AutoML: Beyond AutoML

Overview: Algorithm Configuration

Bernd Bischl   Frank Hutter   Lars Kotthoff
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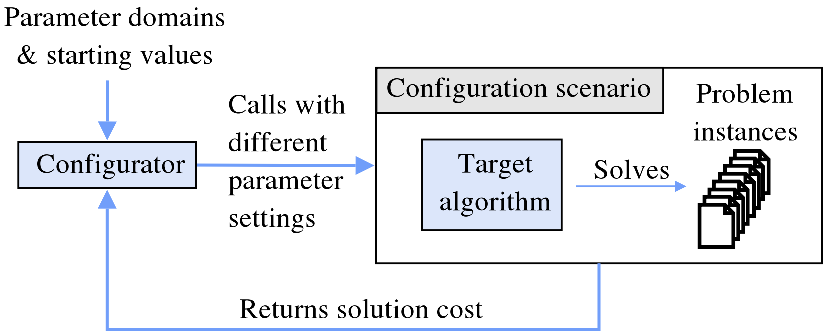
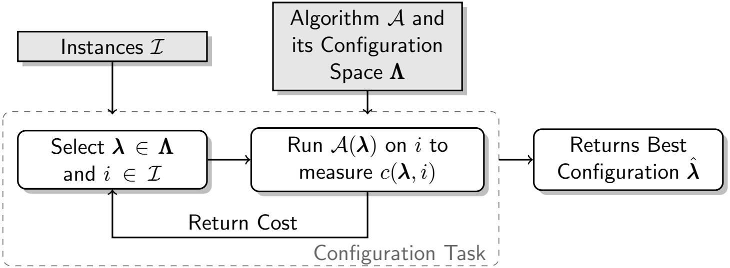
$\rightsquigarrow$ Algorithm configuration

Algorithm Configuration Visualized



Algorithm Configuration – in More Detail



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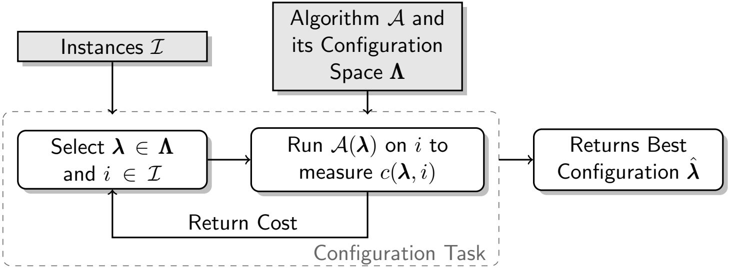

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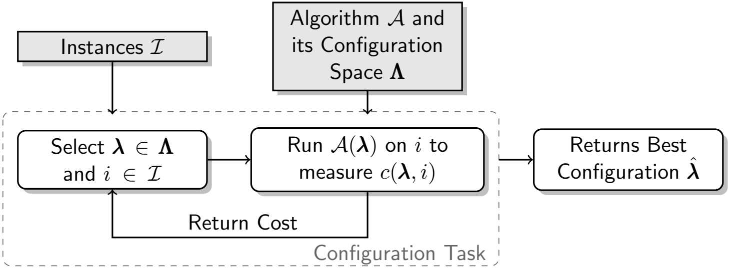

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Given a parameterized algorithm $\mathcal{A}$ with possible (hyper-)parameter settings $\boldsymbol{\Lambda}$, a set of training problem instances $\mathcal{I}$, and a cost metric $c : \boldsymbol{\Lambda} \times \mathcal{I} \rightarrow \mathbb{R}$,

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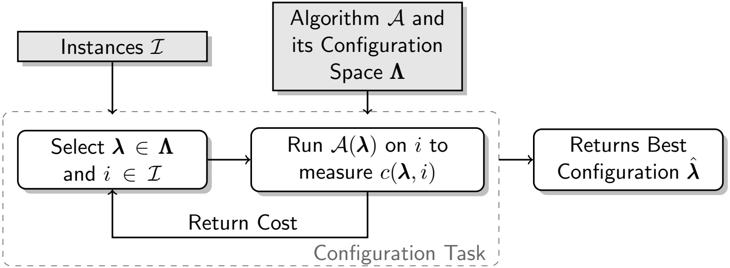

Definition

Given a parameterized algorithm $\mathcal{A}$ with possible (hyper-)parameter settings $\boldsymbol{\Lambda}$, a set of training problem instances $\mathcal{I}$, and a cost metric $c : \boldsymbol{\Lambda} \times \mathcal{I} \to \mathbb{R}$, the algorithm configuration problem is to find a parameter configuration $\boldsymbol{\lambda}^* \in \boldsymbol{\Lambda}$ that minimizes c across the instances in $\mathcal{I}$.

