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HDS-LEE Course on Hyperparameter Optimization

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What are hyperparameters?

“*In machine learning, a **hyperparameter** is a parameter whose value is set before the learning process begins. By contrast, the values of other parameters are derived via training*.” [Source: Wikipedia]

- Model Hyperparameters
  - Configures the model (model selection)
- Algorithm Hyperparameters
  - Configures learning process (speed and quality)

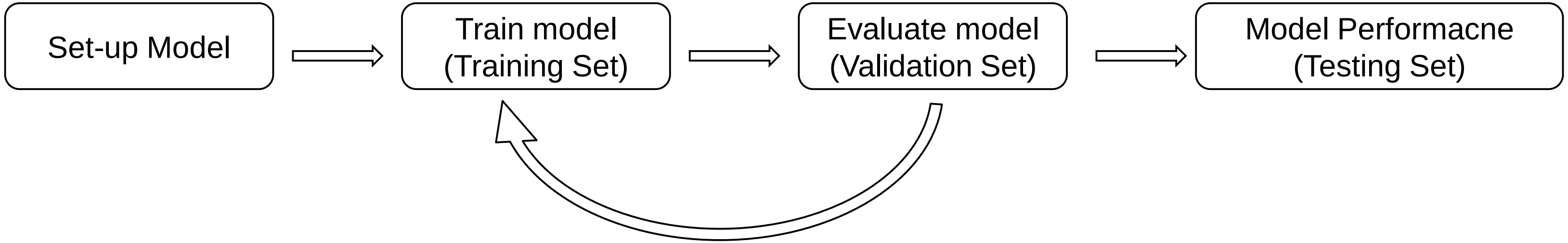
What are hyperparameters?

Examples for Hyperparameters in ML Models (other than NN)

Machine Learning Process	Hyperparameter	Model vs Algorithm HP ?
Logistic Regression	Regularization	Algorithm HP
K-means clustering	K (number of clusters)	Model HP
SVM	ζ (margin distance/Slack variable)	Model HP
Decision Tree	Impurity Metric (i.e. Gini impurity)	Algorithm HP
Random Forest	Number of trees	Model HP
	bootstraping	Algorithm HP
Neural Networks	Number of hidden layers	Model HP
	Mini-batch size	Algorithm HP
Stochastic Gradient Descent	Learning Rate	Algorithm HP

The „Validation Dataset“

- In machine learning tasks: 3 Datasets
  - Training → to train the model
  - Testing → unseen dataset, to evaluate trained model performance
  - …
  - Validation→ Evaluation of trained model for a HP configuration
    Model is evaluated on validation set (substitute to get the expected performance on the true distribution of the data)



Hyperparameter optimization

Find the model hyperparameters with the best score on the valdation set

- Hyperparameters $\vec{x}$
- Objective / loss function $f(\vec{x})$ → Validation score
- We need…
  - A validation set
  - A search space for the hyperparameters χ
  - An optimization algorithm (aka tuning method)

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Exhaustive search

Grid Search
Random Search

Exhaustive search

Grid Search

1. Discretize search space of hyperparameters (Cartesian grid)
2. Train model for every hyper-parameter configuration
3. Evaluate loss for every configuration
4. Select the best configuration

- Trivial to parallelize (train several models at the same time)
- Curse of dimensionality

Random Search

1. Define Search space
2. Randomly draw samples for hyperparameters
3. Evaluate loss

➢ Run number of trials (time budget)

4. Select best option

- If two hyper-parameters are little correlated, optima of each parameter more precisely found

Exhaustive search

- Grid search and random search: blindly try a new configuration in the search space or make an educated guess of where the most interesting configuration might be

Problem: For every different hyperparameter configuration, we have to train the model (training set), make predictions (validation set), and then calculate the validation metric

> Expensive!!! → Model training

Bayesian Inference

Choose the next sample x in an *informed manner* based on previous observations

- Probabilistic model that maps hyperparameters to a probability of objective function score

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Surrogate-based optimization using Baysian inference

„Let machine learning figure out the hyperparameters!“
(Snoek, Larochelle, Adams, NIPS 2012)

Black-Box optimization

$$\vec{x}^* = \arg\min_{\vec{x}\in\chi} f(\vec{x})$$

- We don‘t have access to the true form of the objective function $f(x)$
  - ➢ No gradients
- We can only observe function values
  - ➢ Query $f(x)$ with an input value x and get some output y

