Hands-On Session: Practical Hyperparameter Optimization with SMAC3

Carolin Benjamins, Alexander Tornede

Who Are We? Alexander Tornede

- From 10/2018 - 06/2023 PhD student with Prof. Dr. Eyke Hüllermeier at Paderborn University on the topic of Algorithm Selection
- Since 09/2022 PostDoc in Prof. Dr. Marius Lindauer's group at Leibniz University Hannover
- Head of SMAC's dev team
- Member of the automl.org supergroup
- Collaborations with other research groups
- Focus on interactive and explainable AutoML and LLMs x AutoML
- Background: Computer Science
- I love playing board games with friends

Who Are We? Carolin Benjamins

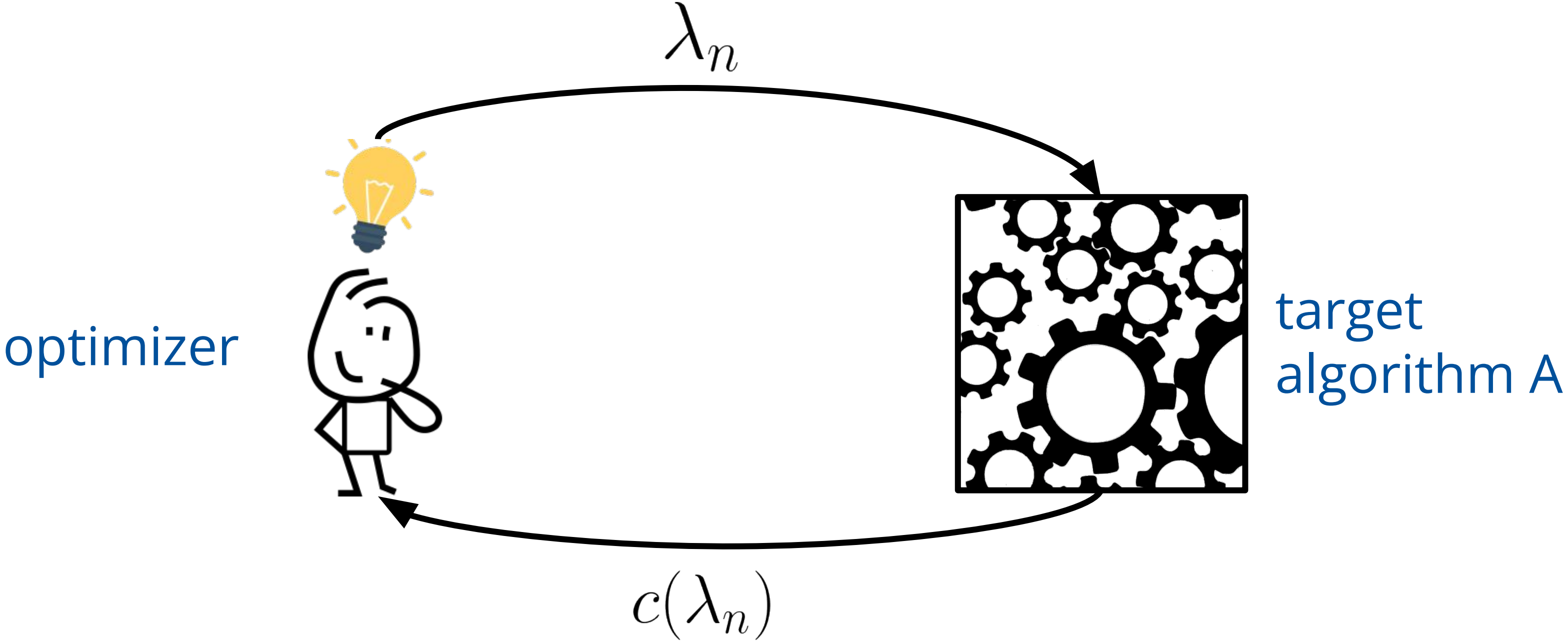
- ⏳ Since 2020 PhD student with Prof. Dr. Marius Lindauer at Leibniz University Hannover
- 👩‍💻 Member of SMAC’s dev team
- 👥 Member of the automl.org supergroup
- 🤝 Collaborations with other research groups
- ⚡ Focus on AutoML, Dynamic Algorithm Configuration, Bayesian Optimization. Interested in robotics and Contextual Reinforcement Learning.
- 🤖 Background: Mechatronics & Robotics
- 💜 I love automation and making complex algorithms more accessible!

🎲 Today's Game Plan

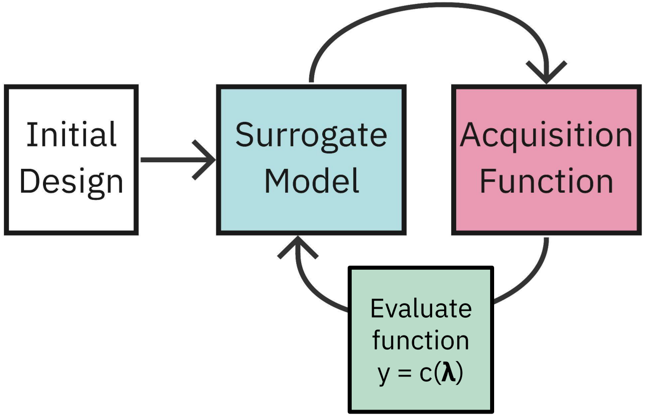
1. 14:00 - 14:25: Introduction of SMAC
2. 14:20 - 15:15: Hands-on Notebook Session
3. 15:15 - 15:30: Wrap-Up: What did we learn?

