Practical Methodology

Baraa Hassan and Keanu Buschbacher February 9, 2021

- [Performance Metrics](#page-3-0)
- 2 [Default Baseline Models](#page-11-0)
- **3** [Determine Wether to Gather More Data](#page-15-0)
- 4 [Debugging Strategies](#page-20-0)
- **5** [Selecting Hyperparameters](#page-21-0)
	- **[Manually](#page-24-0)**
	- **[Automatically](#page-30-0)**
	- [Model-based](#page-36-0)

6 [Example: Multi-Digit Number Recognition](#page-37-0)

Model Performance

Question

How to test your model performance?

Is it using:

2 **Error Rate**?

Cost/Loss Function:

It gives you a numerical evaluation of how your model output is deviated from the target output, on the current state (train/dev./test).

Error Rate

It shows the rate of the dissimilarity between the model output and the target output.

The Cost Function's output is not an interpretable number for the accuracy, in the same time the Error Rate is not enough to address the performance of the model.

Let's see in the examples why.

We can have 4 scenarios for this system output:

Email Spam Detection System has 2 kinds of mistakes:

- Classifying legitimate message as a spam
- Allow spam message to appear in the inbox

In case of performance evaluation the first mistake is catastrophic and needed much more to be prevented than the second one

Our classifier is a binary classifier for a rare disease that happens once in a million people.

Our classifier can achieve accuracy of 99.9999%, by only output false for all input cases.

Although the classifier doesn't achieve the expected goal (detecting the patients catching this disease)

Confusion Matrix:

You should choose your performance metrics (that address your model accuracy) according to your expected goal from the model.

- To achieve our goal in Spam Detection System:
	- we can compute FPR (Type 1 Error) = $\frac{FP}{FP+TN}$ (to evaluate the first catastrophic mistake).
- To achieve our goal in Rare Disease Classifier:
	- we can compute Recall (True Positive Rate) = $\frac{TP}{TP+FN}$ (to get how many real patient were detected).
	- we can compute Precision (Positive Prediction Value) = $\frac{TP}{TP+FP}$ (to get how much of the detected values were right).

Precision and Recall are inversely proportional; in case of all the output are non-patient you will get a good precision but zero recall, and vice versa.

To get the mean of the two metrics you can compute F1 = ²∗*Precision*∗*Recall Precision*+*Recall* .

There are many different metrics that you can use to achieve your goal:

- For Classification:
	- FPR
	- FNR
	- Recall
	- Precision
- For Regression:
	- Mean Absolute Error(MAE)
	- Mean Squared Error(MSE)
	- Root Mean Squared Error(RMSE)

End-to-end System Development

Determine Wether to Gather More Data

Question When to decide to collect more data ?

Taking into consideration the cost of collecting more data.

In the next flowchart we will discuss when to collect more data

Wether to Gather More Data Model Debugging

Wether to Gather More Data Model Debugging

[\[NG, 2018\]](#page-45-0)

Analysing Your Software Defects

To debug your train model method to check if you have software defect or under-fitting problem:

- Visualize the model in action
- Visualize the worst mistakes
- Fit a tiny dataset
- Compare back-propagated derivatives to numerical derivatives
- Mintor histograms of activations and gradient

Sometimes it is hard to find the source of the problem; as the machine learning models are composed of adaptive parts, if one went wrong the other parts can adapt and achieve roughly acceptable performance.

Selecting Hyperparameters

Hyperparameters control different aspects of how your model behaves.

- 1 **Costs**: time and memory requirements during training *(and inference)*
- **Quality:** performance during training process and on new inputs

Some parameters actually influence both!

Goal

Find hyperparameters that minimize the generalization error, s.t. they do not exceed our runtime and memory requirements.

There are two kinds of strategies:

- **1** Manual hyperparameter tuning
	- No additional (explicit) computational complexity
	- Requires knowledge about hyperparameters...
- 2 Automatic hypterparameter tuning
	- Less need to understand hyperparameters
	- But computationally costly...

We want the capacity of our model to match the complexity of our task. The effective model capacity consists of three factors:

Representational capacity What functions can my model represent?

Cost function capacity Can the learning algorithm minimize my cost function?

Regularization capacity How strong do training and cost function regularize my model?

Baraa Hassan and Keanu Buschbacher Practical Methodology 25 / 47

Effects of Hyperparameters

Manual Hyperparameter Tuning

Source: CS231n Convolutional Neural Networks for Visual Recognition.¹

The learning rate is a very important hyperparameter.

- too large: gradient descent can increase training error
- too low: slower training, more likely to get stuck in local minima

The model capacity is highest if the learning rate is set correctly!

