AutoML: Bayesian Optimization for HPO

Extensions of Bayesian Optimization

Bernd Bischl   Frank Hutter   Lars Kotthoff
Marius Lindauer   Joaquin Vanschoren

Beyond the Standard Bayesian Optimization Setting

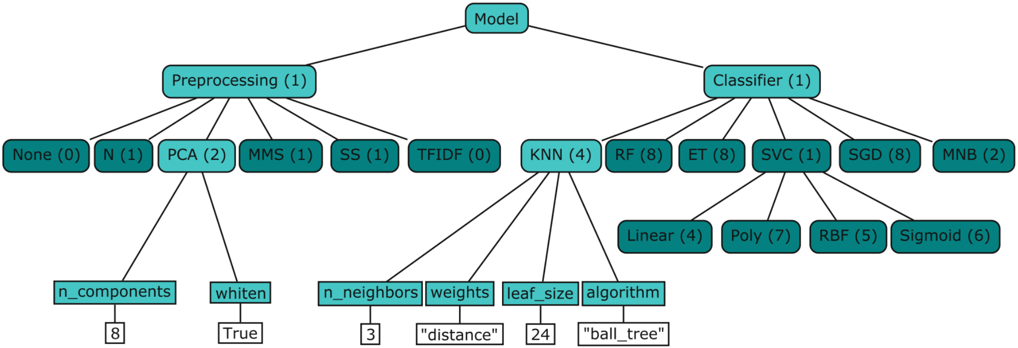
Standard Bayesian optimization problems

- Low-dimensional functions
- Continuous, smooth functions
- Sequential optimization

Extensions

- Structured search spaces: categorical & conditional hyperparameters
- High dimensions
- Parallel evaluations
- Optimization with constraints

Structured Search Spaces: Categorical & Conditional Hyperparameters

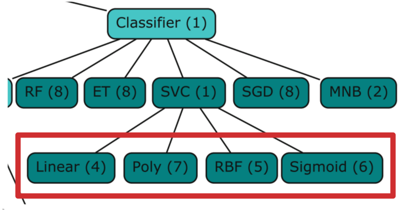


Example of a structured search space (Source: Figure 5.1 of the [AutoML book])

Structured Search Spaces: Categorical Hyperparameters

Properties of categorical hyperparameters:

- Finite, discrete set of values
- No natural order between values
- Potentially different distances between values



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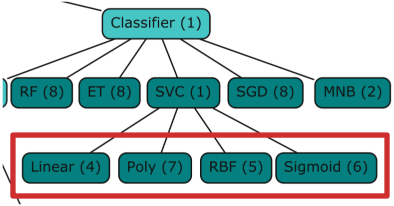


This has to be taken into account by the surrogate model:

- Random Forests natively handle categorical inputs [Hutter et al, 2011]
- *One-hot* encoding provides a simple general solution
- Gaussian Processes can use a (weighted) Hamming Distance Kernel [Hutter 2009]:

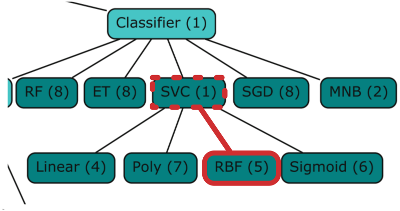
$$\kappa_\theta(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_j) = \exp \sum_{l=1}^{d} (-\theta \cdot \delta(\lambda_{i,l} \neq \lambda_{j,l}))$$

- Neural networks can learn entity embeddings for categorical inputs [Guc et al. 2016]

Structured Search Spaces: Conditional Hyperparameters

Conditional hyperparameters:

- Are only relevant if certain other hyperparameters take on certain values
- Should be ignored by the model if not active



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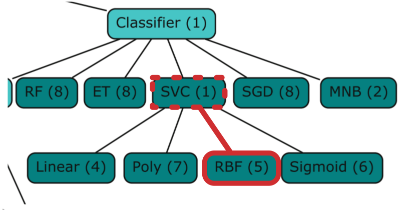

Modelling conditional hyperparameters:

- Setting the values for inactive hyperparameter to a specific value (e.g. 0)
- Random Forests [Hutter et al. 2011] and Tree Parzen Estimators [Bergstra et al. 2011] can natively handle conditional inputs
- There exist several kernels for Gaussian Processes to handle conditional inputs [Hutter et al. 2013] [Lévesque et al. 2017] [Jenatton et al. 2017]

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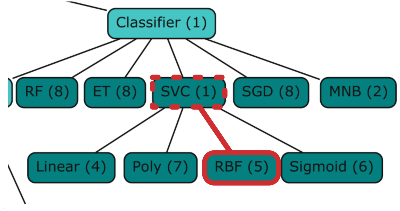

