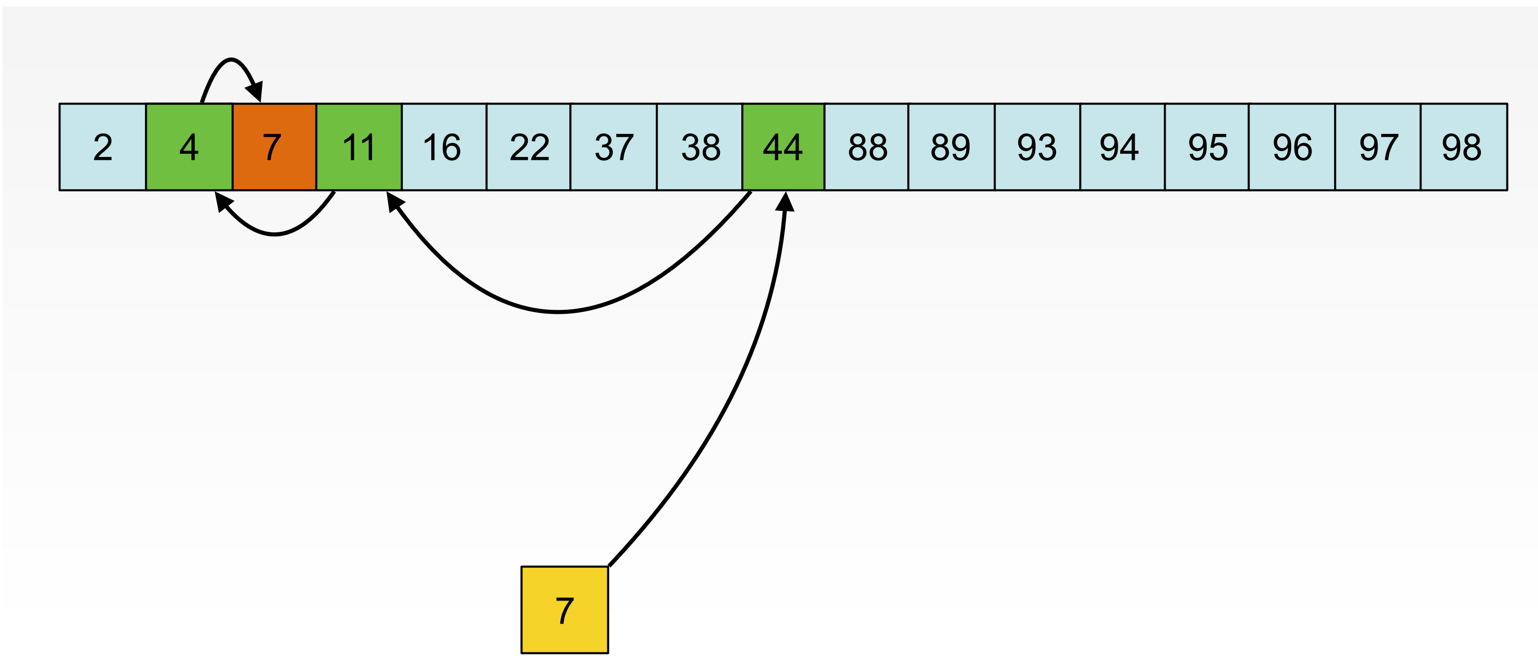
Machine Learning is Transforming Society

- Has not fundamentally changed combinatorial optimization
- However, could it?

Optimization Augmented with Machine Learning

Motivating Example
[Kraska et al. SIGMOD 2018]

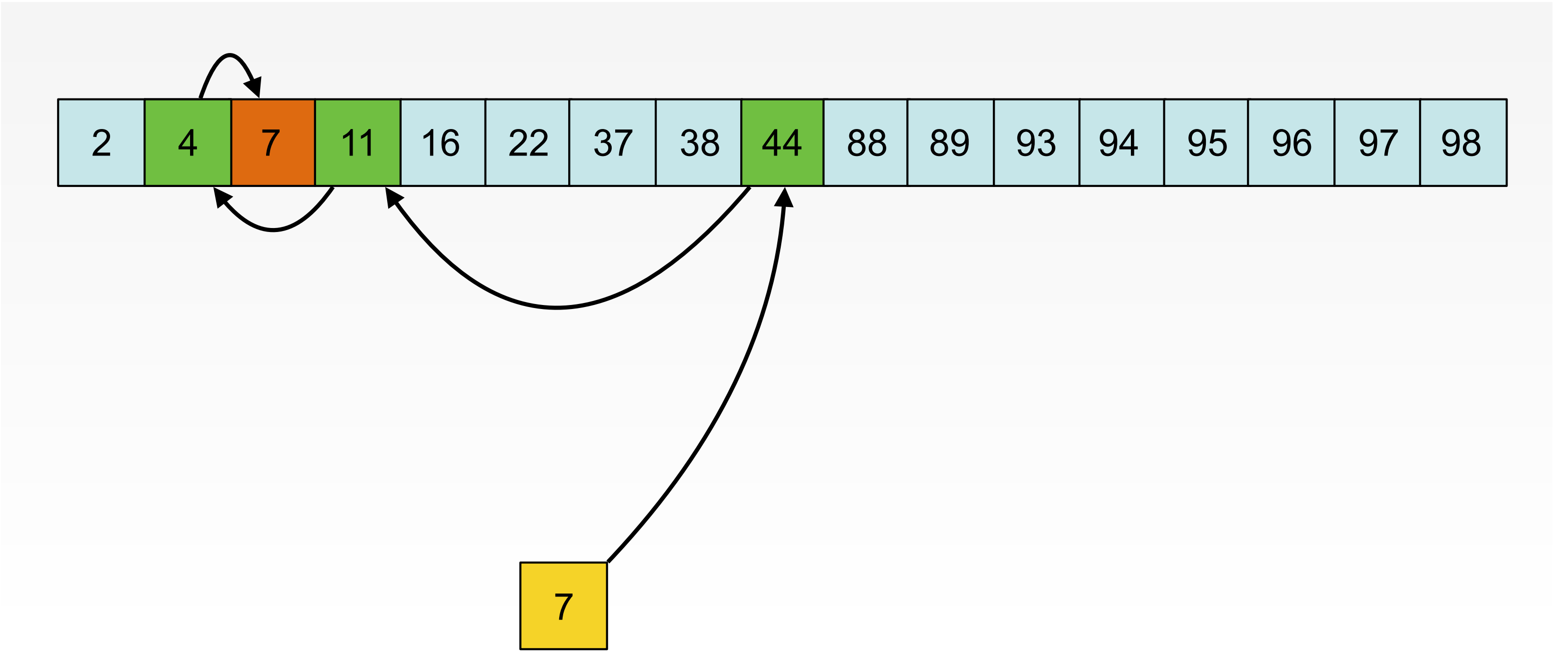
- Array of n integers A
- Over time queries arrive asking if q is in A



