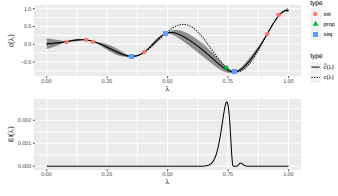
# Introduction to Machine Learning

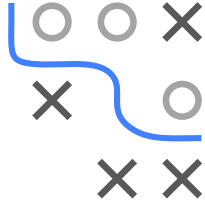
## Hyperparameter Tuning
## Advanced Tuning Techniques



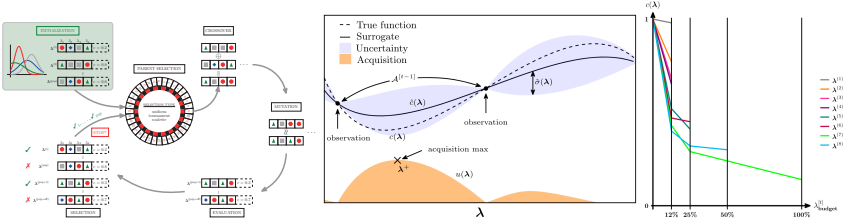

**Learning goals**

- Basic idea of evolutionary algorithms
- and Bayesian Optimization
- and hyperband

# HPO – MANY APPROACHES



- Evolutionary algorithms
- Bayesian / model-based optimization
- Multi-fidelity optimization, e.g. Hyperband

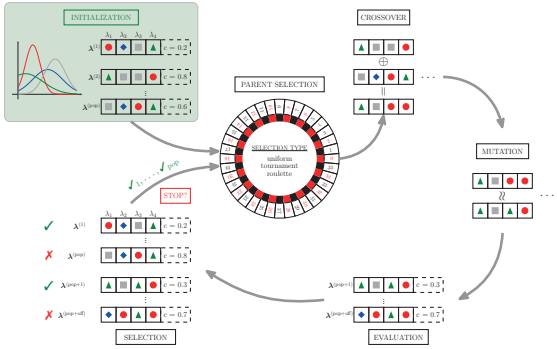


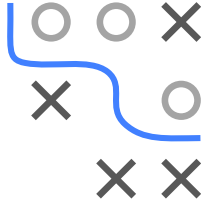

HPO methods can be characterized by:

- how the exploration vs. exploitation trade-off is handled
- how the inference vs. search trade-off is handled

Further aspects: Parallelizability, local vs. global behavior, handling of noisy observations, multifidelity and search space complexity.

# EVOLUTIONARY STRATEGIES

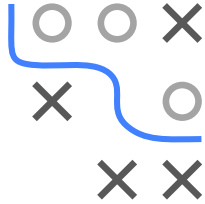


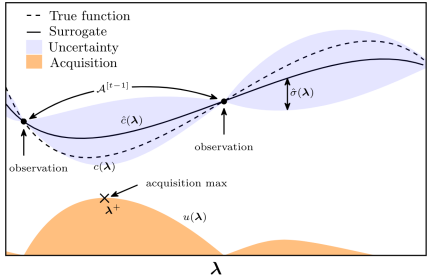
- Are a class of stochastic population-based optimization methods inspired by the concepts of biological evolution
- Are applicable to HPO since they do not require gradients
- Mutation is the (randomized) change of one or a few HP values in a configuration.
- Crossover creates a new HPC by (randomly) mixing the values of two other configurations.

# BAYESIAN OPTIMIZATION

BO sequentially iterates:

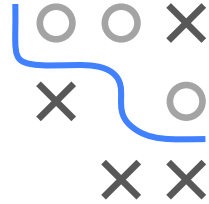


1. **Approximate** $\boldsymbol{\lambda} \mapsto c(\boldsymbol{\lambda})$ by (nonlin) regression model $\hat{c}(\boldsymbol{\lambda})$, from evaluated configurations (archive)
2. **Propose candidates** via optimizing an acquisition function that is based on the surrogate $\hat{c}(\boldsymbol{\lambda})$
3. **Evaluate** candidate(s) proposed in 2, then go to 1