Input x $\longrightarrow$ Black-box $f(x)$ $\longrightarrow$ Noisy output y

➢ Sequential strategy which maps collected data to the next query point
Sequential Model-Based Optimization (SMBO)

Sequential Model-Based Optimization (SMBO)

1. Build a model of what the objective function might look like
   - **Surrogate probability (Prior)**: Initial view of the world
2. Find the hyperparameters that perform best on the surrogate
   - **Acquisition/Selection Function**: What are the points that we should evaluate next?
3. Apply these hyperparameters to the true objective function
4. Update surrogate model incorporating the new results
   - **Posterior**: Updated view of the world
5. Repeat

- Keep track of past evaluation results

Surrogate model of the objective function: Prior

- Model:
  - Make predictions
  - Maintain a measure of uncertainty over those predictions
  - Incorporate prior knowledge
- Find a distribution over the possible **functions** $f(x)$ that are consistent with the observed data

➢ **Gaussian Processes**

Gaussian Processes

- Distributions over functions $f(x)$ of which the distribution is defined by a mean function $\mathrm{m}(x)$ and positive definite covariance function $\Sigma = k(X, X')$, with (X, X') all possible pairs in the input domain $\mathrm{x} \in X$, $f(x) \sim \mathcal{GP}(m(x), k(x, x'))$

  where for any finite subset $X = \{x_1, \dots, x_n\}$, the marginal distribution is a multivariate Gaussian distribution

  $$f(X) \sim \mathcal{N}(m(X), k(X, X))$$

- ➢ Multivariate Gauss: captures a finite number of jointly distributed Gaussians
- ➢ Gaussian Process: mean and covariance are defined by a function;
  → Infinite dimensional Gaussian random variable

- Specification of covariance function (kernel) implies a distribution over functions $f(x)$
  - E.g exponential quadratic function (RBF)
  - ➢ Set prior information on this distribution

$$k(x_a, x_b) = \exp\left(-\frac{1}{2\sigma^2}\|x_a - x_b\|^2\right)$$

Gaussian Processes

- Flexible model of continuous functions
  - If you have no Idea about the effects of the hyperparameters
  - consider every possible function that matches the data
- Side note: Inference with GP requires matrix inversion (negligible for expensive model evaluations)

Exploration Strategy

- Policy which maps a model to the next query point
  (criteria for evaluating which hyperparameters to choose next from the surrogate model)

➢ Acquisition/Selection function
  - <u>Probability of improvement</u>: evaluates f at the point most likely to improve upon this value
  - <u>Expected Improvement</u>: evaluates f at the point that, in expectation, improves upon f' (the minimal value of f observed so far) the most
  - <u>Entropy search:</u> minimize the uncertainty we have in the location of the optimal value
  - <u>Upper confidence bound</u>
  - …

- Maximize the acquisition function → Find best new sample point

Exploration – Exploitation Trade-off

Improve on an already good sample point

vs.

Evaluation new points in unexplored areas

- Next point is not necessarity better point (with respect to the objective function), but a point that yields *most information*

Surrogate-based optimization

- Bayesian model-based optimization:
  - Build a probability model of the objective function to propose smarter choices for the next set of hyperparameters
- Sequential model-based optimization
  - Formalization of Bayesian Approach
  - More efficient at finding the best hyperparameters compared to random or grid search.

<u>Problem:</u>

- Sequentiallity
- Sampling strategy = Optimization → Computationally expensive
- *Exploration vs. Exploitation trade-off*

