Learning near-optimal hyperparameters with minimal overhead

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DeepMind

Workshop on Automated Algorithm Design

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Introduction

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  - No structure assumed over the parameter space.

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  - the chosen configuration; and
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- Goal: find a near-optimal configuration solving $1 - \delta$ fraction of the problems in the least expected time.
  - Since some instances (δ fraction) are hopelessly hard; don't want to solve those.

Problem formulation

Given: n configurations, distribution Γ of problem instances.

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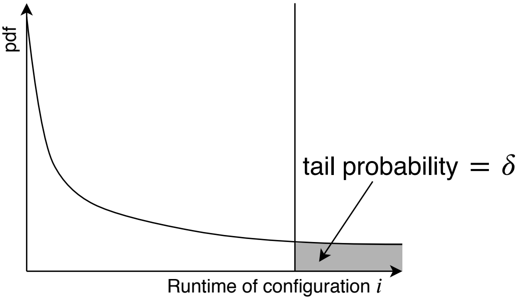

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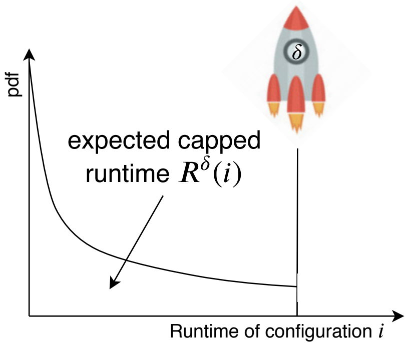

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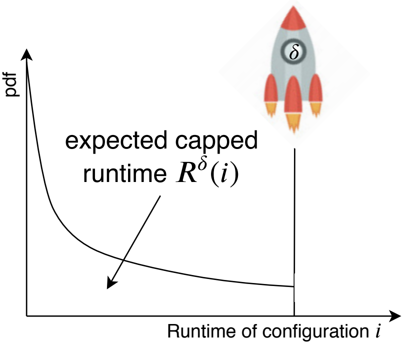

Runtime of the optimal capped configuration:

$$\mathrm{OPT}_{\delta} = \min_{i} R^{\delta}(i)$$

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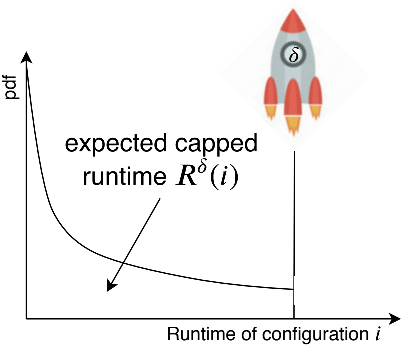

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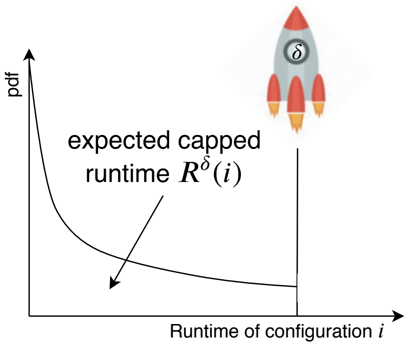

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Note that $\mathrm{OPT}_\delta \leq \mathrm{OPT}_{\delta/2} \leq \mathrm{OPT}_0$ – gaps can be large!

Previous work (before ICML'19)

Structured Procrastination

(Kleinberg et al., 2017)

- Relaxed goal: Find i with $R^{\delta}(i) \leq (1+\varepsilon)\mathrm{OPT}_0$
- Worst-case lower bound: runtime must be at least $\Omega\left(\mathrm{OPT}_0 \frac{n}{\varepsilon^2\delta}\right)$
- With probability $1-\zeta$, returns an (ε, δ)-optimal configuration in worst-case time

$$\mathcal{O}\left(\mathrm{OPT}_0 \, \frac{n}{\varepsilon^2\delta} \log\left(\frac{n \log \bar{\kappa}}{\zeta\varepsilon^2\delta}\right)\right)$$

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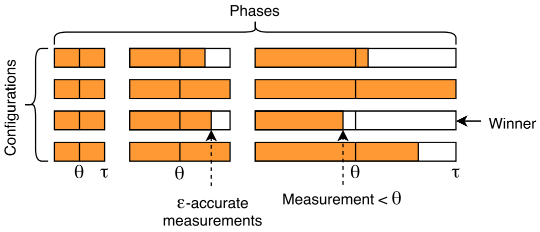
Can we remove $\bar{\kappa}$?