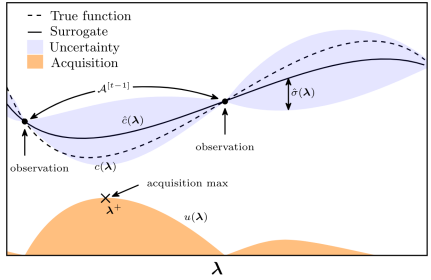

Important trade-off: **Exploration** (evaluate candidates in under-explored areas) vs. **exploitation** (search near promising areas)

# BAYESIAN OPTIMIZATION



**Surrogate Model**:

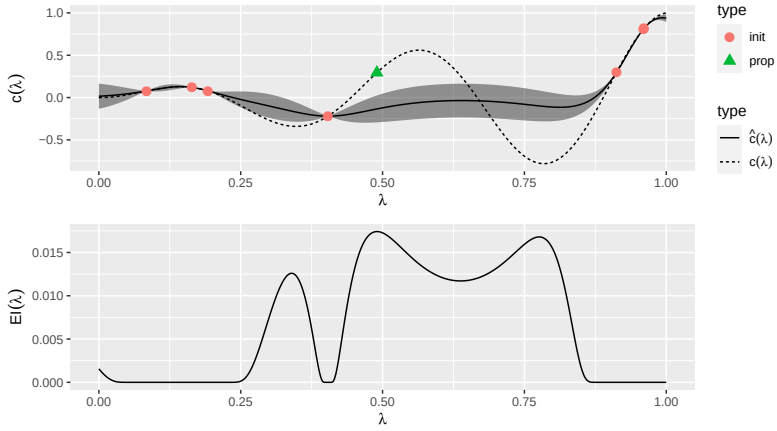
- Probabilistic modeling of $C(\boldsymbol{\lambda}) \sim (\hat{c}(\boldsymbol{\lambda}), \hat{\sigma}(\boldsymbol{\lambda}))$ with posterior mean $\hat{c}(\boldsymbol{\lambda})$ and uncertainty $\hat{\sigma}(\boldsymbol{\lambda})$.
- Typical choices for numeric spaces are Gaussian Processes; random forests for mixed spaces

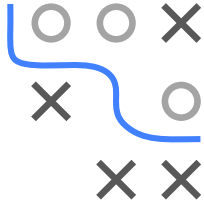



**Acquisition Function**:

- Balance exploration (high $\hat{\sigma}$) vs. exploitation (low $\hat{c}$).
- Lower confidence bound (LCB): $a(\boldsymbol{\lambda}) = \hat{c}(\boldsymbol{\lambda}) - \kappa \cdot \hat{\sigma}(\boldsymbol{\lambda})$
- Expected improvement (EI): $a(\boldsymbol{\lambda}) = \mathbb{E}\left[\max\left\{c_{\text{min}} - C(\boldsymbol{\lambda}), 0\right\}\right]$ where ($c_{\text{min}}$ is best cost value from archive)
- Optimizing $a(\boldsymbol{\lambda})$ is still difficult, but cheap(er)

# BAYESIAN OPTIMIZATION



Upper plot: The surrogate model (black, solid) models the *unknown* relationship between input and output (black, dashed) based on the initial design (red points).

Lower plot: Mean and variance of the surrogate model are used to derive the expected improvement (EI) criterion. The point that maximizes the EI is proposed (green point).

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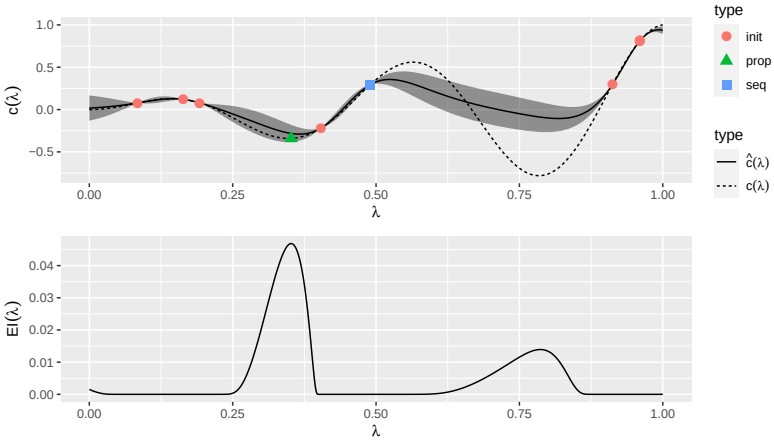