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Evolutionary Strategies

Generic population-based metaheuristic optimization algorithms

Evolution … Survival by adaptation to environment

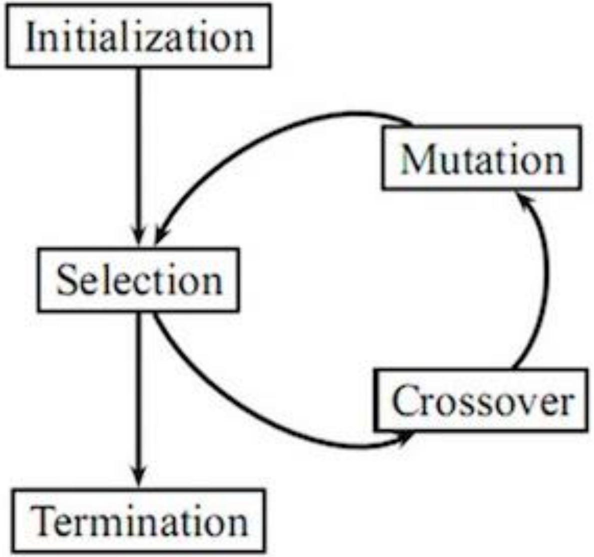
- **Population**
- **Genome**: Properties of each individual
- **Fitness**: measure of degree of adaptation of organism to environment
- **Reproduction**: Adaptation to Selection
  - **Recombination/Crossover**:
    How two individuals combine to form offspring
  - ➢ Inheritence of parental properties
- **Mutation**: introduces new „features“ → Variability
  - Can have positive, negative, or no effect
- **Selection**: the „weakest“ are removed from the gene pool (aka get eaten)

Evolutionary Strategies

```
P = Create_Population(N)

P.Calc_Fitness()

While (it < numberIterations):
    p1, p2 = Choose_Parents(P)
    child =
    Create_Offspring(p1, p2)
    Mutate_Offspring(child)
    fitness =
    Rate_Offspring(child)
    P.add(child, fitness)
    Remove_Unfittest(P)
    Next
```



Evolutionary Strategies

- No assumption about the underlying “fitness landscape”
  → ability to approximate solutions to all types of problems
- Populations evolving in different niches can independently develop different (but similar) solutions to the same problem
- Solutions may reach a local optimum
- But: possibility that populations leave local optimum and find better solution
- Fitness of individuals may depend on the other individuals in the population
- Historically four “flavors”: genetic algorithms, evolutionary algorithms, genetic programming, evolutionary programming
  - differ in genetic representation, implementation details, nature of particular applied problem

Putting it all together…

Frameworks offering Hyperparameter optimization

Framework	Description	Grid/ Random	SMBO	Evolutionary
scikit-learn	Python package	✓	(✓) Auto-sklearn	(✓) sklearn-deap
Tune	Python library for distributed HP tuning	✓		✓
Talos	For Keras	✓		
Keras Tuner	For Keras / Tensorflow	✓ (Random)	✓	
hyperopt (hyperas, hyperopt-sklearn)	Python packages	✓	✓	
Katib	Kubernetes-native system	✓	✓	
Optuna	Python package for black box optimization		✓	
tuneRanger	R package for tuning random forests using MBO		✓	
SMAC	Python/Java library		✓	
deap	Python framework for general evolutionary computation			✓
BOCS	Matlab package for minimizing a black-box function		✓	

References & Acknowledgements

- Ajay Uppili Arasanipalai “How To Make Deep Learning Models That Don’t Suck” https://nanonets.com/blog/hyperparameter-optimization/
- Matthew Hoffman „Bayesian Optimization“, UAI 2018 https://www.youtube.com/watch?v=C5nqEHpdyoE
- Oskar Knagg „An intuitive guide to Gaussian processes” https://towardsdatascience.com/an-intuitive-guide-to-gaussian-processes-ec2f0b45c71d
- Görtler, Kehlbeck ‚Deussen „ A Visual Exploration of Gaussian Processes” https://distill.pub/2019/visual-exploration-gaussian-processes/
- Manuel Ernst „Evolutionary Algorithms 101“ otsconf 2015, https://www.youtube.com/watch?v=t3XofbN2HgE
- Alois Bissuel „Hyper-parameter optimization algorithms: a short review” https://medium.com/criteo-labs/hyper-parameter-optimization-algorithms-2fe447525903
- Rakesh Sukumar “Introduction to Automatic Hyperparameter Optimization with Hyperopt” https://medium.com/analytics-vidhya/introduction-to-automatic-hyperparameter-optimization-with-hyperopt-e0b9c84d1059
- Wikipedia, XKCD, Sci-Kit Learn documentation
- …

