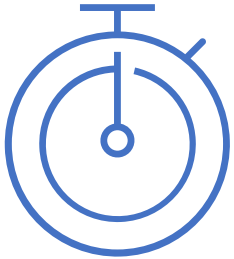
Hyperparameter Tuning

Bert Gollnick

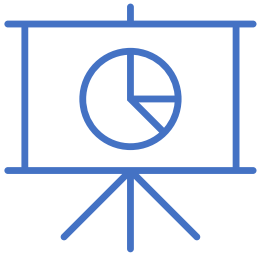
Hyperparameter Tuning

Introduction

Reasons for tuning parameters



training / inference time



improving results

convergence

Hyperparameter Tuning

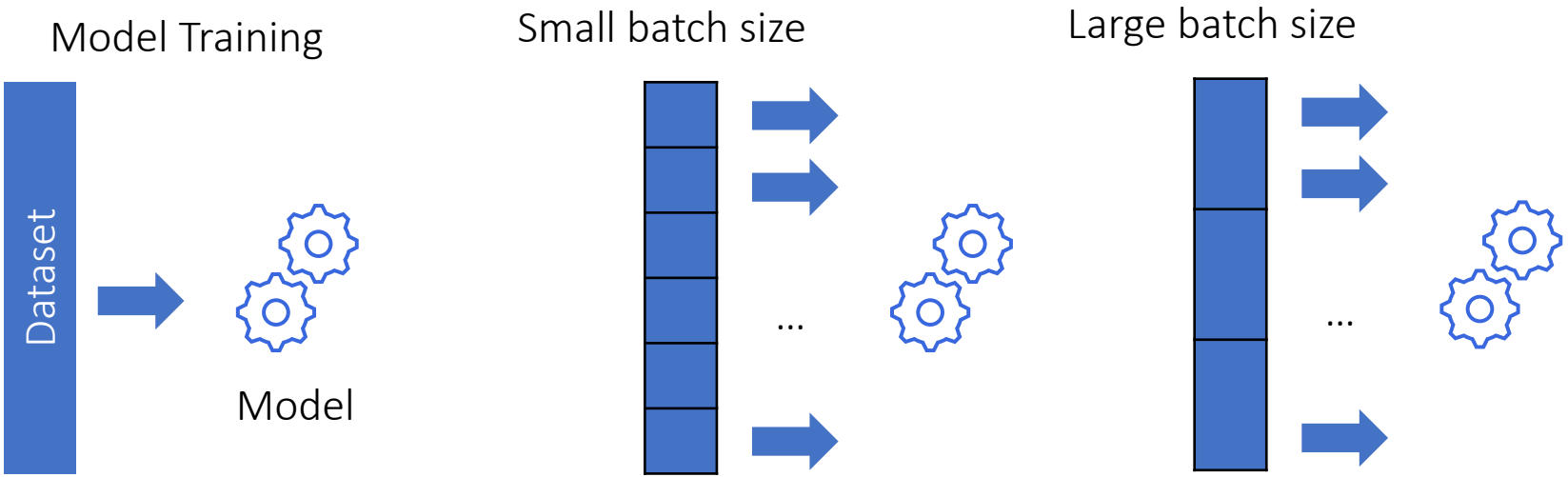
Tunable Hyperparameters

- Hyper-parameters huge impact on model performance
- Intuition…check multiple combinations of parameters and pick the best
- available packages: RayTune, Optuna, skorch
- Hyperparameters

network topology	number of nodes	layer types	activation functions	…
network objects	loss function	optimizer		
model training	learning rate	batch size	number epochs	

Hyperparameter Tuning

batch size



Best practice often: 32

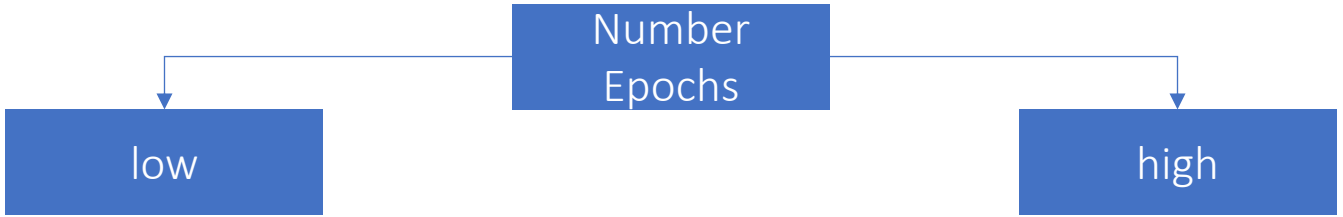
↓ GPU utilization ↑

↑ Iterations ↓

↑ Training-Stability ↓

Hyperparameter Tuning

Epochs



low		high
↓	Training Time	↑
-	Inference Time	-
↓	Model performance	↑ (but dimishing)
↑	Stability	↓ (instability possible)

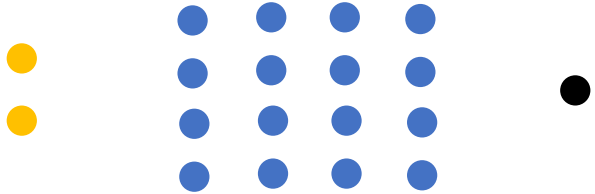
Hyperparameter Tuning

Hidden Layers

Few Hidden Layers

Input Layer
Hidden Layer
Output Layer

Many Hidden Layers



Input Layer
Hidden Layer
Output Layer

↓	Ability to learn complex patterns	↑
↓	Training Time	↑
↓	Inference Time	↑
↓	Risk of Overfitting	↑

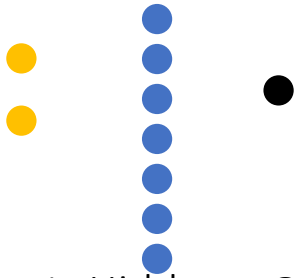
Hyperparameter Tuning

Nodes within a Layer

Few Nodes

Input Layer | Hidden Layer | Output Layer

Many Hidden Layers



Input Layer | Hidden Layer | Output Layer

↓	Ability to learn complex patterns	↑
↓	Training Time	↑
↓	Inference Time	↑
↓	Risk of Overfitting	↑

Hyperparameter Tuning

Types of Search

- grid search
  - define search space (set of parameters with limiting values)
  - evaluate each possible combination
  - e.g. learning_rate = [0.1, 0.2],
    batch_size = [2, 4, 8]
  - good for checking well-known parameters

Run	learning_rate	batch_size
0	0.1	2
1	0.2	2
2	0.1	4
3	0.2	4
4	0.1	8
5	0.2	8

- random search
  - picks a point from configuration space
  - good for discovery

Hyperparameter Tuning

skorch

- skorch…A scikit-learn compatible neural network library that wraps PyTorch.
- Repo: https://github.com/skorch-dev/skorch
- Works like a scikitlearn wrapper for PyTorch
- Can be integrated into
  - sklearn pipeline
  - grid search


```
from sklearn.model_selection import GridSearchCV


# deactivate skorch-internal train-valid split and verbose logging
net.set_params(train_split=False, verbose=0)
params = {
    'lr': [0.01, 0.02],
    'max_epochs': [10, 20],
    'module__num_units': [10, 20],
}
gs = GridSearchCV(net, params, refit=False, cv=3, scoring='accuracy', verbose=2)

gs.fit(X, y)
print("best score: {:.3f}, best params: {}".format(gs.best_score_, gs.best_params_))
```