Algorithm Configuration – Full Formal Definition

Definition

An instance of the algorithm configuration problem is a 5-tuple $(\mathcal{A}, \mathbf{\Lambda}, \mathcal{D}, \kappa, c)$ where:

- $\mathcal{A}$ is a parameterized algorithm;
- $\mathbf{\Lambda}$ is the (hyper-)parameter configuration space of $\mathcal{A}$;
- $\mathcal{D}$ is a distribution over problem instances with domain $\mathcal{I}$;

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The cost of a candidate solution $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ is $f(\boldsymbol{\lambda}) = \mathbb{E}_{i \sim \mathcal{D}}(c(\boldsymbol{\lambda}, i))$.
The goal is to find $\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} f(\boldsymbol{\lambda})$.

Distribution of Instances

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Like in machine learning

- We split the instances into a training set and a test set
- We configure algorithms on the training instances
- We only use the test instances afterwards

  $\rightarrow$ unbiased estimate of generalization performance for unseen instances

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  $\leadsto$ combination of algorithm configuration and selection

$\leadsto$ Hyperparameter optimization is a subproblem of algorithm configuration

[Eggensperger et al. 2019]

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Racing for Algorithm Configuration

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State-of-the-art Algorithm Configuration

SMAC: Sequential Model-based Algorithm Configuration [Hutter et al. 2011]

- Bayesian Optimization +
- aggressive racing +
- adaptive capping (for optimizing runtime)

SMAC: Overview [Hutter et al. 2011]

Algorithm 1 SMAC

Input : instance set $\mathcal{I}$, Algorithm $\mathcal{A}$ with configuration space $\mathbf{\Lambda}$, Initial configuration $\boldsymbol{\lambda}_0$, performance metric c, Configuration budget b

run history $\mathcal{D}_{\text{Hist}} \leftarrow$ initial design based on $\boldsymbol{\lambda}_0$; // $\mathcal{D}_{\texttt{Hist}} = (\boldsymbol{\lambda}, i, c(i, \boldsymbol{\lambda}))_i$

while b *remains* **do**

SMAC: Overview [Hutter et al. 2011]

Algorithm 2 SMAC

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- $\mathbf{\Lambda}_{challengers} \leftarrow$ select configurations based on $\hat{c}$;
- $\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\text{Hist}} \leftarrow$ intensify($\mathbf{\Lambda}_{challengers}$, $\hat{\boldsymbol{\lambda}}$); // `racing and capping`

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return $\hat{\boldsymbol{\lambda}}$

Comparisons on N instances [Hutter et al. 2009]

- Basic(N) uses a pretty basic comparison: *better*$_N(\boldsymbol{\lambda}', \boldsymbol{\lambda})$:
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  - Problem of large N: evaluations are slow
  - Problem of small N: overfitting to a small set of instances

  $\leadsto$ Tradeoff: Choose N of moderate size

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If we sampled different instances for each configuration:

- Some configurations would randomly get easier instances
- Those configurations would look better than they really are

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(Different Basic(N) runs can use different instances and seeds.)

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More pronounced for heterogeneous benchmark sets

- But it even happens for very homogeneous sets
- Indeed, one can even overfit on a single instance, to the seeds used for training

Overtuning Visualized

- Example: minimizing SLS solver runlengths for a single SAT instance
- Training cost, e.g., with N=100:
  average runlengths across 100 runs with different seeds
- Test cost of $\hat{\boldsymbol{\lambda}}$ here based on 1000 new seeds

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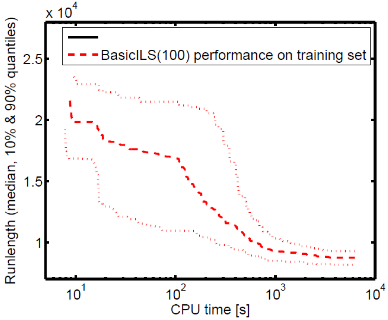

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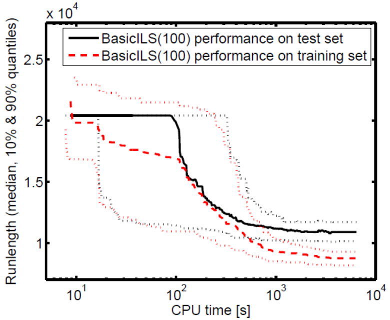

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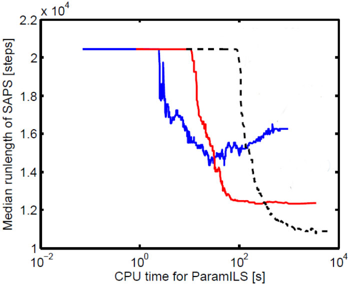

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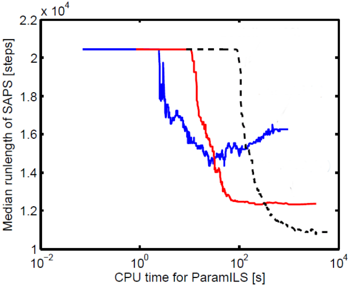