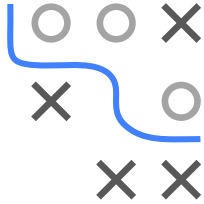

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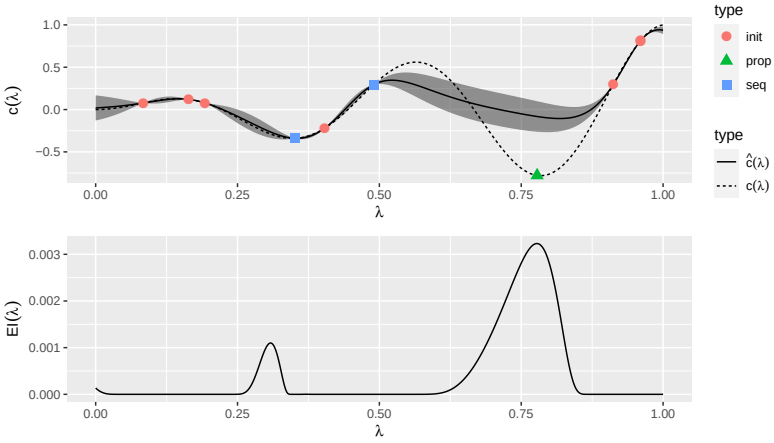


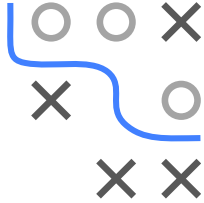

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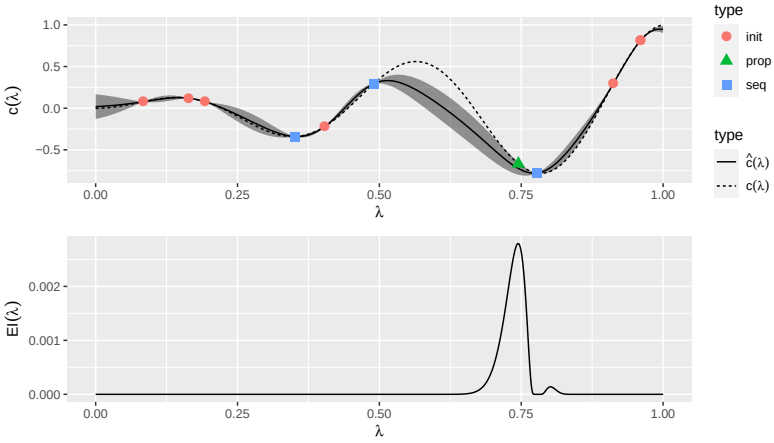


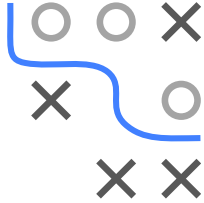

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# BAYESIAN OPTIMIZATION / 2

Since we use the sequentially updated surrogate model predictions of performance to propose new configurations, we are guided to "interesting" regions of $\mathbf{\Lambda}$ and avoid irrelevant evaluations:

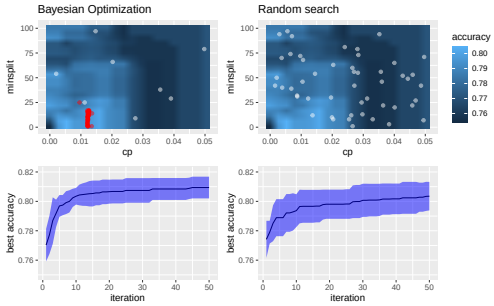
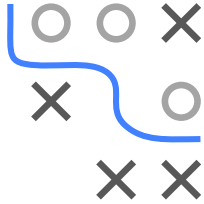
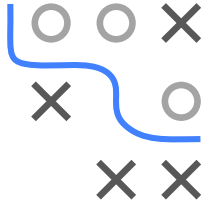



**Figure:** Tuning complexity and minimal node size for splits for CART on the `titanic` data (10-fold CV maximizing accuracy).
Left panel: BO, 50 configurations; right panel: random search, 50 iterations.
Top panel: one run (initial design of BO is white); bottom panel: mean $\pm$ std of 10 runs.