Can we improve runtime when problem is easier?

LEAPSANDBOUNDS

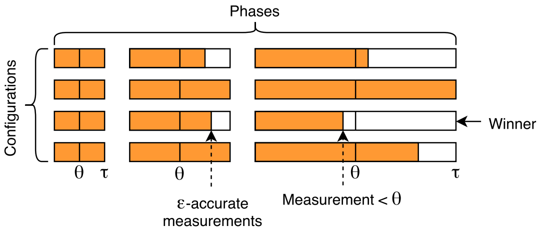
(Weisz et al., 2018)

1. Guess a value θ of OPT, starting from a low value
2. Test whether $R^\delta(i) \leq \theta$ for some configuration i:
   - For each i, run $b = \tilde{\mathcal{O}}(\frac{1}{\delta\varepsilon^2})$ instances with instance-wise timeout $\tau = \frac{4\theta}{3\delta}$, abort if empirical average exceeds θ.
3. Return the configuration with the smallest mean amongst successful configurations. If no test succeeded, double θ, continue from Step 2.



Average runtime budget and its use across different configurations and phases

Why does this work?



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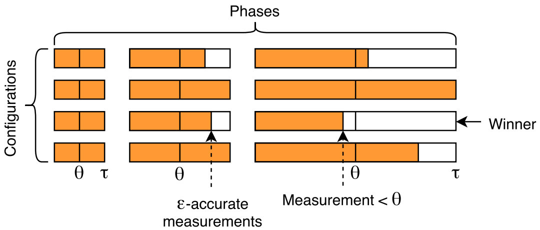

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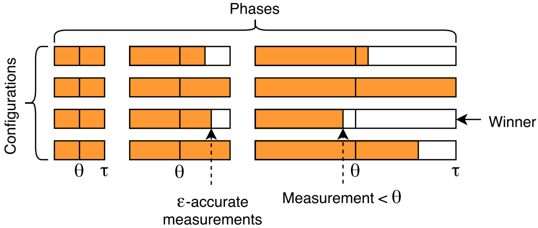

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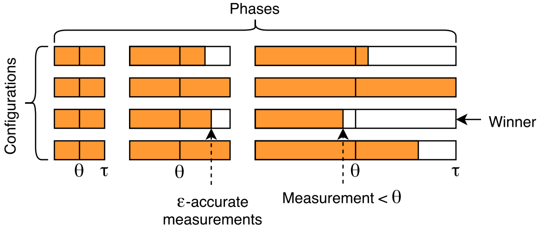

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  - if runs complete within θ average runtime:
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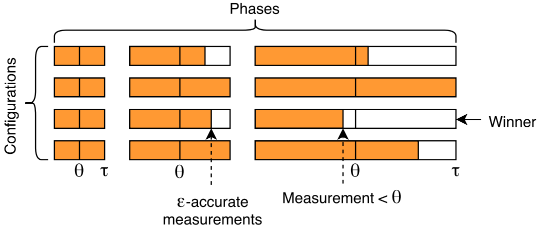

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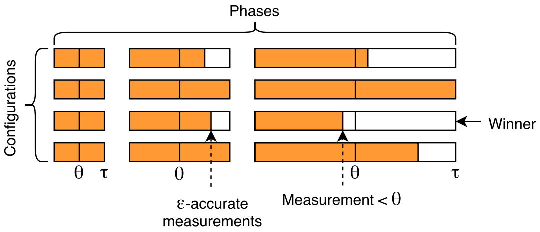

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- Thus, if for any configuration i, $\bar{R}_i < \theta$, then for $i^* = \operatorname{argmin}_i \bar{R}_i$, $R^\delta(i^*) \leq (1+\varepsilon)\mathrm{OPT}_0$ w.h.p.

Guarantees

Theorem

With high probability,

(i) the algorithm finds an (ε, δ)-optimal configuration;

(ii) the worst case runtime is $\mathcal{O}\left(\mathrm{OPT}_0 \frac{n}{\varepsilon^2 \delta} \log\left(\frac{n \log \mathrm{OPT}_0}{\zeta}\right)\right)$.