Hyperparameter Optimization

Goal: Find the best performing configuration: $\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} c(\boldsymbol{\lambda}) = \arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \mathcal{L}(\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{val}}; \boldsymbol{\lambda})$



Recap: Bayesian Optimization



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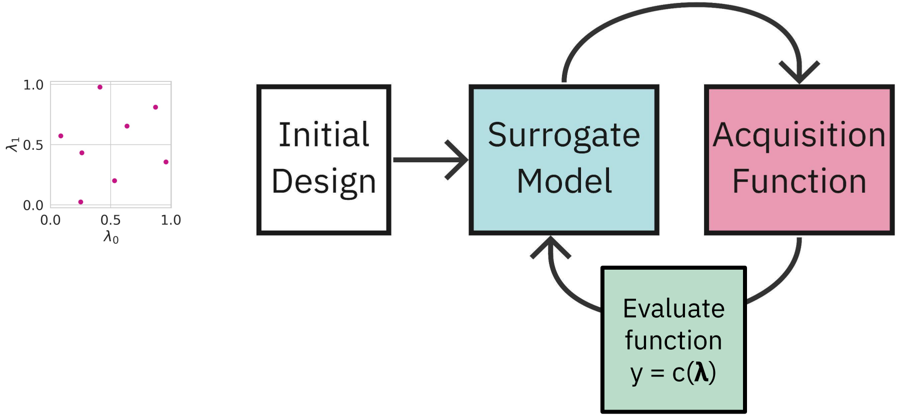

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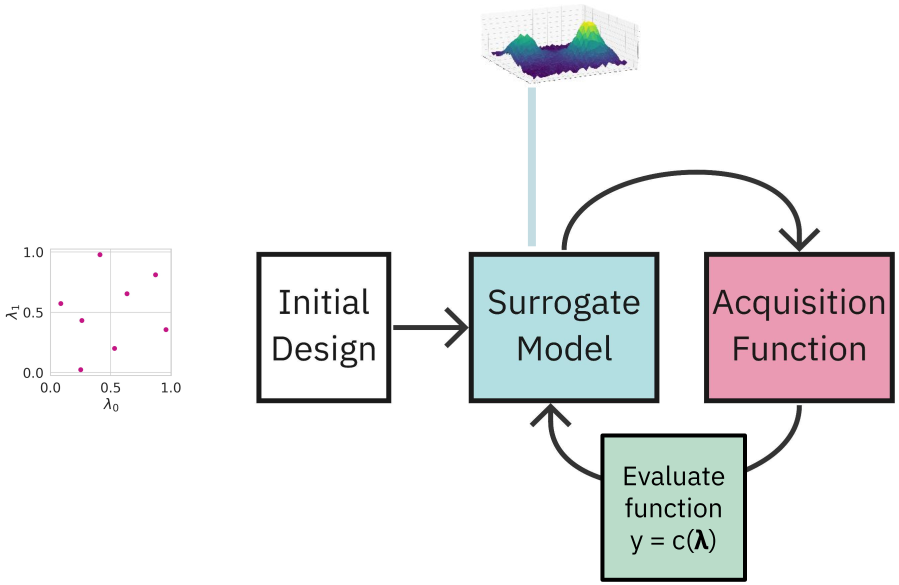

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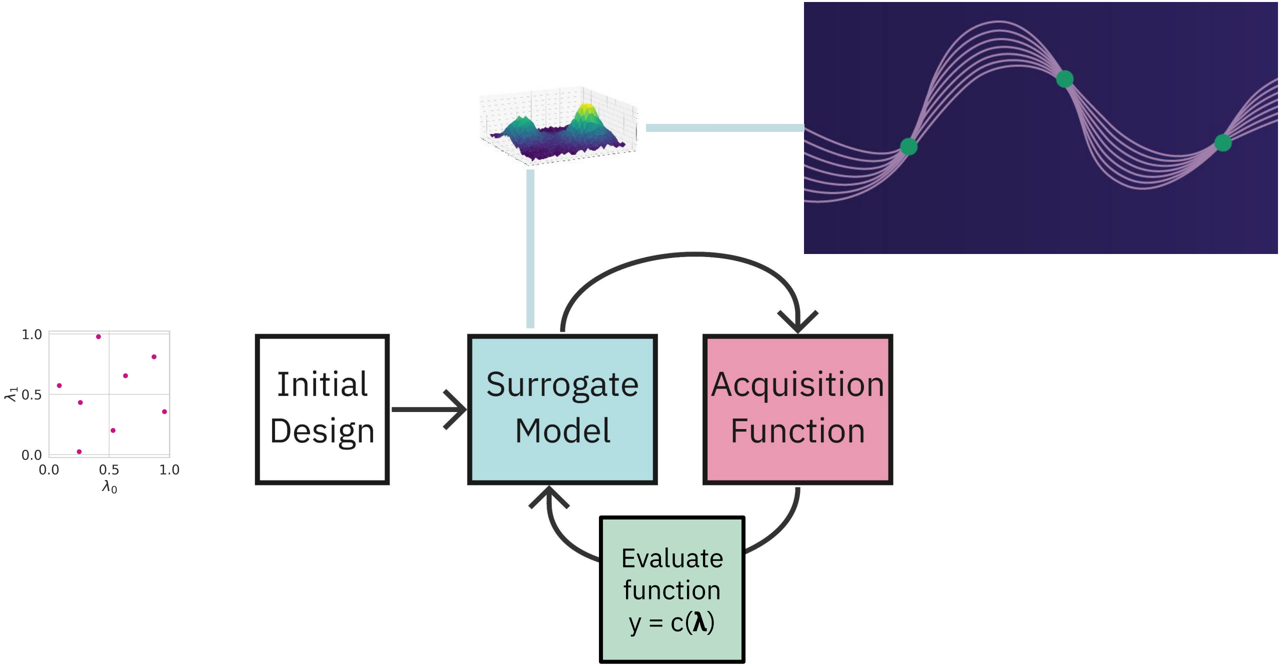