# BAYESIAN OPTIMIZATION / 3

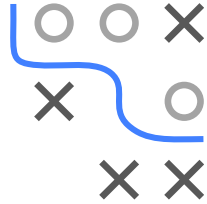


# MULTIFIDELITY OPTIMIZATION

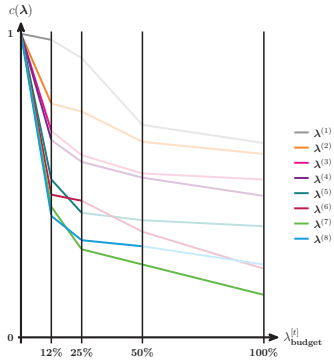


- Prerequiste: Fidelity HP $\lambda_{\text{fid}}$, i.e., a component of $\boldsymbol{\lambda}$, which influences the computational cost of the fitting procedure in a monotonically increasing manner
- Methods of multifidelity optimization in HPO are all tuning approaches that can efficiently handle a $\mathcal{I}$ with a HP $\lambda_{\text{fid}}$
- The lower we set $\lambda_{\text{fid}}$, the more points we can explore in our search space, albeit with much less reliable information w.r.t. their true performance.
- We assume to know box-constraints of $\lambda_{\text{fid}}$, so $\lambda_{\text{fid}} \in [\lambda_{\text{fid}}^{\text{low}}, \lambda_{\text{fid}}^{\text{upp}}]$, where the upper limit implies the highest fidelity returning values closest to the true objective value at the highest computational cost.

# SUCCESSIVE HALVING



- Races down set of HPCs to the best
- Idea: Discard bad configurations early
- Train HPCs with fraction of full budget (SGD epochs, training set size); the control param for this is called **multi-fidelity HP**
- Continue with better $1/\eta$ fraction of HPCs (w.r.t $\widehat{\mathrm{GE}}$); with $\eta$ times budget (usually $\eta = 2, 3$)
- Repeat until budget depleted or single HPC remains



# MULTIFIDELITY OPTIMIZATION – HYPERBAND

**Problem with SH**

- Good HPCs could be killed off too early, depends on evaluation schedule

**Solution: Hyperband**

- Repeat SH with different start budgets $\lambda_{\text{fid}}^{[0]}$ and initial number of HPCs $p^{[0]}$
- Each SH run is called bracket
- Each bracket consumes ca. the same budget

For $\eta = 4$

bracket 3

| $t$ | $\lambda_{\text{fid}}^{[t]}$ | $p_3^{[t]}$ |
|---|---|---|
| 0 | 1 | 82 |
| 1 | 4 | 20 |
| 2 | 16 | 5 |
| 3 | 64 | 1 |

bracket 2

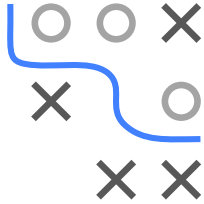
| $t$ | $\lambda_{\text{fid}}^{[t]}$ | $p_2^{[t]}$ |
|---|---|---|
| 0 | 4 | 27 |
| 1 | 16 | 6 |
| 2 | 64 | 1 |

bracket 1

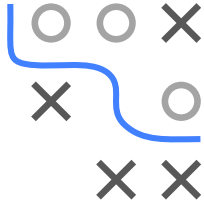
| $t$ | $\lambda_{\text{fid}}^{[t]}$ | $p_1^{[t]}$ |
|---|---|---|
| 0 | 16 | 10 |
| 1 | 64 | 2 |

bracket 0

| $t$ | $\lambda_{\text{fid}}^{[t]}$ | $p_0^{[t]}$ |
|---|---|---|
| 0 | 64 | 5 |



# MORE TUNING ALGORITHMS:



Other advanced techniques besides model-based optimization and the hyperband algorithm are:

- Stochastic local search, e.g., simulated annealing
- Genetic algorithms / CMAES
- Iterated F-Racing
- Many more . . .

For more information see *Hyperparameter Optimization: Foundations, Algorithms, Best Practices and Open Challenges*, Bischl (2021)