No Free Lunch Theorem

No algorithm exists which outperforms every other algorithm for every problem

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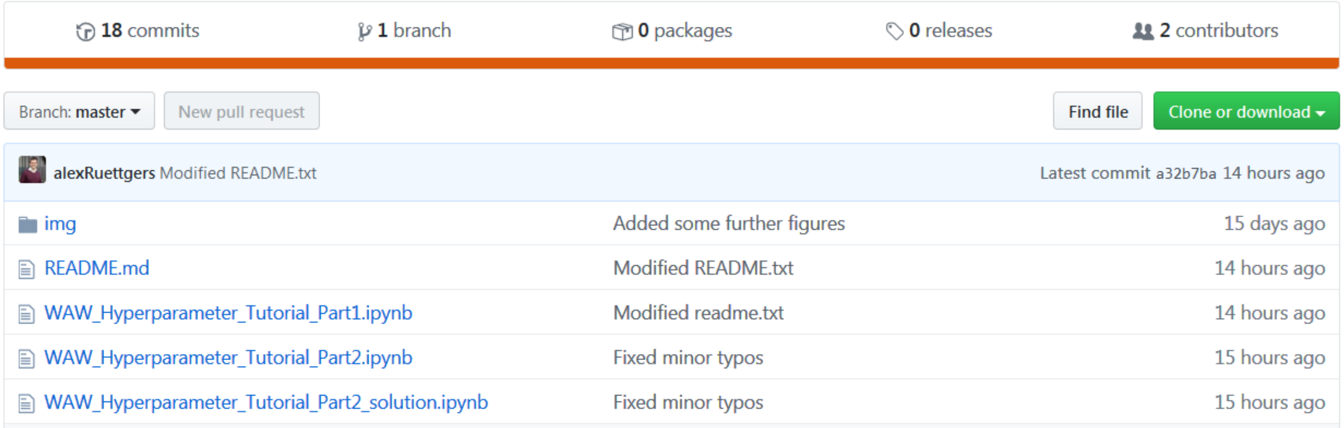
Hyperparameter Optimization

Part II: hands-on course

Excercises

- **Aim:** hyperparameter optimization of a regression problem:
  - **manual approach** (1st Jupyter notebook)
  - **machine-assisted approach** (2nd Jupyter notebook)

- **Download:** https://github.com/DLR-SC/Hyperparameter_tutorial



1st Jupyter notebook

(https://github.com/DLR-SC/Hyperparameter_tutorial/*/WAW_Hyperparameter_Tutorial_Part1.ipynb)

The aim of this notebook is the following:

- Introduction of the Boston house price regression problem.
- A (very) short introduction of Keras.
- Manual approach to optimize hyperparameters (i.e. one exercise).

Excercise 1:

- Play around with the different hyperparameters to build a better regression model
- Can you achive a better result as `build_better_model()`

```
from keras import regularizers

def build_better_model_task():

    model = models.Sequential()

    # replace 'number_of_neurons' with a value of your choice, e.g. 8, 16, 32, 64, 128
    number_of_neurons = 32
    model.add(layers.Dense(number_of_neurons, activation='relu', input_shape=(train_data.shape[1],
)))
    # maybe add a second hidden layer?
    # model.add(layers.Dense(XXX, activation='relu'))
```

2nd Jupyter notebook

(https://github.com/DLR-SC/Hyperparameter_tutorial/*/WAW_Hyperparameter_Tutorial_Part2.ipynb)

- The aim of the 2nd notebook is:
  - Introduction of Talos and machine-assisted hyperparameter optimization
  - Give general guidelines on hyperparameter optimization
- Due to the limited computing time (i.e. we want to have lunch at 12pm) you will consider a „toy problem“ with all its drawbacks (low number of training samples, …)
- Instead of focusing too much on the specific problem, the important aspect is understanding the machine-assisted approach itself.
- Try to solve the exercises yourself and do not directly look at *WAW_Hyperparameter_Tutorial_Part2_solution.ipynb*

Thank you for your attention and enjoy!

Wrap-up: Guidelines on machine-assisted hyperparameter optimization

- Hyperparameter optimization is an iterative process.
  - find out the important parameters for your specific problem (i.e. that correlate with performance metric)
  - the parameter boundaries should decrease with every iteration
- Avoid a full grid parameter search. Use other search strategies such as random search instead.
- Use an additional validation set for finding adequate hyperparameters, not the test set.
- Important to first get some kind of understanding which model architecture might be adequate.

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Thank you for your participation!

We hope that you have enjoyed this tutorial.

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