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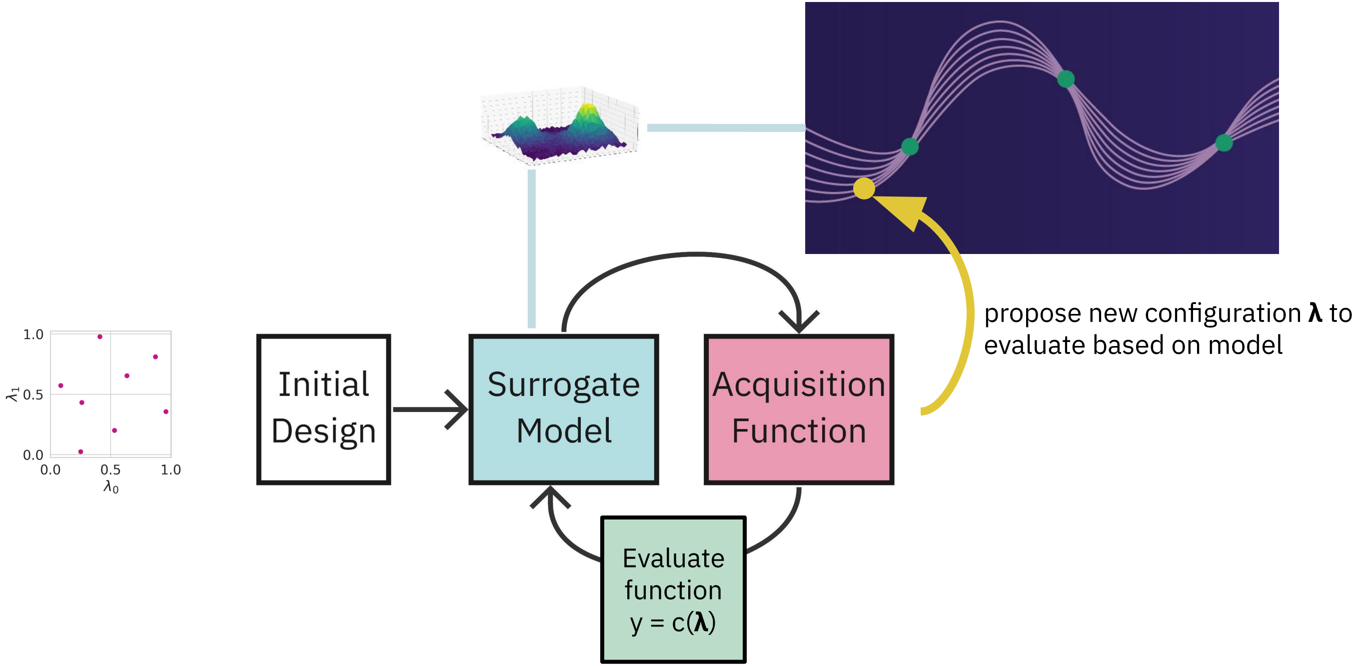


SMAC3 - A Versatile Bayesian Optimization Package for Hyperparameter Optimization

Original authors:

New team members:

Funded by:

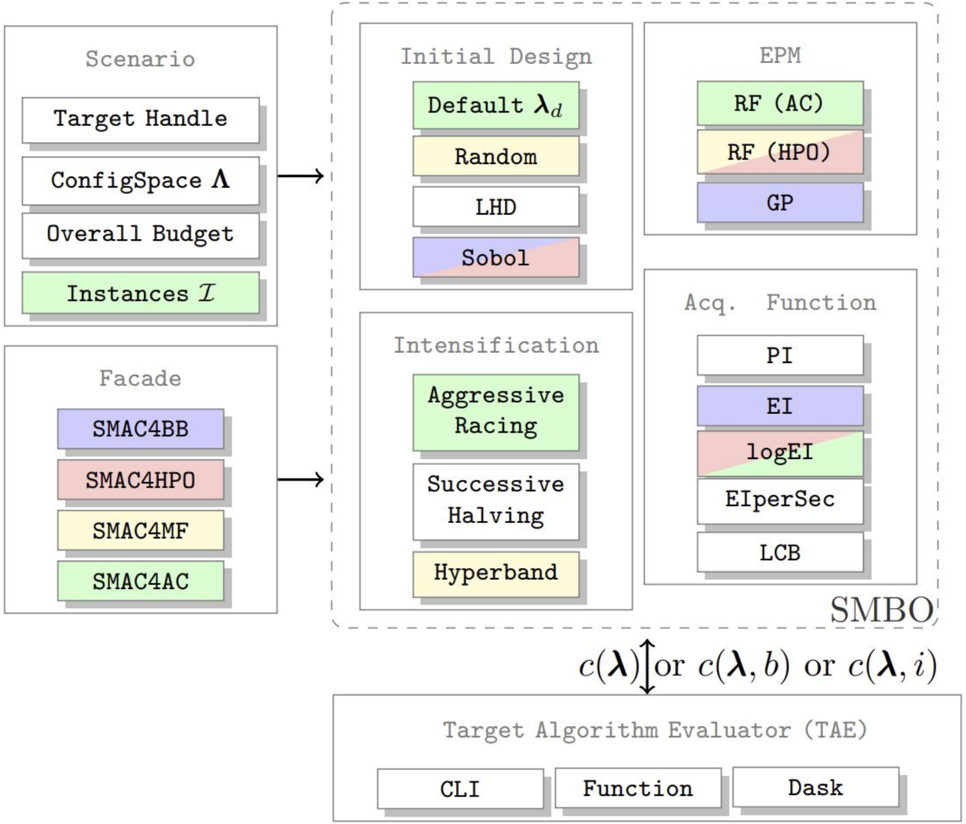
🎁 SMAC Features (1)

- Open source + active maintenance
- Rich search space with floats, ordinals, categoricals and conditions
- Ask-and-Tell Interface
- Continue and Warmstart Optimization
- Intensification mechanism to efficiently compare configurations
- User priors

🎁 SMAC Features (2)

- Parallelization, local and on a cluster with Dask
- Multi-fidelity optimization, e.g. when we can evaluate our function with different resolutions
- Multi-objective optimization with ParEGO
- Optimization across many tasks (aka algorithm configuration)
- Function to optimize can either be pythonic or called via a script
- Easily extensible with callbacks

Modular Design



SMAC for Black-Box Functions

$$\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} c(\boldsymbol{\lambda})$$

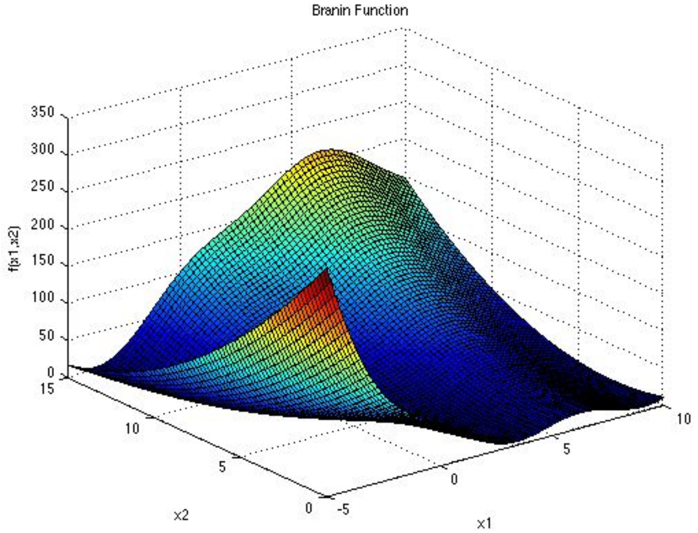
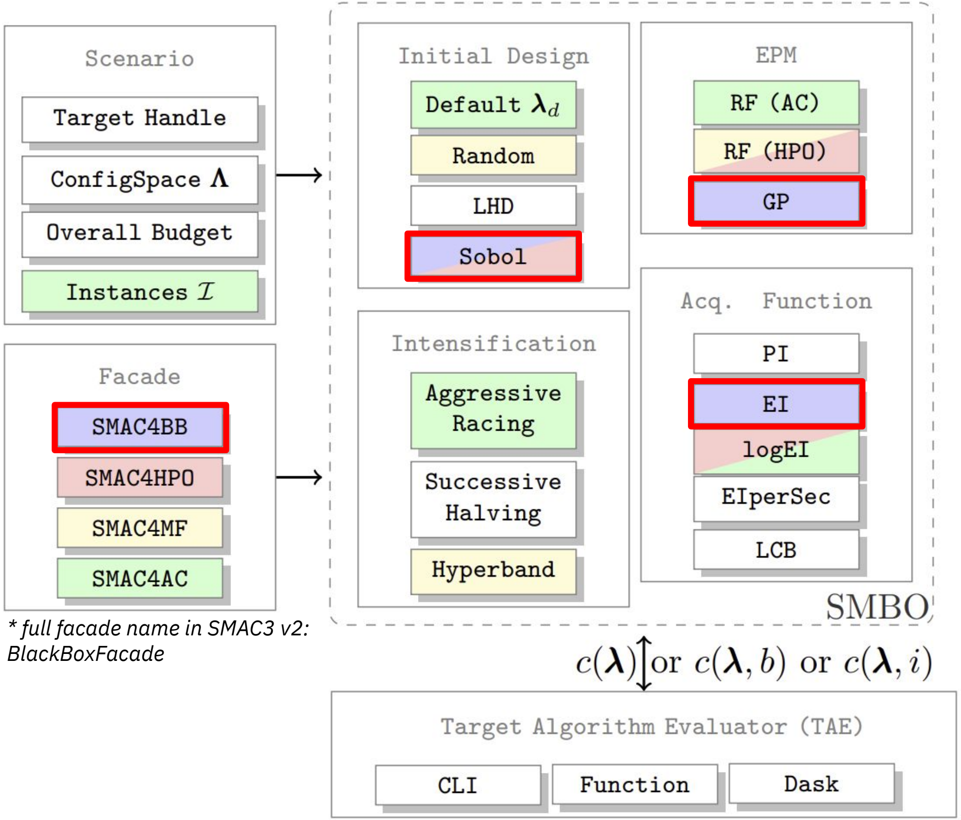


