浙江大学爱丁堡大学联合学院
ZJU-UoE Institute

Lecture 17 - Hyperparameter tuning

Nicola Romanò - nicola.romano@ed.ac.uk

Learning objectives

- Give examples of hyperparameters and explain what are the issues with hyperparameters in deep learning.
- Discuss and compare different methods of tuning hyperparameters.
- Implement these methods in Python.

Introduction

What are hyperparameters?

Hyperparameters are values that are used by a ML model to control the learning process.

Examples include:

- Structural parameters
    - Number of layers
    - Number of units in each layer
    - Number of filters, their kernel size, stride and padding
    - Type of activation function
    - ...
- Learning parameters
    - Type of optimizer
    - Learning rate α
    - Schedule of learning rate
    - Loss function
    - Dropout rate
    - Weight regularization
    - ...
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Other **parameters** such as weights and biases are learned by the network during training; these will be affected by the choice of hyperparameters.

Problems with choosing hyperparameters

- Deep network have an extremely large number of hyperparameters.
- The search space is extremely large but often the "good solution" only covers a small region of this space.
- We cannot try all possible combinations.
- No definitive strategy exists.

So... how do we choose hyperparameters?

Choosing hyperparameters

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Manual methods

What did others do?

We can look at the hyperparameters of published models that performed similar tasks and start from there.

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Cons

- It might be difficult to find a model doing exactly the same task.

Manual tweaking

- Start with a reasonable choice of hyperparameters
- Modify one parameter at a time to improve model performance

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Pros

- It generates high-quality results, when done by an expert.
- Humans can integrate knowledge from several sources and previous experience to make the best changes to hyperparameters.

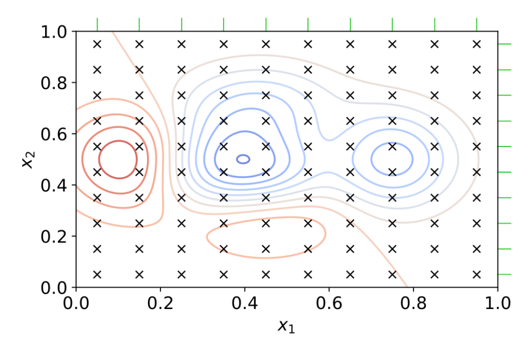
Cons

- It is not obvious to find a good starting point.
- It is extremely time-consuming.
- There is no guarantee to find the optimal model.
- Difficult process to replicate.

Choosing hyperparameters

Automated methods

Grid search is the simplest method to use and is an exhaustive search over a defined parameter search space.



Grid search - In this example we tune hyperparameters x_1 and x_2 in the range [0, 1] - source Wikipedia

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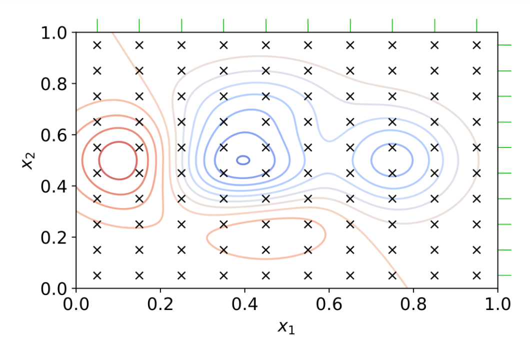

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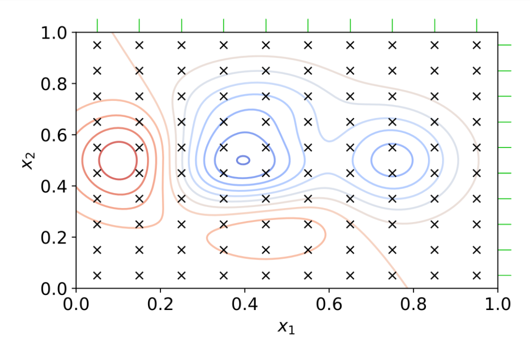

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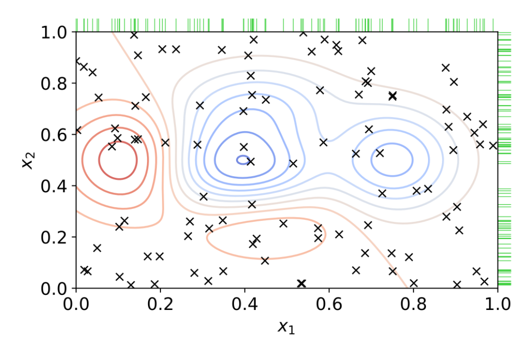
Cons

- It is computationally expensive -> early stop and parallelism help.
- Need to choose a range.
- It does not scale well; 5 hyperparameters with 10 values each, give 10^5 combinations.
- A lot of wasted computation time to sample low-accuracy combinations.

We will now see a simple implementation of grid search in Python.

See the attached `GridSearch.ipynb` notebook.

In **random search**, we randomly sample hyperparameters from the search space, rather than exploring a fixed grid.