Motivating Example

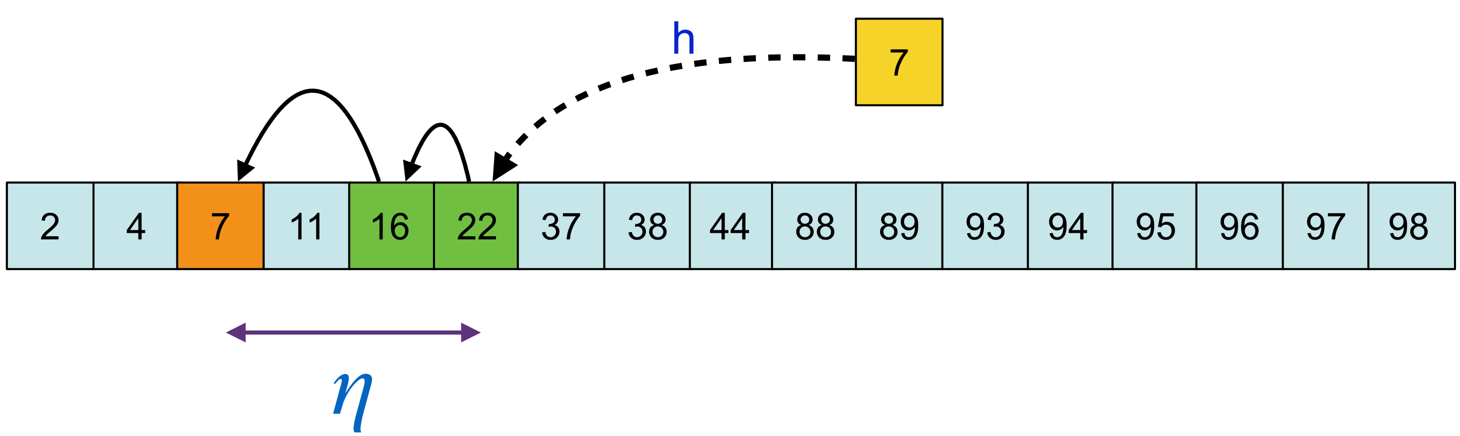
- Array of n integers A
- Over time queries arrive asking if q is in A

O(log n) lookup time



Motivating Example

- Train a predictor h(q) to predict where q is in the array
    - Estimates where the integer is based on prior queries
- Could be wrong, but hopefully not too far off
    - Use doubling binary search from prediction



Motivating Example

- Analysis
  - Let η be the value of $|h(q) - OPT(q)|$, the error in the prediction
  - Run time is $O(\log \eta)$
- Need to be careful about overhead of the prediction
  - Can make this work in practice

Learning Augmented Algorithm

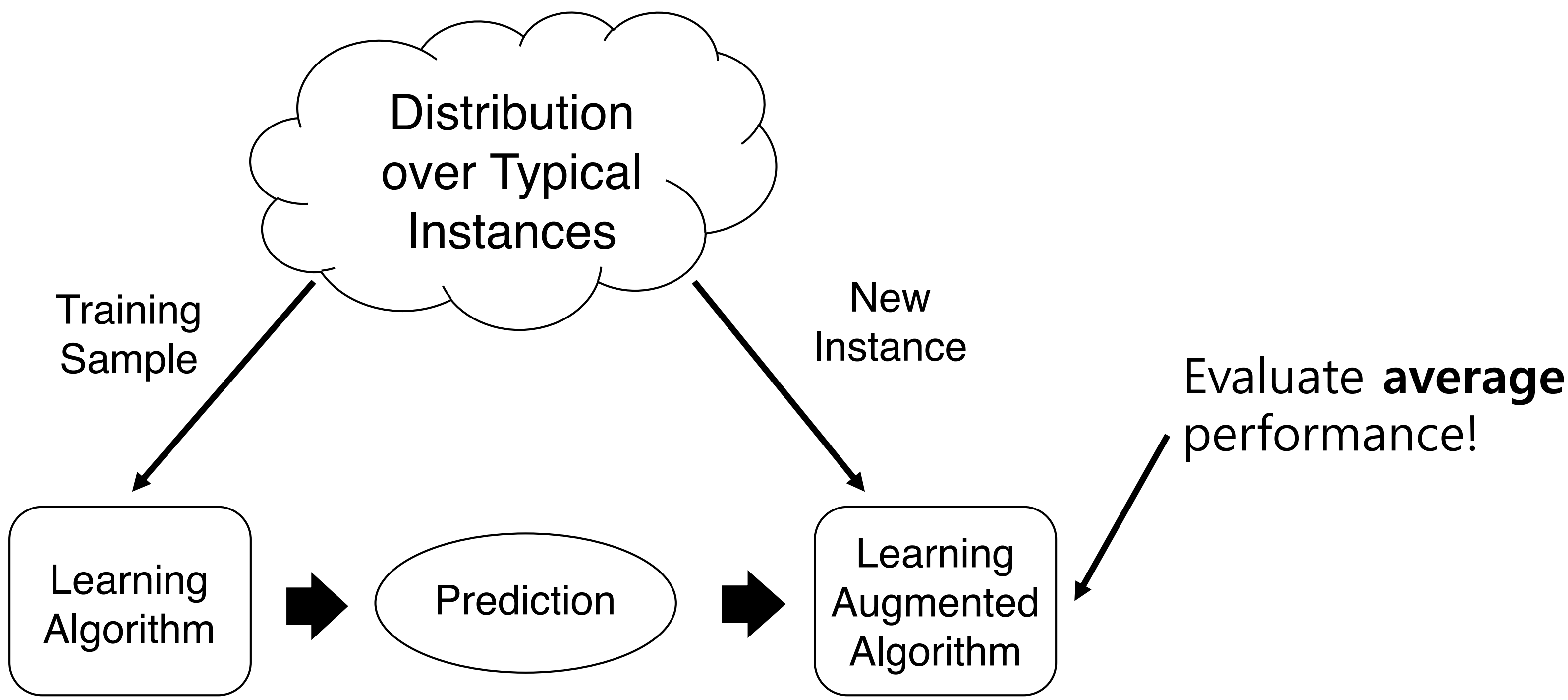
- Run time binary search O(log n)
- Run time prediction O(log η)