Image credit [Derek Bingham]()

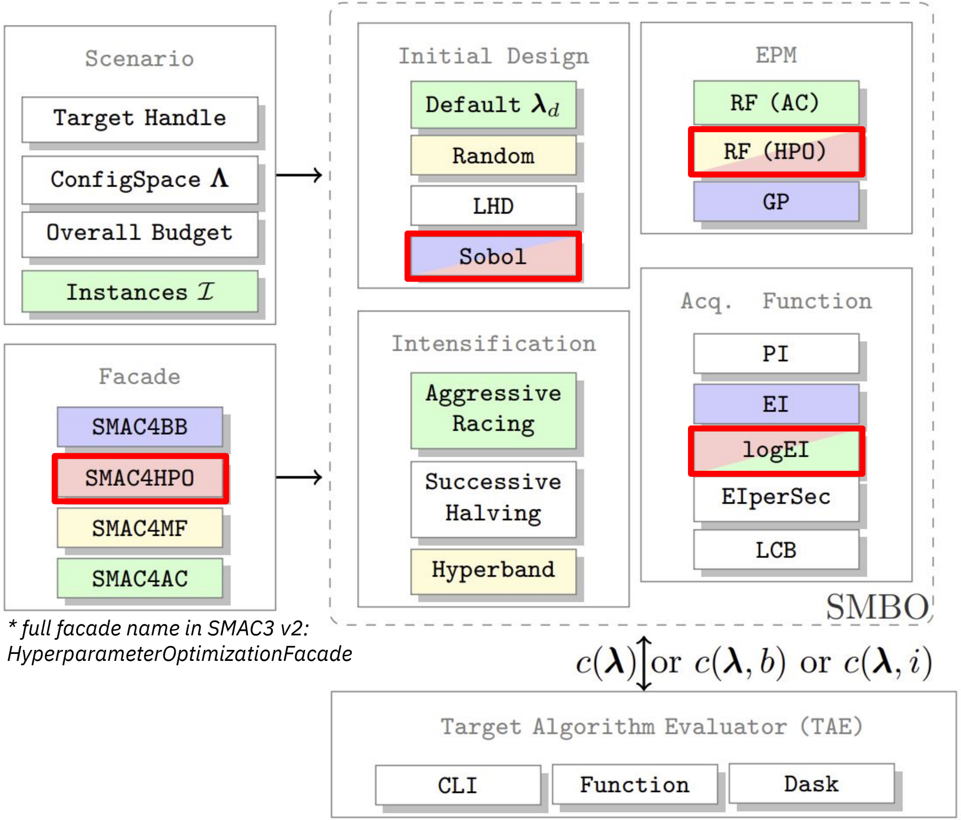


** full facade name in SMAC3 v2: BlackBoxFacade*

SMAC for CASH and Structured Hyperparameter Optimization

$$(A^*, \boldsymbol{\lambda}^*) \in \underset{A_i \in \mathbf{A}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_i}{\arg\min} \; c(A_i, \boldsymbol{\lambda}) =$$

$$\underset{A_i \in \mathbf{A}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda}_i}{\arg\min} \; \mathcal{L}(\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{val}}; A_i(\boldsymbol{\lambda})).$$