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- Runtime:

$$\mathcal{O}\left[\mathrm{OPT}_0 \sum_{i=1}^{n} \max\left(\frac{\sigma_{i,k}^2}{\varepsilon^2 R_{\tau_k}^2(i)}, \frac{1}{\varepsilon\delta}, \frac{1}{\delta}\log\frac{1}{\delta}\right)\left(\log\frac{n \log \mathrm{OPT}_0}{\zeta} + \log\frac{1}{\varepsilon R_{\tau_k}(i)}\right)\right].$$

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- Huge improvement if the variances are small: $\frac{\sigma_{i,k}^2}{R_{\tau_k}^2} \ll \frac{1}{\delta}$.

Experiments

- Configuring the minisat SAT solver (Sorensson and Een, 2005)
- 1K configurations, 20K nontrivial problem instances
- Compare with Structured Procrastination by Kleinberg et al. (2017)
- Code and (83 CPU years worth of @ year 2018 CPUs) data:
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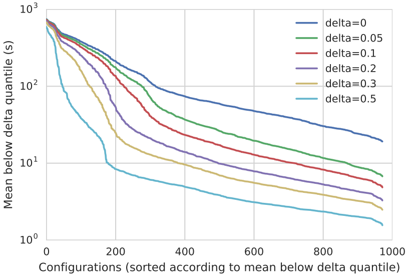

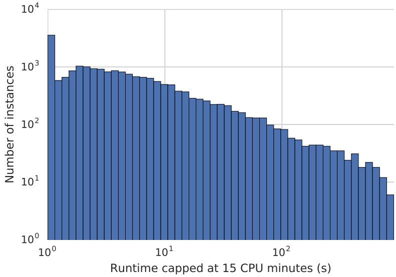

Results

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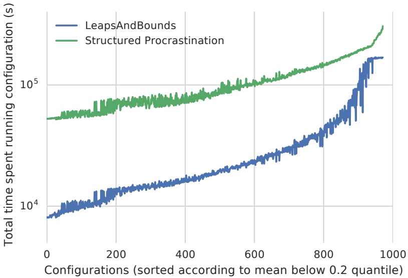

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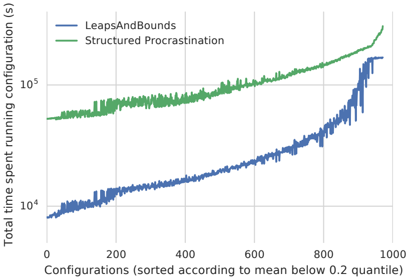
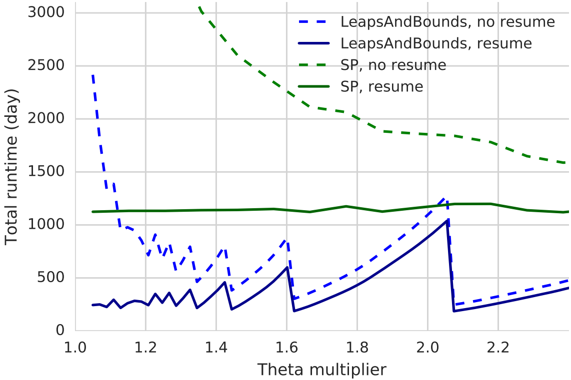


3–20-times improvement in total work
(also across different choices of ε and δ)

Effect of the multiplier of θ



(cost of pause/resume is not modeled)

Current work (ICML'19)

CapsAndRuns algorithm (Weisz et al., 2019)

For all configurations i, in parallel:

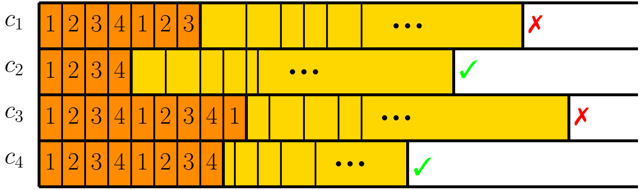
Phase I: Find $t_\delta(i) \le \tau_i \le t_{\delta/2}(i)$:

- Run $\Theta(1/\delta)$ instances in parallel until $1 - \frac{3}{4}\delta$ fraction of them finishes.