- Perfect predictions give constant lookup
- Worst case same as the best classical algorithm
    - Gracefully degrades to the worst case

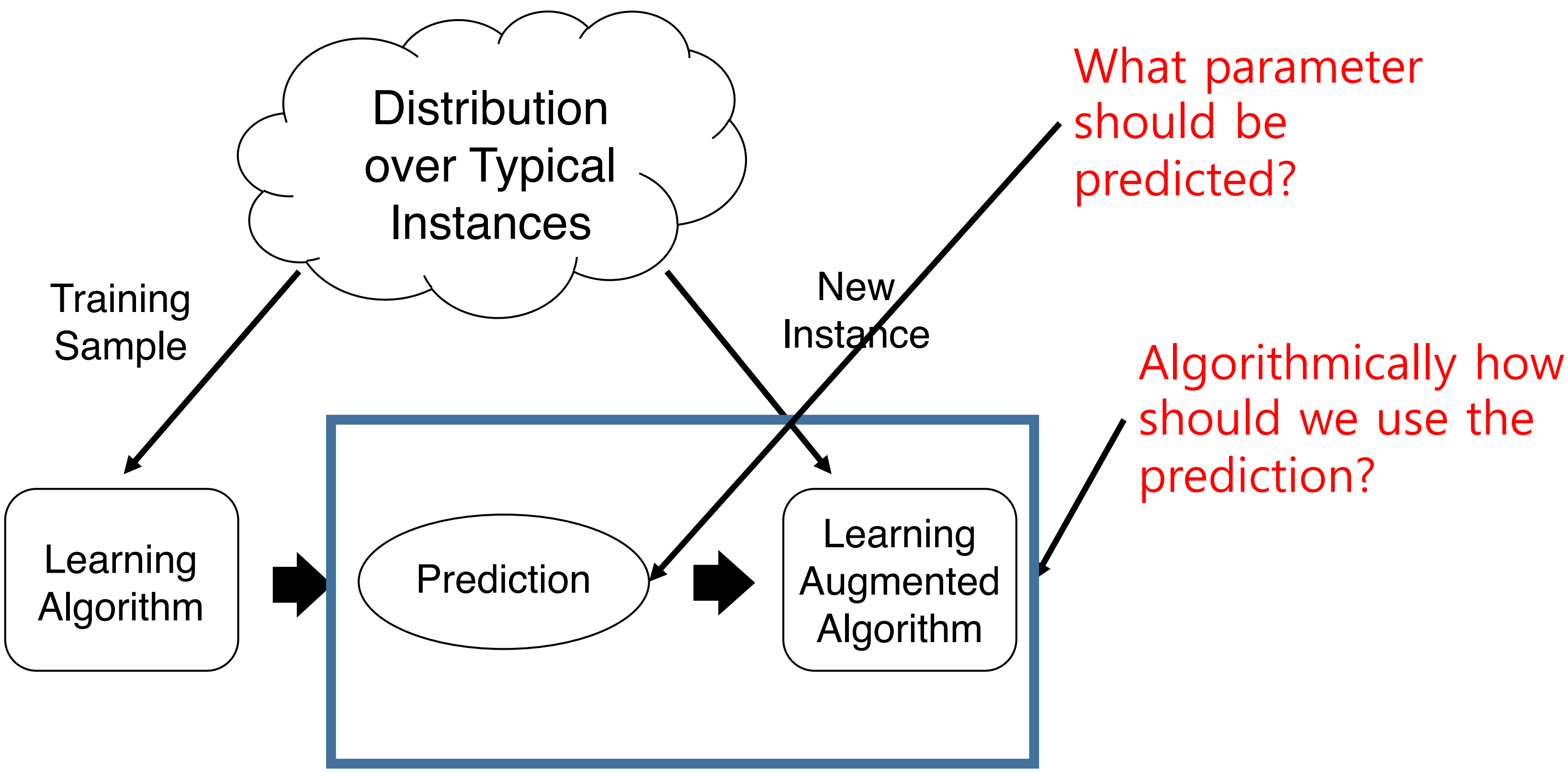
Learning Augmented Algorithms

- Punchline:
  - Machine learning can be combined with classical algorithms to obtain better results
  - Gives us new widely applicable models for beyond worst-case analysis