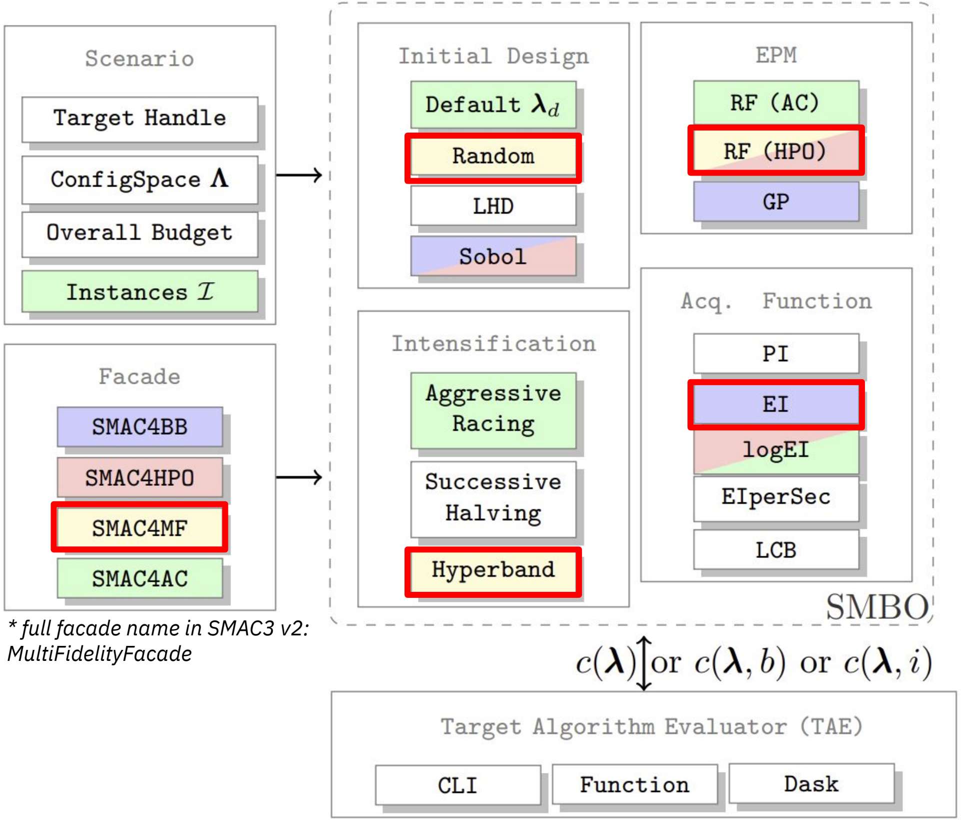


** full facade name in SMAC3 v2: HyperparameterOptimizationFacade*

SMAC for Expensive Tasks and Automated Deep Learning

$$\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} c(\boldsymbol{\lambda}, b_{max}) =$$

$$\arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} \mathcal{L}(\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{val}}; \boldsymbol{\lambda}, b_{max}).$$