Phase II: Find $R_{\tau_i}(i)$ with ε relative accuracy:

- Run sufficiently many instances with timeout τ_i until we get an ε-accurate estimate of $R_{\tau_i}(i)$ ('Bernstein stopping' ala Mnih et al. 2008).

Return: Of the configurations not rejected, select the one with the smallest average capped runtime



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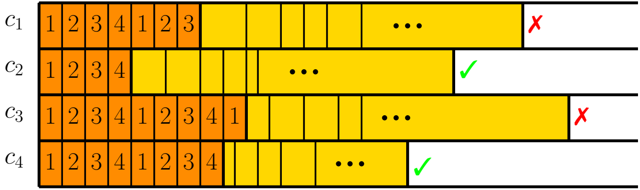

Global variables

Set $\mathcal{N}$ of n algorithm configurations
Precision parameter $\varepsilon \in (0, \frac{1}{3})$
Quantile parameter $\delta \in (0, 1)$
Failure probability parameter $\zeta \in (0, \frac{1}{6})$
Instance distribution Γ
$b \leftarrow \left\lceil 48 \frac{1}{\delta} \log\left(\frac{3n}{\zeta}\right) \right\rceil$
$T \leftarrow \infty$ ▷ Time limit, updated continuously by all parallel processes

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Algorithm 2 QUANTILEEST

1: **Inputs:** i
2: **Initialize:** $m \leftarrow \left\lceil (1 - \frac{3}{4}\delta) b \right\rceil$
3: Run configuration i on b instances, in parallel, until m of these complete. Abort if total work $\geq 2Tb$.
4: $\tau \leftarrow$ runtime of m^{th} completed instance
5: **return** τ

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Algorithm 3 RUNTIMEEST

Inputs: i, τ
Initialize: $j \leftarrow 0$
while True **do**
    Sample j^{th} instance J from Γ
    Let Y be τ capped runtime of i on J
    Update $\bar{Y}$, $\bar{\sigma}^2$, sample mean and variance
    $C = c(\bar{\sigma}, n, j, \zeta, \tau)$
    if $\bar{Y} - C > T$ **then**
        return reject i
    end if
    $T \leftarrow \min\{T, \bar{Y} + C\}$ ▷ lowest upper confidence
    if $C \leq \frac{\varepsilon}{3}(2\bar{Y} - C)$ **then**
        return accept i with runtime estimate $\bar{Y}$
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    $j \leftarrow j + 1$
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Algorithm 1 CAPSANDRUNS

$\mathcal{N}' \leftarrow \mathcal{N}$ ▷ Pool of competing configurations
for configuration $i \in \mathcal{N}$, in parallel **do**
// Phase I:
Run $\tau_i \leftarrow$ QUANTILEEST (i)
// Phase II:
if QUANTILEEST (i) aborted **then**
Remove i from $\mathcal{N}'$
else
Run RUNTIMEEST (i, τ_i), abort if $|\mathcal{N}'| = 1$
if RUNTIMEEST (i, τ_i) rejected i **then**
Remove i from $\mathcal{N}'$
else
$\bar{Y}(i) \leftarrow$ return value of RUNTIMEEST (i, τ_i)
end if
end if
end for
return $i^* = \text{argmin}_{i \in \mathcal{N}'} \bar{Y}(i)$ and τ_{i^*}

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CapsAndRuns theory

Theorem

With probability $1-\zeta$,

(i) the algorithm finds an (ε,δ)*-optimal configuration;*

(ii) the total work is

$$\tilde{O}_\zeta\left(n\,\mathrm{OPT}_{\delta/2}\left(\frac{1}{\delta}+\max\left\{\frac{\sigma^2}{\max\{\varepsilon^2,\Delta^2\}},\frac{r}{\max\{\varepsilon,\Delta\}}\right\}\right)\right),$$

Refined result

- Gap: $\Delta_i = 1 - \frac{\mathrm{OPT}_{\delta/2}}{R^{\delta}(i)}$.
- Variance of $R(i, j, \tau), j \sim \Gamma$: $\sigma_\tau^2(i)$.
- Maximum relative variance: $\hat{\sigma}^2(i) = \sup_{\tau \in [t_\delta(i), t_{\delta/2}(i)]} \frac{\sigma_\tau^2(i)}{R_\tau^2(i)}$.
- Relative range $r(i) = \sup_{\tau \in [t_\delta(i), t_{\delta/2}(i)]} \frac{\tau}{R_\tau(i)}$.
- Among the set of configurations $\mathcal{N}_1$ not rejected by QuantileEst, let $i_* = \mathrm{argmin}_{i \in \mathcal{N}_1} R_{\tau_i}(i)$.