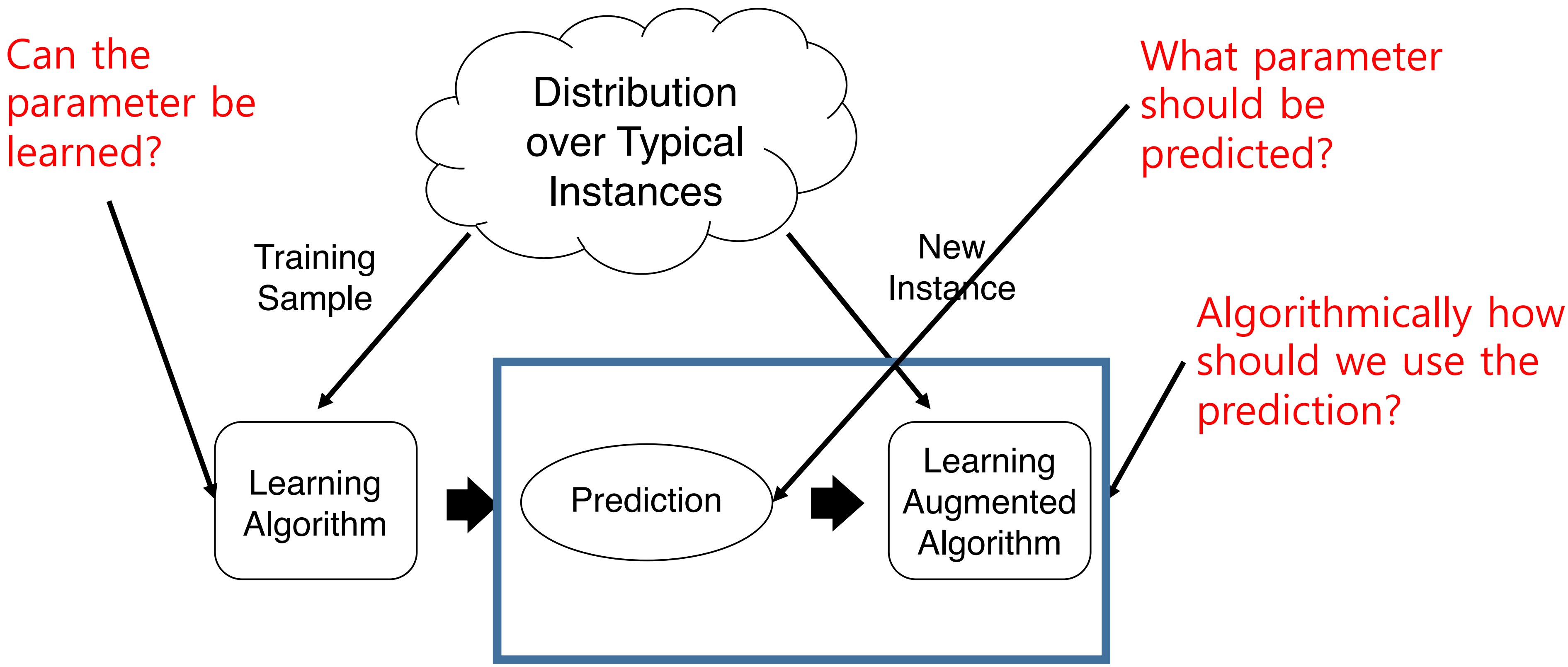
Learning Augmented Algorithms



Learning Augmented Algorithms



Learning Augmented Algorithms



Current Status

ERL: Desirable Analysis Framework

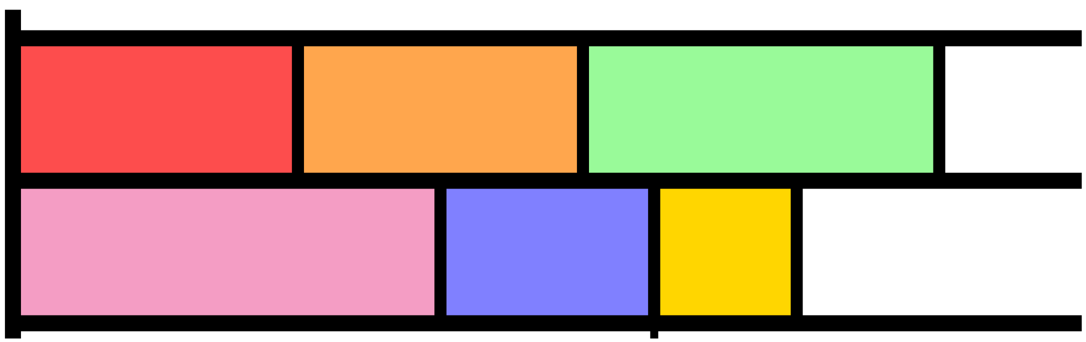
- **Existence:** Predictions should allow the algorithm to go beyond worst-case bounds
  - Good example: Location in the array
  - What to predict is often the main question
- **Robustness**: Algorithms are robust to minor changes in the problem input
  - Good example: Algorithm is robust to incorrect location in the array
  - Bad example: yes/no if an item is in the array
- **Learnability**: Predictions should be learnable if data is coming from a distribution
  - Example: PAC-Learning

Beyond Worst-Case Analysis Frameworks

- Online algorithm design
  - Competitive ratio parameterized by error in the predictions
- Running time
  - Worst case run time parameterized by error in the predictions

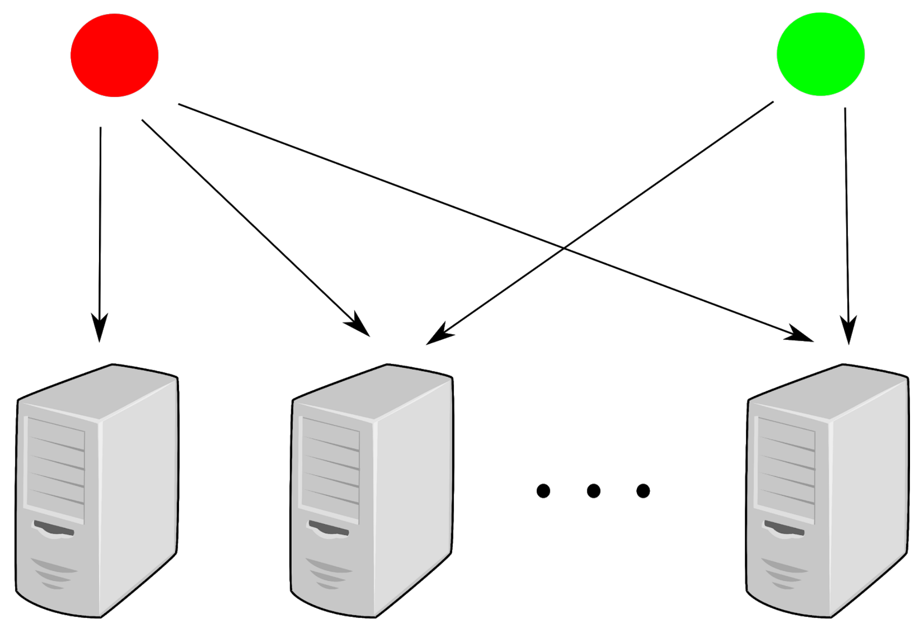
Online Restricted Assignment Makespan Minimization

- Client Server Scheduling
  - Processed in m machines in the **restricted assignment** setting (some results hold for **unrelated machines**)
  - Jobs arrive over time in the **online-list** model
    - **All arrive at time 0**
    - **Jobs revealed one at a time**
  - Assign jobs to the machines to minimize **makespan**



Restricted Assignment Makespan Minimization

- m machines
- n jobs
  - Online list: a job must be immediately assigned before the next job arrives
  - N(j): feasible machines for job j
  - p(j): size of job j (complexity essentially the same if ***unit sized***)
- Minimize the maximum makespan
  - Optimal makespan is T



Online Competitive Analysis Model

- c-competitive $$\frac{ALG(I)}{OPT(I)} \leq c$$
- Worst case relative performance on each input I
- Problem well understood:
  - A $\Omega(\log m)$ lower bound on any online algorithm
  - Greedy is a $O(\log m)$ competitive algorithm [Azar, Naor, and Rom 1995]

Beyond Worst Case via Predictions

- Reasonable assumption:
  - Access to last week's job sequence
  - What should be predicted?
  - How can it be used?