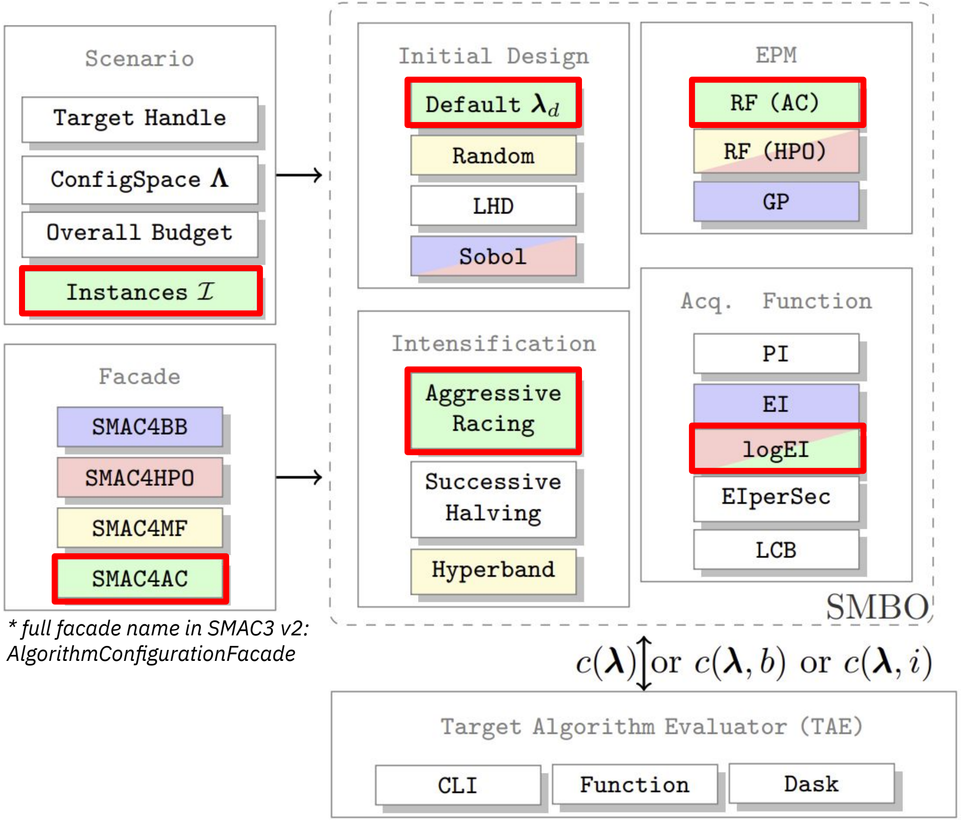


** full facade name in SMAC3 v2: MultiFidelityFacade*

SMAC for Algorithm Configuration

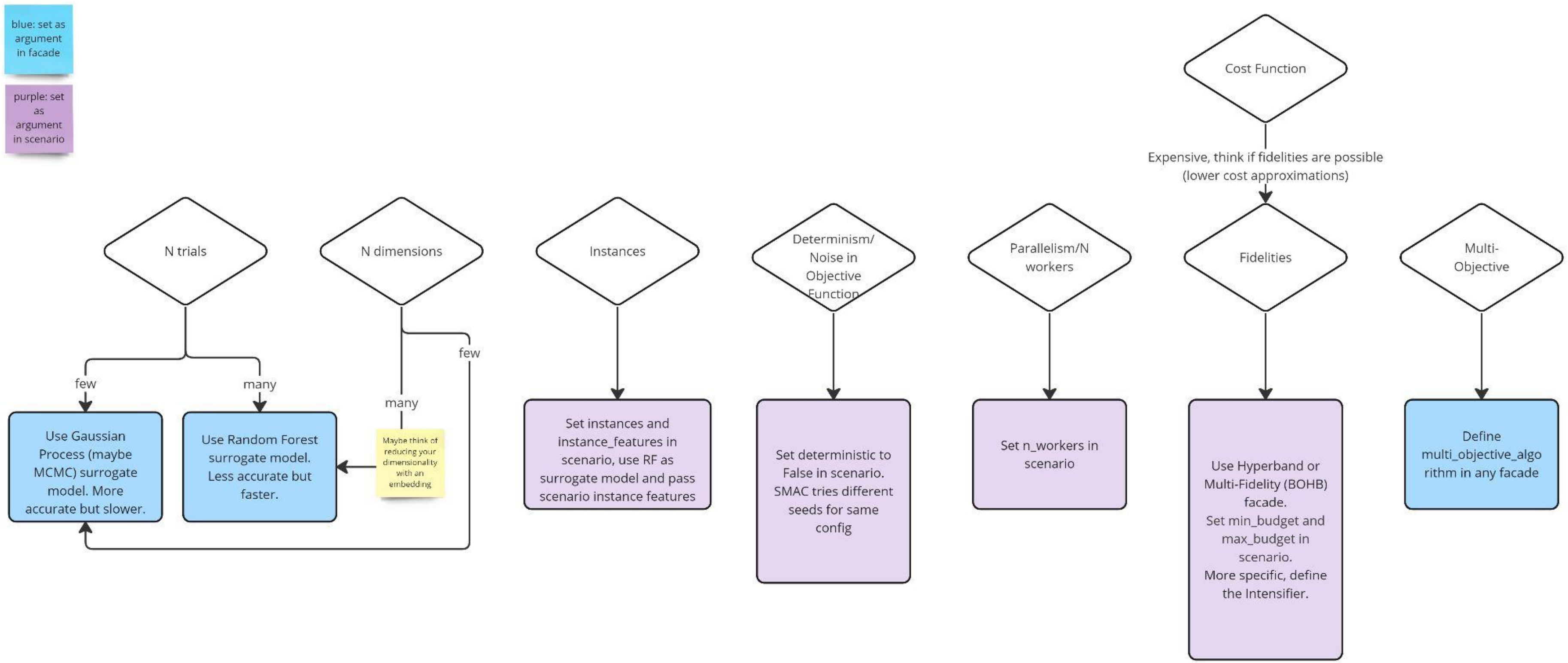
$$\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} c(\boldsymbol{\lambda}) =$$

$$\arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} \sum_{i\in\mathcal{I}} c'(\boldsymbol{\lambda}, i)$$



** full facade name in SMAC3 v2: AlgorithmConfigurationFacade*

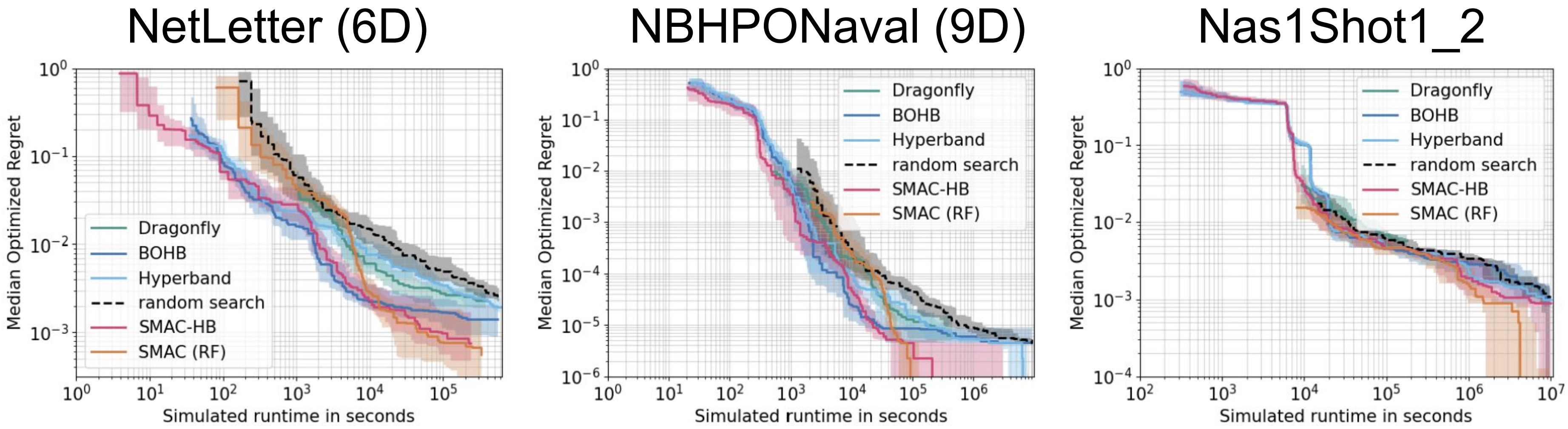
🌳 Facades Are Only Shortcuts!