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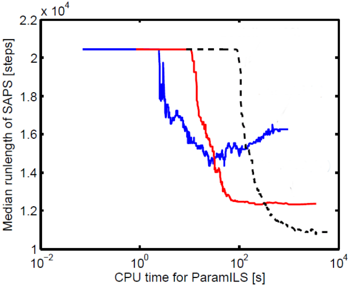

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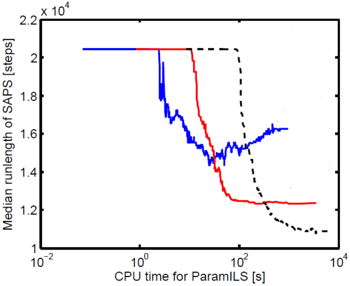

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Correct Answer: 1

Aggressive Racing (inspired by FocusedILS) [Hutter et al. 2009]

Intuition: get the best of both worlds

- Perform more runs for good configurations
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In the beginning: $N(\boldsymbol{\lambda}) = 0$ for every configuration $\boldsymbol{\lambda}$

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$\boldsymbol{\lambda}^{(1)}$ dominates $\boldsymbol{\lambda}^{(2)}$ if

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- Over time: perform extra runs of $\hat{\boldsymbol{\lambda}}$ to gain more confidence in it

Toy Example

- Let $\hat{\boldsymbol{\lambda}}$ be the incumbent (evaluated on $i^{(1)}, i^{(2)}, i^{(3)}$)
- We'll look at challengers $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}''$

	$i^{(1)}$	$i^{(2)}$	$i^{(3)}$
$\hat{\boldsymbol{\lambda}}$	3	2	10

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	$i^{(1)}$	$i^{(2)}$	$i^{(3)}$
$\hat{\boldsymbol{\lambda}}$	3	2	10
$\boldsymbol{\lambda}'$			

Toy Example

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$\boldsymbol{\lambda}'$	2	10	
	$\rightarrow$ reject, since $\hat{c}_2(\boldsymbol{\lambda}') = 6 > \hat{c}_2(\hat{\boldsymbol{\lambda}}) = 2.5$		

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$\boldsymbol{\lambda}''$	3		

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$\boldsymbol{\lambda}''$	3	1	

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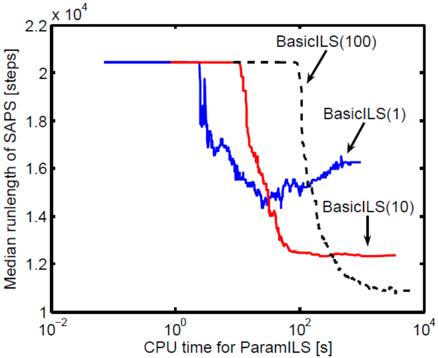
$\boldsymbol{\lambda}''$	3	1	5

- new incumbent: $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}''$
- Perform an additional run for new $\hat{\boldsymbol{\lambda}}$ to increase confidence over time

Racing achieves the best of both worlds

Aggressive racing (aka FocusedILS): Fast progress and no overtuning

Test performance



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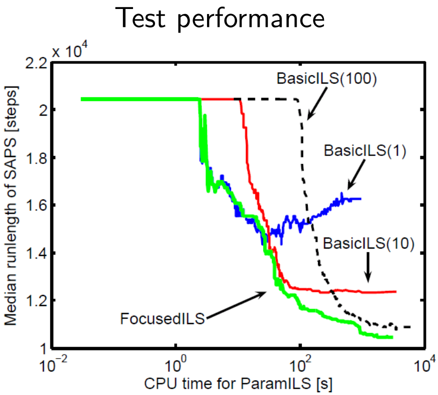

Overview of Racing

Input : candidate configurations $\boldsymbol{\Lambda}_{new}$, cutoff κ_{max}, previously evaluated runs $\mathcal{D}_{\mathsf{Hist}}$, budget T, incumbent $\hat{\boldsymbol{\lambda}}$

while $\boldsymbol{\Lambda}_{new}$ *not empty* **do**

  $\boldsymbol{\lambda}^{(t)} \leftarrow$ getNext($\boldsymbol{\Lambda}_{new}$);

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  $i, s \leftarrow$ instance and seed drawn uniformly at random;

  $c \leftarrow$ EvaluateRun($\hat{\boldsymbol{\lambda}}, i, s, \kappa_{max}$);

  $\mathcal{D}_{\text{Hist}} \leftarrow \mathcal{D}_{\text{Hist}} \cup (\hat{\boldsymbol{\lambda}}, i, s, c)$;

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if *average cost of* $\boldsymbol{\lambda}^{(t)} >$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *across* $\mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)}$ **then**

break;

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    - break;
  - **else if** *average cost of* $\boldsymbol{\lambda}^{(t)} <$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *and* $\mathcal{I}^{+} = \mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)} = \mathbf{s}^{+}$ **then**
    - $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}^{(t)}$;
- **if** *time spent exceeds* T *or* $\mathbf{\Lambda}_{new}$ *is empty* **then**
  - **return** $\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\mathit{Hist}}$