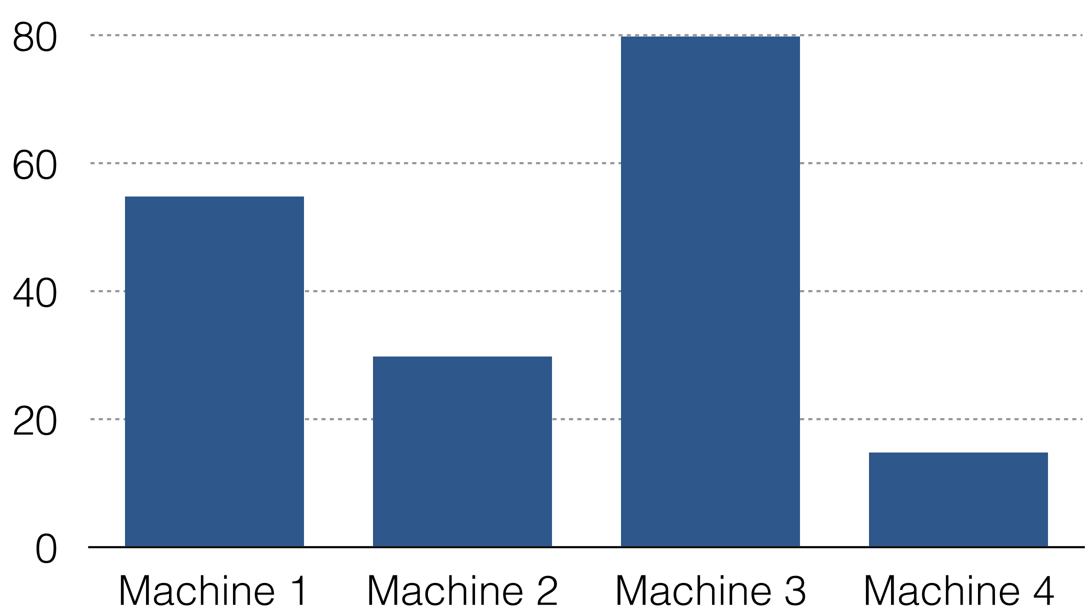
Existence

- First show natural predictions that fail
- Next give a good parameter to predict

What (not) to Predict?

- **Number of jobs assigned to machines** in the optimal solution?
  - Perhaps we can identify the contentious machines?

optimal solution

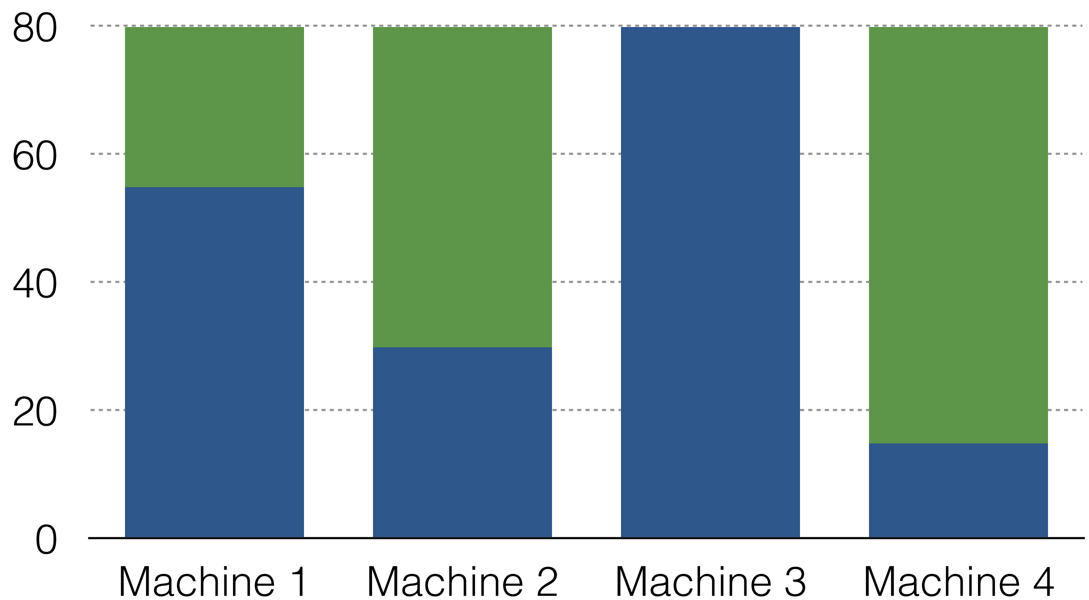


makespan 80

What (not) to Predict?

- **Load** of the machines in the optimal solution?
  - Perhaps we can identify the contentious machines? **No**

optimal solution



new instance padded with dummy jobs

loads the **same**

What (not) to Predict?

- Predict **dual variables**
- Known to be useful for **matching** in the **random order model** [Devanur and Hayes, Vee et al.]
  - Read a portion of the input
  - Compute the duals
  - Prove a primal assignment can be (approximately) constructed from the duals online
  - Use duals to make assignments on remaining input

What (not) to Predict?

- Predict **dual variables** for makespan scheduling
  - Can derive primal based on dual
  - Sensitive to small error (e.g. changing a variable by a factor of $1+1/\mathrm{poly}(n)$ has the potential to drastically change the schedule)

What to Predict?