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Overall, structured search spaces are still an active research topic and far from solved

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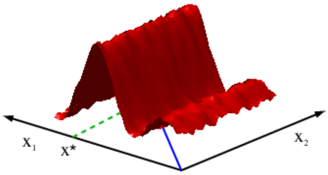

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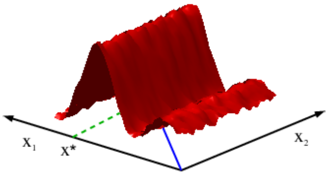
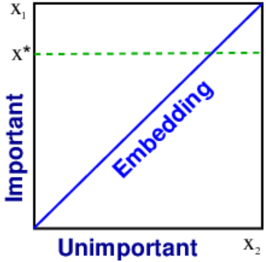
  - Many optimization problems have low effective dimensionality
  - Not all dimensions interact with each other
- Possible solutions
  - Optimize in a lower-dimensional embedding [Wang et al. 2016]
  - Fit additive models on subsets of dimensions [Kandasamy et al. 2015]
  - Use other models; e.g., random forests





Parallel Bayesian Optimization: Multi-point Acquisition Functions

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- To select a batch of q points in parallel, we need to compute the multi-point acquisition function. E.g., for expected improvement:

$$q\text{-}\mathsf{EI}(\boldsymbol{\lambda}_{1,\ldots,q}) = \mathbb{E}\left[c(\hat{\boldsymbol{\lambda}}^{(t)}) - \min_{i=1,\ldots,q} \hat{c}(\boldsymbol{\lambda}_i)\right]$$

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- For EI and KG, this requires *expensive-to-compute* q-dimensional Gaussian cumulative distributions [Ginsbourger et al. 2007], [Wu et al. 2018], [Wang et al. 2019]
- Nevertheless, multi-point acquisition functions can be optimized efficiently with gradient descent via the reparameterization trick [Wilson et al. 2018]

Asynchronous Parallel Bayesian Optimization with Pending Evaluations

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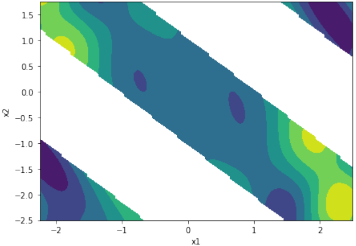
  - Monte Carlo Fantasies
    - Sample pending evaluations from the model
    - Update copy of the model with these samples
    - Compute acquisition function under each updated copy
    - Define acquisition function as an average over these sampled acquisition functions

Bayesian Optimization with Constraints

Several types of constraints

1. Known constraints:
   can be accounted for when optimizing u
2. Hidden constraints: no function value is observed due to a failed function evaluation [Lee and Gramacy 2010]
3. Unknown constraints: there's an additional, but unknown constraint function (e.g., memory used), which can be observed and modeled



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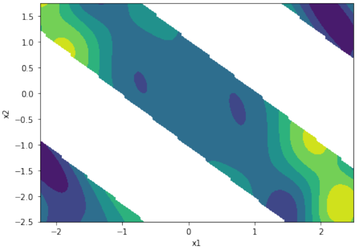

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Most general solution: Expected Constrained Improvement [Lee and Gramacy 2010]:

$$ECI(\boldsymbol{\lambda}) = EI(\boldsymbol{\lambda})h(\boldsymbol{\lambda}),$$

where $h(\boldsymbol{\lambda})$ is the probability that $\boldsymbol{\lambda}$ is a valid configuration.

Further literature in [Frazier 2018] and [Feurer and Hutter 2019].

Even more extensions

Bayesian optimization has been extended to numerous scenarios:

- Multi-task, Multi-fidelity and Meta-learning $\rightarrow$ separate lecture
- Multi-objective Bayesian optimization $\rightarrow$ separate lecture
- Bayesian optimization with safety guarantees [Sui et al. 2015]
- Directly optimizing for ensemble performance [Lévesque et al. 2016]
- Combination with local search methods [Taddy et al. 2009] [Eriksson et al. 2019]
- Optimization of arbitrary spaces that can be described by a kernel (e.g., neural network architectures [Kandasamy et al. 2018] or molecules [Griffiths et al. 2017])
- Many more (too many to mention)

Questions to Answer for Yourself / Discuss with Friends

- Discussion. What would happen if you treat a categorical hyperparameter as continuous (e.g., $\{A, B, C\}$ as $\{0, 0.5, 1\}$), in Bayesian optimization using a Gaussian Process?
- Repetition. Which methods can you use to impute values for outstanding evaluations? What are advantages and disadvantages of each method?
- Discussion. What are worst case scenarios that could happen if you ignore the noise during Bayesian optimization?