Comparison to Other Packages

Package	Complex Hyperparameter Space	Multi-Objective	Multi-Fidelity	Instances	Command-Line Interface	Parallelism
HyperMapper	✅	✅	❌	❌	❌	❌
Optuna	✅	✅	✅	❌	✅	✅
Hyperopt	✅	❌	❌	❌	✅	✅
BoTorch	❌	✅	✅	❌	❌	✅
OpenBox	✅	✅	❌	❌	❌	✅
HpBandSter	✅	❌	✅	❌	❌	✅
SMAC	✅	✅	✅	✅	✅	✅

Exemplary Results



Take-Aways:

1. SMAC with a RF as black-box HPO approach *"SMAC (RF)"* outperforms other approaches with TPE and GP models
2. SMAC's implementation of BOHB [Falkner et al. 2018] *"SMAC-HB" (also using a RF as surrogate) has a very strong any-time performance*

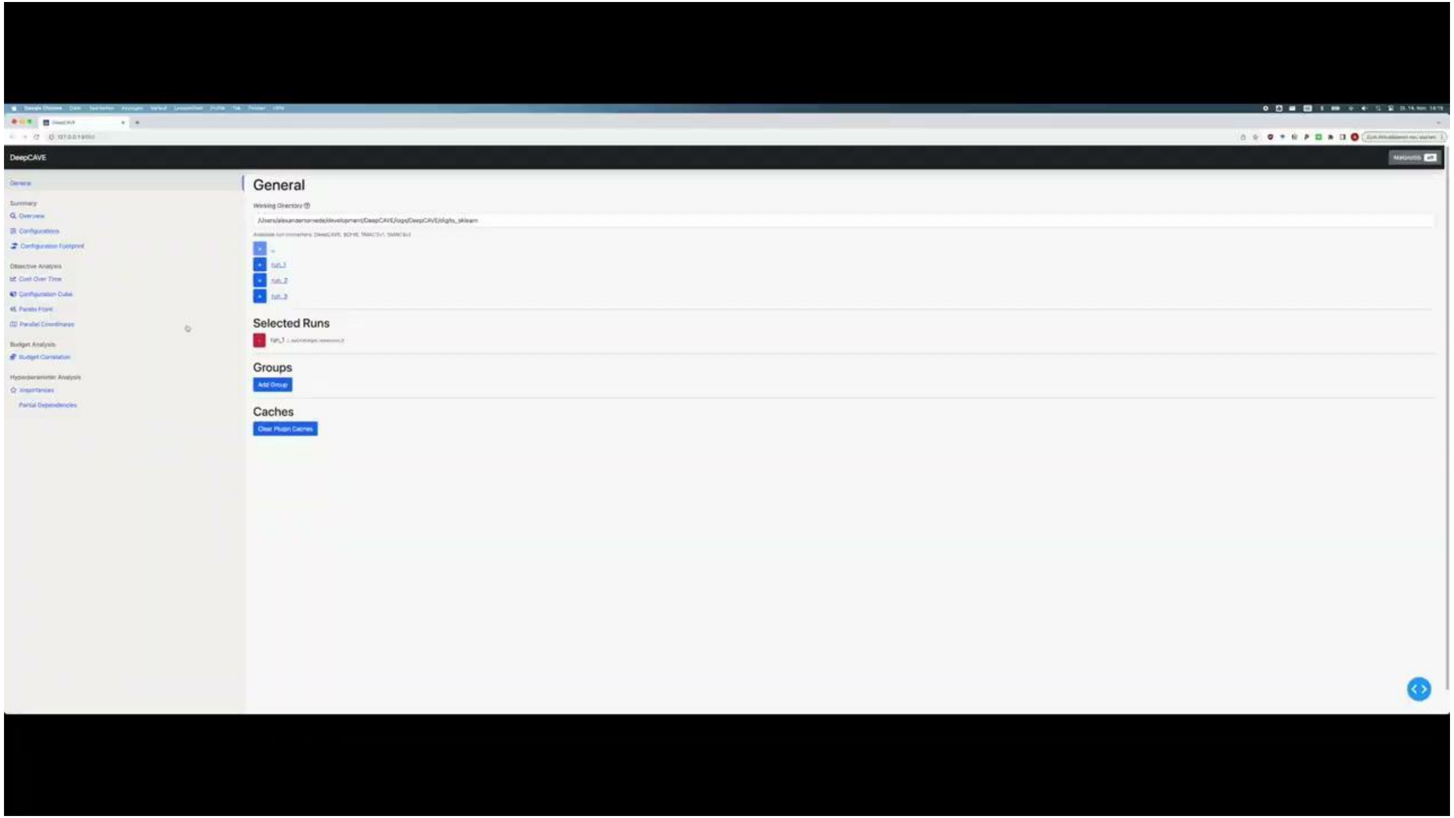
Hands-On Notebook Session

https://tinyurl.com/fallschoolsmac

Wrap-Up: What Did We Learn?

- How to perform HPO with SMAC
- SMAC is highly modularized offering many customization options
- SMAC offers different facades for easy usages in many use cases
- We welcome collaborations and contributions 😊

DeepCave Sneak Peek



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