- Idea: capture **contentiousness** of a machine
  - Seems like the most important quantity besides types of jobs

Prediction: Machine Weights

- Predict a weight for each machine
  - **Single** number (compact)
  - Lower weight means more restrictive machine
  - Higher weight less restrictive
- Framework:
  - Predict machine **weights**
  - Using to construct **fractional** assignments online
  - **Round** to an **integral** solution online

Fractional Assignments via Weights

- Each machine i has a weight w_i

- Job j is assigned to machine i **fractionally** as follows:

$$x_{i,j} = \frac{w_i}{\sum_{i' \in N(j)} w_{i'}}$$

Existence

- **Theorem (existence of weights)**: Let T be optimal max load. For any $\varepsilon > 0$, there **exists** machine weights such that the resulting fractional max load is at most $(1+\varepsilon)T$.

- **Theorem (rounding assignments) [Li, Xian ICML 2021]**: There exists an online algorithm that takes as input fractional assignments and outputs integer assignments for which the maximum load is bounded by $O((\log\log(m))T')$, where T' is maximum fractional load of the input. The algorithm is randomized and succeeds with probability at least $1 - 1 / m^c$

- **Theorem (tightness of rounding)**: Any randomized online rounding algorithm has worst case load at least $\Omega(T' \log \log m)$

- **Large makespan case:** [fractional makespan larger than $\log(m)$]

    - Randomized rounding gives gives a $(1+\varepsilon)T'$ where T' is maximum fractional load of the input with probability at least $1 - 1 / m^c$.

Results on Robustness

- **Theorem:** Given predictions of the machine weights with **maximum relative error** $\eta > 1$, there exists an online algorithm yielding fractional assignments for which the fractional max load is bounded by $O(T \min\{\log(\eta), \log(m)\})$.

- **Corollary**: There exists an $O(\min\{(\log\log(m))\log(\eta), \log m\})$ competitive algorithm for restricted assignment in the online algorithms with learning setting

Learnability

- Unknown distribution model $\mathscr{D}$
  - Instance drawn from unknown distribution
  - Best prediction $y^* := \texttt{argmax}_y \mathbb{E}_{\mathcal{I} \sim \mathcal{D}}[ALG(\mathcal{I}, y)]$
- How many samples s to compute $\hat{y}$ giving the following performance with high probability

$$\mathbb{E}_{\mathcal{I} \sim \mathcal{D}}[ALG(\mathcal{I}, \hat{y})] \geq (1 - \epsilon)\mathbb{E}_{\mathcal{I} \sim \mathcal{D}}[ALG(\mathcal{I}, y^*)]$$

Learnability

- Similar to
  - PAC learning
  - Data-driven algorithm design
- Alternative: competitive analysis
  - Show a small number of samples needed for the following performance with good probability

$$\mathbb{E}_{\mathcal{I}\sim\mathcal{D}}[ALG(\mathcal{I},\hat{y})] \geq (1-\epsilon)\mathbb{E}_{\mathcal{I}\sim\mathcal{D}}[OPT(\mathcal{I})]$$

Learnability

- **Theorem:** Let $\mathscr{D}$ be a product distribution such that $\mathbf{E}_{S\sim\mathscr{D}}[OPT(S)] \geq \Omega(\log m)$. There exists an algorithm that constructs **nearly optimal** weights using a polynomial number of samples in m.

Summary for Restricted Assignment

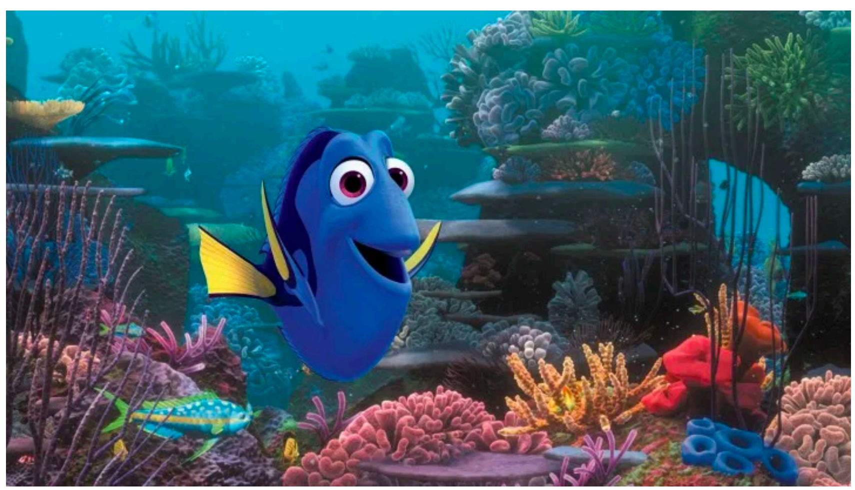
- Existence
  - Weights
- Robustness
  - Near optimal with perfect predictions
  - Bounded by the best worst case performance
- Learnability
  - Low sample complexity

Predictions for Online Algorithms

- Lots of success for online algorithm design
  - Matching
  - Caching
  - Ski-rental
  - Scheduling
  - Online learning
  - Heavy hitters
- **What about the original question of speeding up algorithms offline?**

Warm-Start

- Many problems are solved repeatedly on ‘similar’ instances
  - e.g. scheduling yesterday versus today
- We solve from scratch



Pitfalls

- Robustness
  - Feasibility: The warm start may not be feasible
  - Optimization: The warm start may not be useful
- Learnability: The starting solution may not be learnable

Weighted Bipartite Matching

- Input a bipartite graph $G = (L \cup R, E)$ with edge costs $c_{i,j}$
- Output the minimum cost perfect matching

Existence
What to Predict?

- Idea 1: Edges in optimal solution
  - Brittle
- Idea 2: LP duality

Existence

Primal

$$\min \sum_{e \in E} c_e x_E$$

$$\text{subject to: } \sum_{e \in N(i)} x_e = 1 \qquad \forall i \in V$$

$$x_e \geq 0 \qquad \forall e \in E$$

Dual

$$\max \sum_{i \in V} y_i$$

$$\text{subject to: } y_i + y_j \leq c_{ij} \qquad \forall (i,j) \in E$$

- Dual:
  - Assigns prices to vertices
- Complementary slackness
  - Edges in the matching have tight dual constraints

Existence

Primal

$$\min \sum_{e \in E} c_e x_E$$

$$\text{subject to: } \sum_{e \in N(i)} x_e = 1 \qquad \forall i \in V$$

$$x_e \geq 0 \qquad \forall e \in E$$

Dual

$$\max \sum_{i \in V} y_i$$

$$\text{subject to: } y_i + y_j \leq c_{ij} \qquad \forall (i,j) \in E$$

- Hungarian algorithm (popular in practice)
    - Start with dual values at 0
    - Compute max cardinality matching on tight edges
    - If not done, find a set violating Hall's theorem. Update duals