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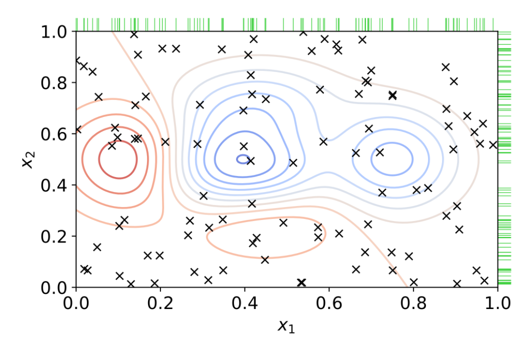

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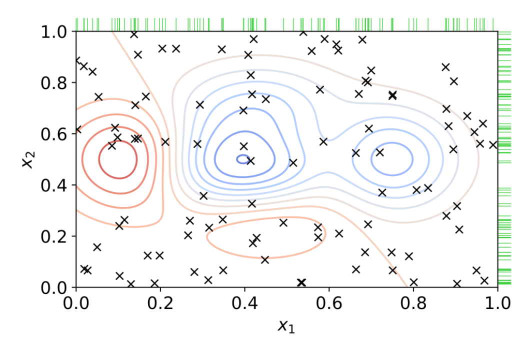

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Pros

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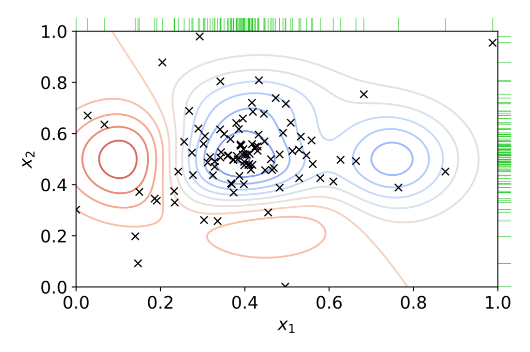
- Helps when dealing with large search spaces.

Cons

- Less reproducible.
- Not guaranteed to hit the optimum.
- Need to choose a range for the hyperparameters.

Bayesian optimization, builds a probability model of the objective function; it uses this model to select the most promising set of hyperparameters. At each iteration, it updates its underlying model, and repeats the process.



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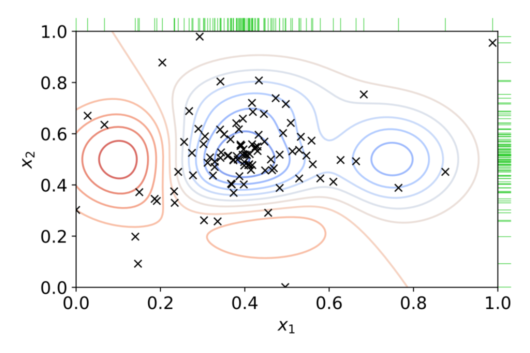

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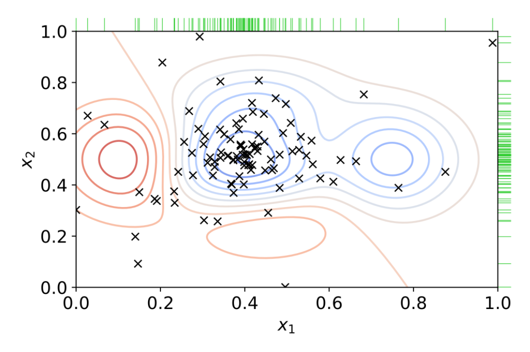

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- Performs better than grid and random search.

Cons

- Can be very computationally expensive when using a lot of hyperparameters.
- Complex to implement.

Early-stopping methods work by early stopping of evaluations on combinations of parameters that are not promising.

Successive Halving algorithm

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Problem: do we consider a small N with a large budget for each configuration, or a large N with a small budget?

Hyperband extends the Successive Halving algorithm by running multiple *brackets* of hyperparameters.

It performs a grid search on the number of configurations N that we are going to choose.

It can be 10-20x faster than Bayesian optimization.

KerasTuner

The **Keras Tuner** library (install via `pip install keras-tuner`) provides a simple way to tune hyperparameters in a Keras model.

It implements the random search, Bayesian optimization and Hyperband strategies.

In order to use Keras Tuner we need to have a function that generates and returns our Keras model. We will pass that function to the tuner class of our choice.

KerasTuner example

```
import tensorflow.keras as keras
import keras_tuner as kt

# hp is an object that contains all the hyperparameters
# it will be automatically passed by the tuner
def build_model(hp):
   model = keras.Sequential()
   # Create an integer hyperparameter, going from 10 to 100
   # We can also have hp.Float, hp.Choice, hp.Bool
   n_units = hp.Int('units', min_value=10, max_value=100, step_size=10)
   model.add(keras.layers.Conv2D(n_units, (3, 3), activation='relu',
       input_shape=(256, 256, 1)))
   ...
   return model
```

```
rs = kt.tuners.RandomSearch(build_model,
       objective='val_accuracy',
       max_trials=10,
       directory="output_dir")

# Instead of calling model.fit we call tuner.search
rs.search(x_train, y_train,
       x_test, y_test,
       epochs=10, batch_size=32)

best_hyperparameter = rs.get_best_hyperparameters(1)[0]
best_model = rs.get_best_models(1)[0]
```

We can now use a model with the best configuration for our task!