AutoML: Beyond AutoML

Capping of Runtimes

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Adaptive capping [Hutter et al. 2009]

- Assumptions
  - optimization of runtime
  - each configuration run has a time limit (e.g., 300 sec)

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- E.g., $\hat{\boldsymbol{\lambda}}$ needed 1 sec to solve i_1
  - Do we need to run $\boldsymbol{\lambda}'$ for 300 sec?
  - Terminate evaluation of $\boldsymbol{\lambda}'$ once guaranteed to be worse than $\hat{\boldsymbol{\lambda}}$

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$\rightsquigarrow$ To compare against $\hat{\boldsymbol{\lambda}}$ based on N runs,
we can terminate evaluation of $\boldsymbol{\lambda}'$ after time $\sum_{k=1}^{N} c(\hat{\boldsymbol{\lambda}}, i_k)$

Toy-Example: Adaptive capping

runtime cutoff $\kappa = 300$, comparison based on 2 instances

	i_1	i_2
$\hat{\boldsymbol{\lambda}}$	4	2

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runtime cutoff $\kappa = 300$, comparison based on 2 instances

	i_1	i_2
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Without adaptive capping		
$\boldsymbol{\lambda}'$	3	

Toy-Example: Adaptive capping

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$\rightarrow$ reject $\boldsymbol{\lambda}'$ (cost: 303)

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With adaptive capping		
$\boldsymbol{\lambda}'$	3	300
	$\rightarrow$ cut off after $\kappa = 4$ seconds, reject $\boldsymbol{\lambda}'$ (cost: 7)	

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$\hat{\boldsymbol{\lambda}}$	4	2
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$\boldsymbol{\lambda}'$	3	300
		$\rightarrow$ reject $\boldsymbol{\lambda}'$ (cost: 303)
With adaptive capping		
$\boldsymbol{\lambda}'$	3	300
	$\rightarrow$ cut off after $\kappa = 4$ seconds, reject $\boldsymbol{\lambda}'$ (cost: 7)	

Note: To combine adaptive capping with BO, we need to impute the censored observations caused by adaptive capping. [Hutter et al. 2011]

Overview of Racing and Adaptive Capping

Input : candidate configurations $\mathbf{\Lambda}_{new}$, cutoff κ_{max}, previously evaluated runs $\mathcal{D}_{\text{Hist}}$, budget T, incumbent $\hat{\boldsymbol{\lambda}}$

while $\mathbf{\Lambda}_{new}$ *not empty* **do**

  $\boldsymbol{\lambda}^{(t)} \leftarrow$ getNext($\mathbf{\Lambda}_{new}$);

  [... add new run for incumbent ...];

  while *true* **do**

    $\mathcal{I}^+, \mathbf{s}^+ \leftarrow$getAlreadyEvaluatedOn($\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\text{Hist}}$);

    $\mathcal{I}^{(t)}, \mathbf{s}^{(t)} \leftarrow$getAlreadyEvaluatedOn($\boldsymbol{\lambda}^{(t)}, \mathcal{D}_{\text{Hist}}$);

    $i^{(t)}, s^{(t)} \leftarrow$ drawn uniformly at random from $\mathcal{I}_+ \setminus \mathcal{I}^{(t)}$ and $\mathbf{s}^+ \setminus \mathbf{s}^{(\mathbf{t})}$;

    $\kappa^{(i)} \leftarrow$ AdaptCutoff($\kappa_{max}, \langle(\boldsymbol{\lambda}^{(j)}, c^{(j)})\rangle_{\boldsymbol{\lambda}^{(j)}=\boldsymbol{\lambda}^+}$) $\cdot\, \xi$;

    $c_i \leftarrow$ EvaluateRun($\boldsymbol{\lambda}^{(t)}, i^{(t)}, s^{(i)}, \kappa^{(i)}$);

    $\mathcal{D}_{\text{Hist}} \leftarrow \mathcal{D}_{\text{Hist}} \cup (\boldsymbol{\lambda}^{(t)}, i^{(t)}, s^{(t)}, c^{(t)})$;

    if *average cost of* $\boldsymbol{\lambda}^{(t)} >$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *across* $\mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)}$ **then**

      break;

    else if *average cost of* $\boldsymbol{\lambda}^{(t)} <$ *average cost of* $\hat{\boldsymbol{\lambda}}$ *and* $\mathcal{I}^+ = \mathcal{I}^{(t)}$ *and* $\mathbf{s}^{(t)} = \mathbf{s}^+$ **then**

      $\hat{\boldsymbol{\lambda}} \leftarrow \boldsymbol{\lambda}^{(t)}$;

  if *time spent exceeds* T *or* $\mathbf{\Lambda}_{new}$ *is empty* **then**

    return $\hat{\boldsymbol{\lambda}}, \mathcal{D}_{\mathit{Hist}}$

AutoML: Beyond AutoML

Structured Procastination

Bernd Bischl Frank Hutter Lars Kotthoff
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Structured Procrastination [Kleinberg et al. 2017]