Existence

Primal

$$\min \sum_{e \in E} c_e x_E$$

$$\text{subject to: } \sum_{e \in N(i)} x_e = 1 \qquad \forall i \in V$$

$$x_e \geq 0 \qquad \forall e \in E$$

Dual

$$\max \sum_{i \in V} y_i$$

$$\text{subject to: } y_i + y_j \leq c_{ij} \qquad \forall (i,j) \in E$$

- Hungarian algorithm (popular in practice)
  - Predict dual values
  - Compute max cardinality matching on tight edges
  - If not done, find a set violating Hall's theorem. Update duals

Robustness
Main Idea

Idea:

- Predict the dual values, i.e. predict $\hat{y}_i$
- "Warm start" Hungarian algorithm from predicted duals.

Feasibility issue:

- Hungarian algorithm slowly increases duals. Always has a feasible solution
- But, predicted dual may be infeasible
- Have an edge s.t.: $\hat{y}_i + \hat{y}_j > c_{ij}$

Approach:

- Minimally reduce predicted duals to attain feasibility
- Must do it quickly (since speed is of the essence)

Robustness
Making Duals Feasible

- Write LP for the feasibility problem:

$$\begin{aligned} &\min \sum_{i \in V} \delta_i \\ \text{subject to: } &\delta_i + \delta_j \geq (\hat{y}_i + \hat{y}_j - c_{ij})^+ \qquad \forall (i,j) \in E \\ &\delta_i \geq 0 \qquad \forall i \in V \end{aligned}$$

Algorithm (greedy):

- Pick any vertex i. Set its δ_i value to the minimum that satisfies all of the constraints
- Remove i from the graph and repeat.
- Theorem: Resulting solution is a 2-approximation for the LP, runs in linear time!

Robustness

Overall approach:

- Obtain (learn) duals: $\hat{y}_1, \ldots, \hat{y}_n$
- Given a new matching instance, $G = (V, E)$ find feasible duals $y'_1, \ldots, y'_n$
- Run Hungarian method starting with $y'_1, \ldots, y'_n$

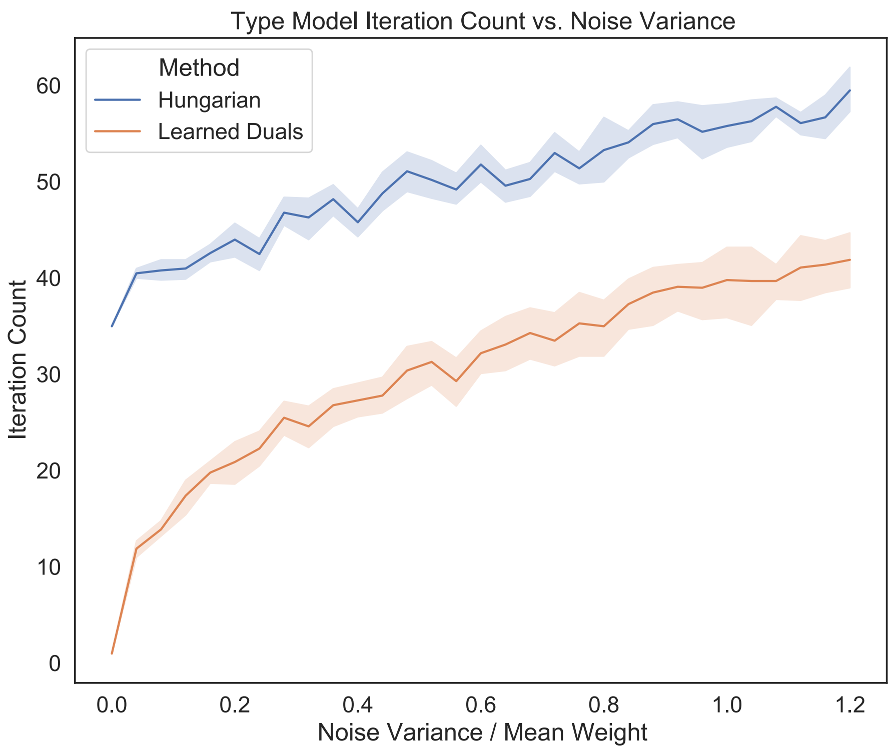
Theorem: The overall running time is: $O(\|\hat{y} - y^*\|_1) \cdot m\sqrt{n}$

- Strictly better when the error is small
- Can prove that it's no worse than vanilla Hungarian algorithm

Does it Work?

Experiment 1(a):

- Start with a bipartite graph with a planted min cost perfect matching
- Generate new instances by adding random noise of increasing magnitude to the edge weights

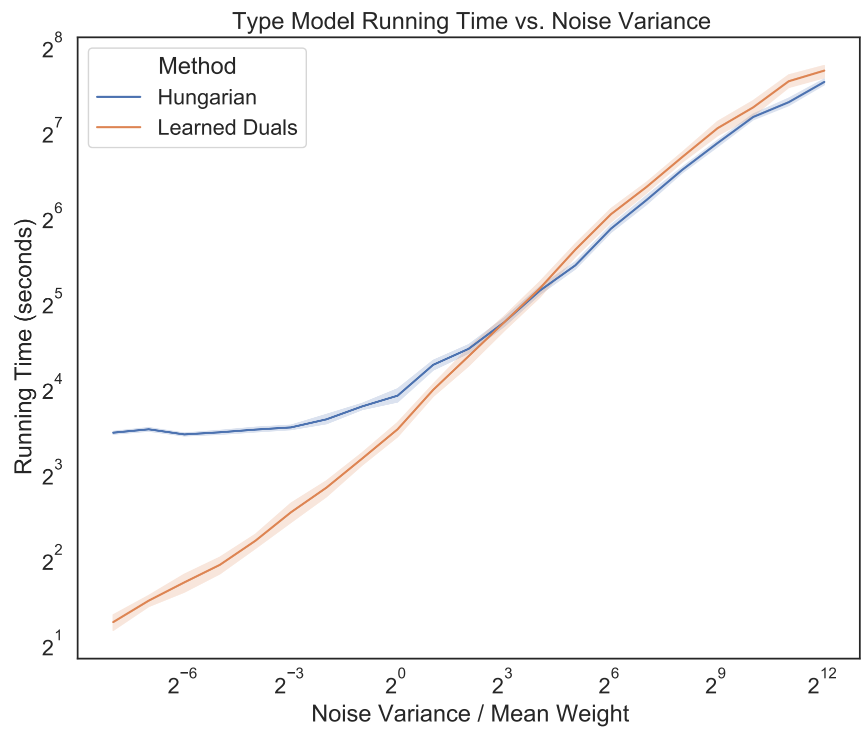


- When noise is low, learning approach dominates.