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Theorem

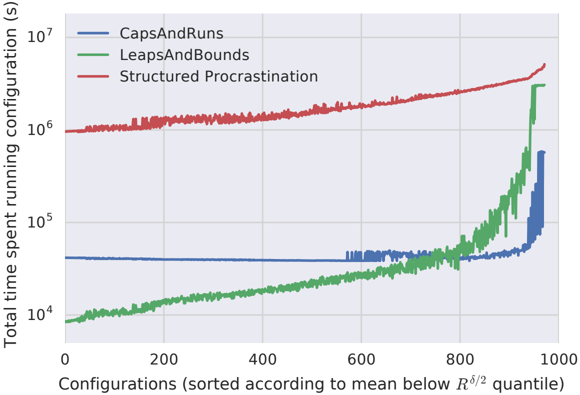
With probability $1 - \zeta$,

(i) *the algorithm finds an* (ε, δ)*-optimal configuration;*

(ii) *the total work is*

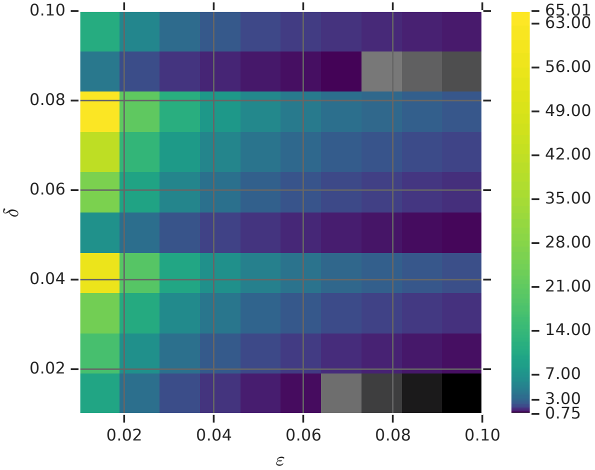
$$\tilde{O}_\zeta\left(\mathrm{OPT}_{\frac{\delta}{2}}\left[\frac{n}{\delta} + \sum_{i \in \mathcal{N}} \max\left\{\frac{\max\left\{\hat{\sigma}^2(i), \hat{\sigma}^2(i_*)\right\}}{\max\{\varepsilon^2, \Delta_i^2\}}, \frac{\max\left\{r(i), r(i_*)\right\}}{\max\{\varepsilon, \Delta_i\}}\right\}\right]\right)$$

Experiments I



STRUCTURED PROCRASTINATION	LEAPSANDBOUNDS	CAPSANDRUNS
20643 (± 5) days	1451 (± 83) days	586 (± 7) days

Experiments II: Speedup compared to LEAPSANDBOUNDS



Recent work (after ICML'19)

Structured proscrastination with confidence

(Kleinberg et al., 2019)

- Anytime guarantee: With some $c, p > 0$ universal, for any (ε, δ), for $t \geq c\,\mathrm{OPT}_0\, n/(\delta\varepsilon^2)$, SPC returns with probability $1 - ct^{-p}$ a config i such that $R^\delta(i) \leq (1+\varepsilon)\mathrm{OPT}_0$

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- Making CapsAndRuns (more) anytime: Fix ε; add outer loop that decreases δ
  - Works because $\mathrm{OPT}_{1/2} \leq \mathrm{OPT}_{1/4} \leq \mathrm{OPT}_{1/8} \leq \cdots \leq \mathrm{OPT}_0$

Structured proscrastination with confidence

(Kleinberg et al., 2019)

- Anytime guarantee: With some $c, p > 0$ universal, for any (ε, δ), for $t \geq c\,\mathrm{OPT}_0\, n/(\delta\varepsilon^2)$, SPC returns with probability $1 - ct^{-p}$ a config i such that $R^\delta(i) \leq (1+\varepsilon)\mathrm{OPT}_0$
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Thank you!

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