Idea

- incumbent driven methods (such as aggressive racing with adaptive capping) provide no theoretical guarantees about runtime

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- task: for a fix set of configuration, identify the one with the best average runtime
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- incumbent driven methods (such as aggressive racing with adaptive capping) provide no theoretical guarantees about runtime
- task: for a fix set of configuration, identify the one with the best average runtime
- instead of top-down capping, use bottom up capping
- start with a minimal cap-time and increase it step by step

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Idea

- incumbent driven methods (such as aggressive racing with adaptive capping) provide no theoretical guarantees about runtime
- task: for a fix set of configuration, identify the one with the best average runtime
- instead of top-down capping, use bottom up capping
- start with a minimal cap-time and increase it step by step
- unsuccessful runs (with too small cap-time) are procrastinated to later

$\leadsto$ worst-case runtime guarantees

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 1 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$

Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`

initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 2 Structured Procrastination

Input : finite (small) set of configurations $\boldsymbol{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
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for each $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 3 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
    determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 4 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
    determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;
    get first element $(i^{(k)}, \kappa)$ from $Q_{\hat{\boldsymbol{\lambda}}}$;

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 5 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
  determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;
  get first element $(i^{(k)}, \kappa)$ from $Q_{\hat{\boldsymbol{\lambda}}}$;
  Run $\hat{\boldsymbol{\lambda}}$ on $i^{(k)}$ capped at κ;
  if *terminates* **then**
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)}) :=$ t;

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 6 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \ldots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
  determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;
  get first element $(i^{(k)}, \kappa)$ from $Q_{\hat{\boldsymbol{\lambda}}}$;
  Run $\hat{\boldsymbol{\lambda}}$ on $i^{(k)}$ capped at κ;
  if *terminates* **then**
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)}) :=$ t;
  else
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)}) := \kappa$;
    Insert $(i^{(k)}, 2 \cdot \kappa)$ at the end of $Q_{\hat{\boldsymbol{\lambda}}}$;

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 7 Structured Procrastination

Input : finite (small) set of configurations $\boldsymbol{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

```
for each λ ∈ Λ initialize a queue Q_λ with entries (i^(k), κ_0);      // small queue in the beginning
initialize a look-up table R(λ, i) = 0;                                // optimistic runtime estimate
while b remains do
    determine the best λ̂ according to R(λ, ·);
      get first element (i^(k), κ) from Q_λ̂;
      Run λ̂ on i^(k) capped at κ;
      if terminates then
        R(λ̂, i^(k)) := t;
    else
        R(λ̂, i^(k)) := κ;
          Insert (i^(k), 2 · κ) at the end of Q_λ̂;
    Replenish queue Q_λ̂ if too small;
```

Structured Procrastination: Outline [Kleinberg et al. 2017]

Algorithm 8 Structured Procrastination

Input : finite (small) set of configurations $\mathbf{\Lambda}$, minimal cap-time κ_0, sequence of instances $i^{(1)}, \dots, i^{(N)}$
Output : best incumbent configuration $\hat{\boldsymbol{\lambda}}$

for each $\boldsymbol{\lambda} \in \mathbf{\Lambda}$ initialize a queue $Q_{\boldsymbol{\lambda}}$ with entries $(i^{(k)}, \kappa_0)$; `// small queue in the beginning`
initialize a look-up table $R(\boldsymbol{\lambda}, i) = 0$; `// optimistic runtime estimate`
while b *remains* **do**
  determine the best $\hat{\boldsymbol{\lambda}}$ according to $R(\boldsymbol{\lambda}, \cdot)$;
  get first element $(i^{(k)}, \kappa)$ from $Q_{\hat{\boldsymbol{\lambda}}}$;
  Run $\hat{\boldsymbol{\lambda}}$ on $i^{(k)}$ capped at κ;
  if *terminates* **then**
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)})$:= t;
  else
    $R(\hat{\boldsymbol{\lambda}}, i^{(k)}) := \kappa$;
    Insert $(i^{(k)}, 2 \cdot \kappa)$ at the end of $Q_{\hat{\boldsymbol{\lambda}}}$;
  Replenish queue $Q_{\hat{\boldsymbol{\lambda}}}$ if too small;
return $\hat{\boldsymbol{\lambda}} := \arg\min_{\boldsymbol{\lambda} \in \mathbf{\Lambda}} \sum_{k=1}^{N} R(\boldsymbol{\lambda}, i^{(k)})$

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- Several extensions and similar ideas:
  - [Kleinberg et al. 2019]
  - [Weisz et al. 2018]
  - [Weisz et al. 2019]

AutoML: Beyond AutoML

Best Practices for Algorithm Configuration

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Pitfalls & Best Practices

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2. using algorithm configuration requires (at least some) expertise in algorithm configuration
3. if done wrong, waste of time and compute resources

Setting up AC

9 Steps to your well-performing algorithm:

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8. Run the configurator on your algorithm and the training instances
9. Validate the eventually returned configuration on your test instances

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We have encountered algorithms that

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Best Practice 1: Never trust your algorithm

Explicitly check and use external software to:

1. ensure resource limitations
2. terminate your algorithm
3. verify returned solutions
4. measure performance

Pitfall 2: File System

Algorithm configurators ...