Does it Work?

Experiment 1(b):

- Start with a bipartite graph with a planted min cost perfect matching
- Generate new instances by adding random noise of increasing magnitude to the edge weights

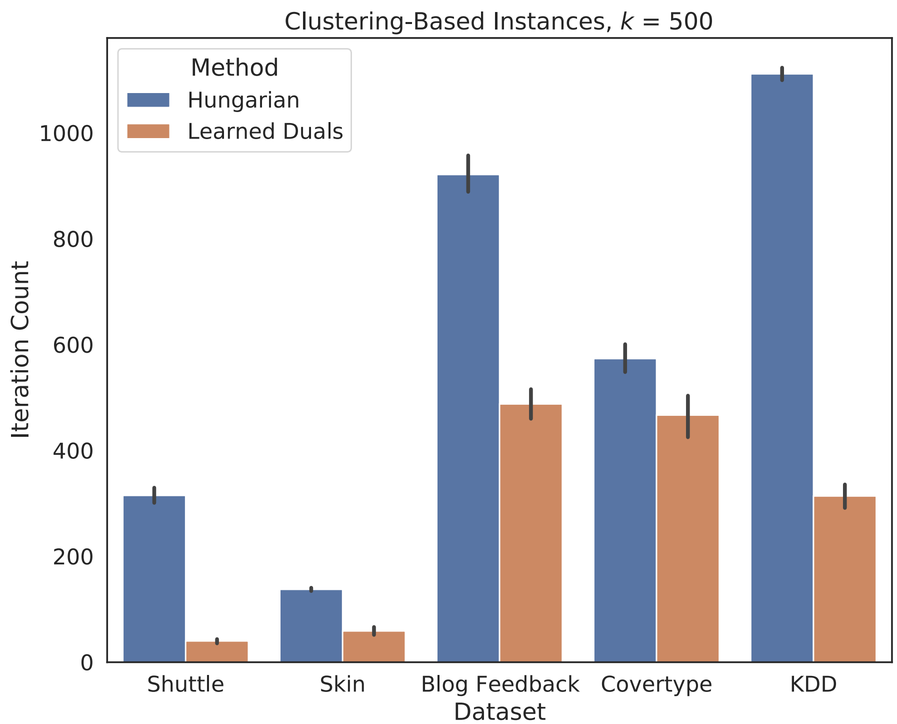


- When noise gets high, nothing to be learned, so converge to Hungarian method.

Does it Work?

Experiment 2:

- Perfect matching problems derived from geometric datasets

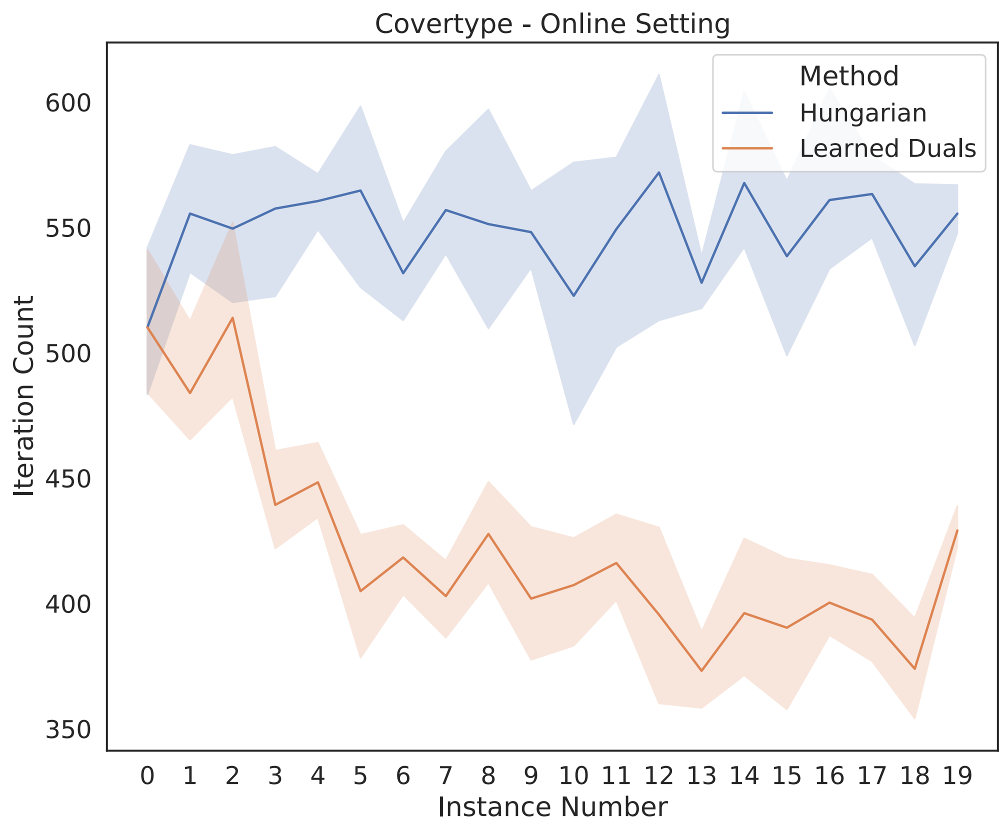


- Learned gains can be substantial (10x in some cases)

Does it Work?

Experiment 3:

- How many samples do you need to learn?



- Many fewer than the theory predicts

Future Work

- Learnability
  - Are unlearnable predictions more useful than learnable predictions
- How useful is this new paradigm empirically and theoretically
  - **Rich area: Online algorithms to cope with uncertainty, running time off-line, other applications?**

https://algorithms-with-predictions.github.io/

Thank you!

Questions?