- often produce quite some log files (e.g., for each algorithm run)
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Best Practice 2: Don't use the Shared File System

To relieve the file system of a HPC cluster:

- design well which files are required and which are not
- use a local (SSD) disc

Pitfall 3: Over-tuning

It's easy to overtune to different aspects, incl.:

- training instances
- random seeds
- machine type

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- training instances
- random seeds
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In practice, it can be hard to prevent over-tuning, e.g., by

- using larger instance sets
- tuning on the target hardware

Best Practice 3: Check for Over-Tuning

Check for over-tuning by validating your final configuration on

- many random seeds
- a large set of unused test instances
- a different hardware

Pitfall 4: Heterogeneous Instance Sets

Algorithm configurators...

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$\rightsquigarrow$ returned configurations often perform worse than default configurations
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Best Practice 4: Ensure Homogeneity

Algorithm configurators should only run on homogeneous instance sets.
Different degrees of homogeneity:

- Strong homogeneity: all instances agree on the ranking of configurations
- Weak homogeneity: all instances agree on the top-performing configurations

More Pitfalls and Best Practices

... can be found in [Eggensperger et al. 2019]

AutoML: Beyond AutoML

Per-Instance Algorithm Configuration

Bernd Bischl Frank Hutter Lars Kotthoff
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Homogeneous vs. Heterogeneous Instances

Assumption of AC: Homogeneous Instance Distribution

- Algorithm configuration tools assume that the instance distribution is homogeneous (see video on "Best Practices for AC")
- Important because
  - there is a well-performing configuration for all (or most) instances
  - the racing algorithm can make educated decisions on subsets

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$\rightsquigarrow$ What should we do with heterogeneous instance distributions?

Why are systems for heterogeneous instance distributions important?

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1. We cannot guarantee homogeneity in practice
   1. Instances might get larger and harder
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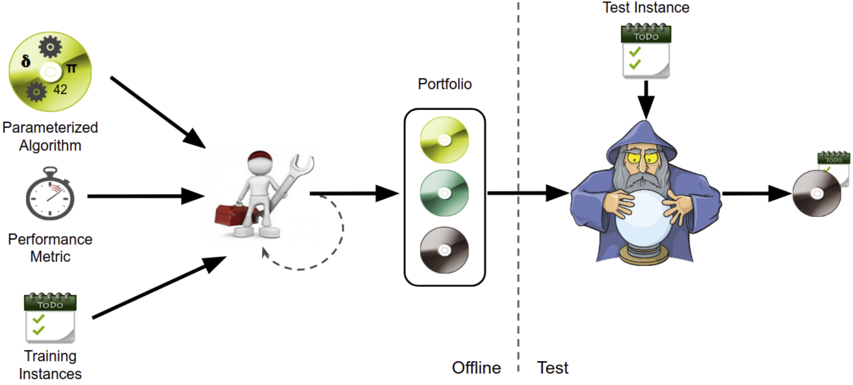
2. We don't want to do algorithm configuration always from scratch
3. An adaptive configuration system would be the holy grail
   - $\leadsto$ hard to achieve

PIAC: Per-Instance Algorithm Configuration



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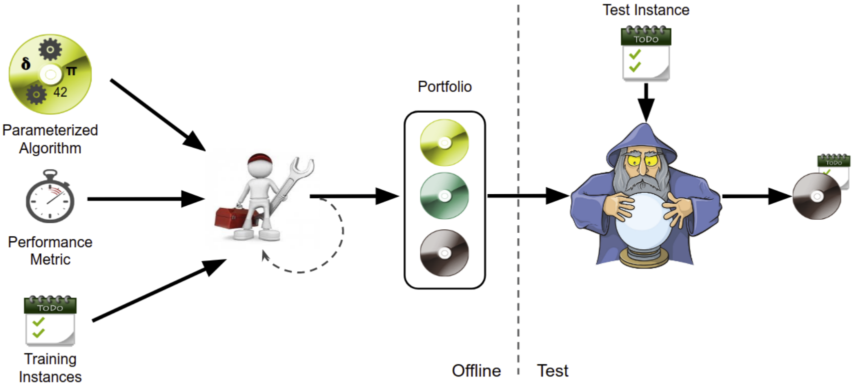

- You can use whichever kind of algorithm selection (wizard) you want
- Challenge: Building a portfolio
- Use case: Instances are heterogeneous

PIAC: Manual Expert Approach

Basic Assumption

Heterogeneous instance set can be divided into homogeneous subsets

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Manual Expert

- An expert knows the homogeneous subsets (e.g., origin of instances)
- Determine a well-performing configuration on each subset
  $\rightarrow$ portfolio of configurations
- Use Algorithm Selection to select a well-performing configuration on each instance

Instance-Specific Algorithm Configuration: ISAC [Kadioglu et al. 2010]

Idea

Training:

1. Cluster instances into homogeneous subsets
   (using g-means in the instance feature space)
2. Apply algorithm configuration (here GGA) on each instance set

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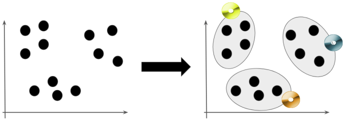
Test:

1. Determine the nearest cluster (k-NN with $k = 1$) in feature space
2. Apply optimized configuration of this cluster



Hydra [Xu et al. 2010]

Idea

- Iteratively add configurations to a portfolio $\mathbf{P}$, start with $\mathbf{P} = \emptyset$
- In each iteration, determine configuration that is complementary to $\mathbf{P}$
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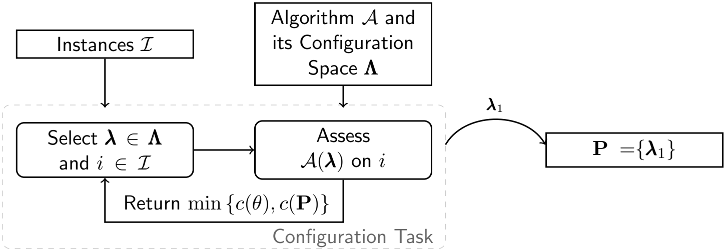

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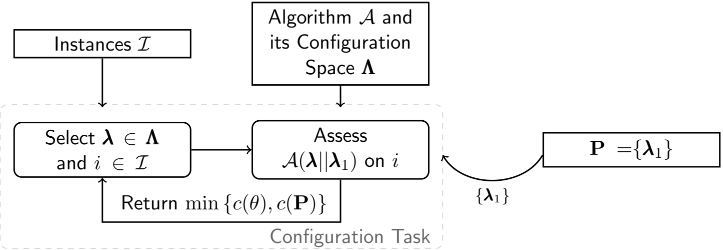

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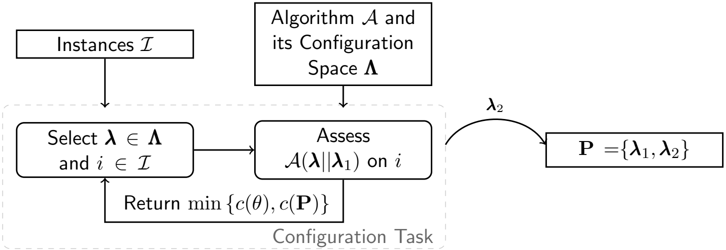

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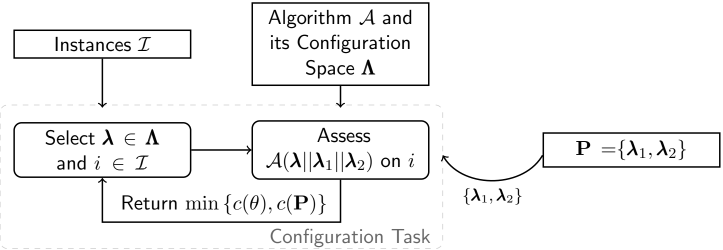
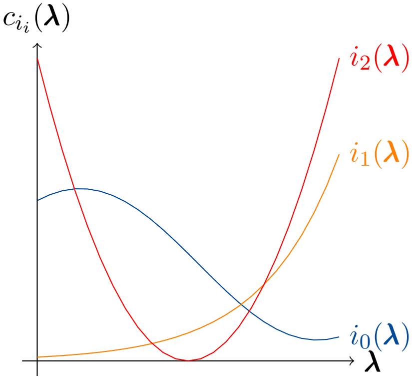


Heterogeneous example



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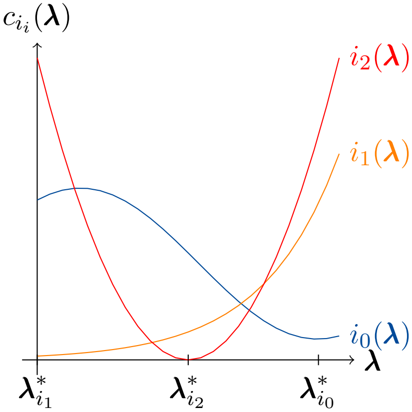

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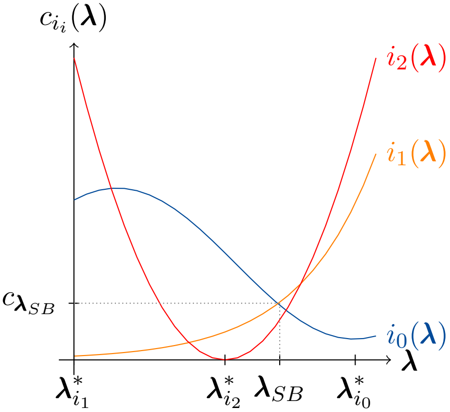

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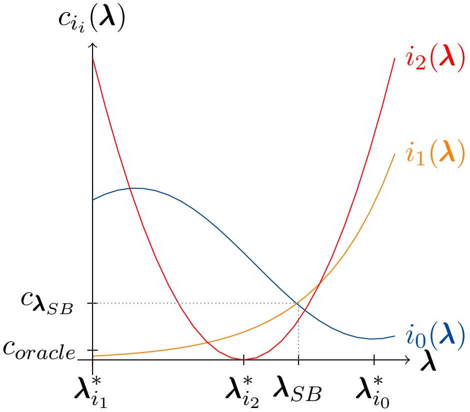
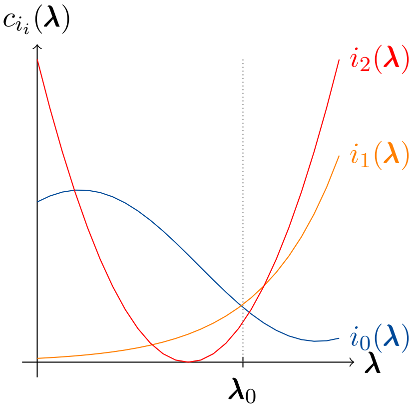


Hydra: Iteration 1



Search initial well performing configuration. Add $\boldsymbol{\lambda}_0$ to $\mathbf{P}$

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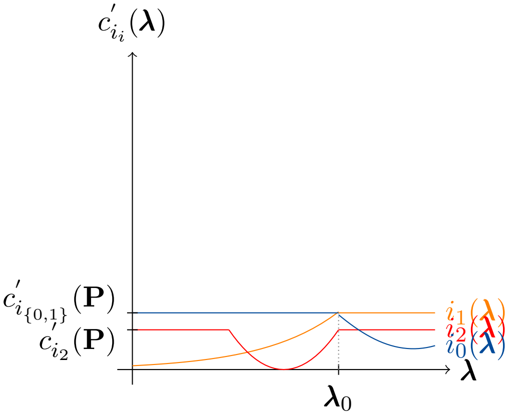
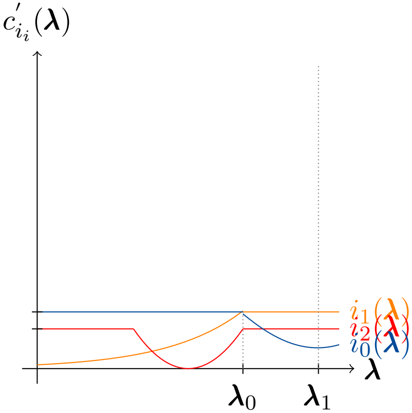


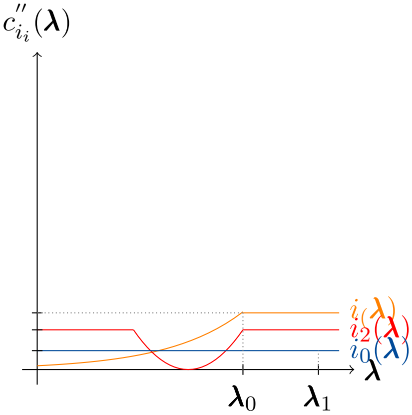
Update metric

Hydra: Iteration 2



Search well performing configuration complementary to $\mathbf{P}$.
Add $\boldsymbol{\lambda}_1$ to $\mathbf{P}$.

Hydra: Iteration 2



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- Iteratively add a configuration with a time slot t to a schedule $\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle$

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- The time slot is a further parameter in the configuration space
- Optimize marginal contribution per time spent:

$$\frac{c(\mathcal{S}) - c(\mathcal{S} \oplus \langle \boldsymbol{\lambda}, t \rangle)}{t}$$

Submodularity

Observation

- Performance metrics of Hydra and Cedalion are submodular
  - Family of functions
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For every $X, Y \subseteq Z$ with $X \subseteq Y$ and every $x \in Z - Y$ we have that
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Advantage

We can bound the error of the portfolio/schedule:
At most away from optimum by factor of 0.63 (see [Streeter and Golovin. 2008])

Dynamic Instance Grouping [Liu et al. 2018]

Idea

- Similar to ISAC: group instances into clusters
- Similar to Hydra: refine clusters and configurations over several iterations

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3. Update clusters based on performance (estimates)
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- increase the configuration budget in each iteration
  - first clusterings will have a poor quality $\rightarrow$ small configuration time
  - later clusterings will be better $\rightarrow$ more configuration time