¹ <https://cs231n.github.io/assets/nn3/learningrates.jpeg> Baraa Hassan and Keanu Buschbacher Practical Methodology 28 / 47

Common Hyperparameters

Manual Hyperparameter Tuning

- Training error too large? **Increase model capacity!**
	- Are you using regularization? \rightarrow Maybe use a bit less.
	- Is your optimization algorithm not performing correctly? \rightarrow Fix it.
	- None of the above? \rightarrow # Hidden Units Kernel size Padding

- Training error is fine, but test error is too large? We need to reduce the generalization gap. **Decrease model capacity!**
	- Add regularization capacity \rightarrow Weight decay Dropout
	- Collect more training data

Choosing hyperparameters is also an optimization: find hyperparameter values that optimize an objective function, e.g. validation error.

Grid Search Automatic Hyperparameter Tuning

Grid Search

- For three or fewer hyperparameters
- Train on every combination of hyperparameter values
- Use best configuration according to validation error

² Bergstra, J., Bengio, Y.: Random search for hyper-parameter optimization. Journal of Machine Learning Research 13, 281–305 (2012) Baraa Hassan and Keanu Buschbacher Practical Methodology 32 / 47

How to pick the hyperparameter values?

 \rightarrow Logarithmic scale: {0.1, 0.01, 10⁻³, 10⁻⁴, 10⁻⁵}

Random Search Automatic Hyperparameter Tuning

Source: Bergestra et al. (2012).³

3
Bergstra, J., Bengio, Y.: Random search for hyper-parameter optimization. Journal of Machine Learning Research 13, 281–305 (2012) Baraa Hassan and Keanu Buschbacher Practical Methodology 34 / 47

Random Search Automatic Hyperparameter Tuning

Source: Bergestra et al. (2012).⁴

Random Search

- Hyperparameter values sampled from random distribution
- Useful also for more than three hyperparameters
- Explores wider parameter space

² Bergstra, J., Bengio, Y.: Random search for hyper-parameter optimization. Journal of Machine Learning Research 13, 281–305 (2012) Baraa Hassan and Keanu Buschbacher Practical Methodology 35 / 47

Random search can be exponentially more efficient than grid search: it reduces validation error much faster w.r.t number of trials.

Trials are not "wasted" if two hyperparameters give the same result.

Example: #Units \in {50, 100} lead to same validation error:

Table: Grid search trials

Table: Random search trials

If gradient $\frac{\partial E}{\partial h}$ is available, we can just follow this gradient.

If not, we can train a model to optimize validation error with our hyperparameters as decision variables.

 \rightarrow Estimates validation error and uncertainty using Bayesian regression

Examples:

- Spearmint [\[Snoek et al., 2012\]](#page-45-1)
- TPE [\[Bergstra et al., 2011\]](#page-45-2)
- SMAC [\[Hutter et al., 2011\]](#page-45-3)

Real-life Application of Practical Methodology

Example: Multi-Digit Number Recognition Street View Transcription System

Goal

Assign digits to pictures of street numbers if model confidence $p(y|x) \ge t$ for some threshold *t*.

Figure: Street view transcription system. [\[Goodfellow et al., 2014\]](#page-45-4)

Baraa Hassan and Keanu Buschbacher Practical Methodology 39 / 47

Example: Multi-Digit Number Recognition

- **1** Choose performance metrics
	- Choose the metrics according to the project's business goal!
	- Here: maps require high, human-level accuracy
	- This meant a high threshold to accept results of the model

Metric is therefore: **coverage**, i.e. percentage of confidences above the threshold (goal: >95%)

Example: Multi-Digit Number Recognition

2 Establish baseline model

- Try to iteratively improve the model!
- Here: *n* different softmax units to predict *n* characters
- each unit trained independently
- $p(y|x)$ obtained by multiplying units together

Improvement idea: **use output layer/cost function that computes log-likelihood instead**

Coverage was still below 90%. Is the problem under- or overfitting?

- **3** Debug model
	- Here: training and test error were identical \rightarrow underfitting or problem with training data
	- Visualize model's worst mistakes

Example: Multi-Digit Number Recognition

Coverage was still below 90%. Is the problem under- or overfitting?

- Debug model
	- Here: training and test error were identical \rightarrow underfitting or problem with training data
	- Visualize model's worst mistakes:
		- \rightarrow Some images were cropped too tightly!

2 vs 239

Solution: **add margin of safety around crops** (+10% coverage)

Example: Multi-Digit Number Recognition

4 Adjust hyperparameters

- Here: train and test error remained equal \rightarrow underfitting
- Model was made larger

Theme by @fseiffarth:

<https://github.com/fseiffarth/LatexBeamerThemeUniBonnStyle>

References

James Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. In J. Shawe-Taylor, R. Zemel, P. Bartlett, F. Pereira, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems*, volume 24, pages 2546–2554. Curran Associates, Inc., 2011. URL [https://proceedings.neurips.cc/paper/2011/file/](https://proceedings.neurips.cc/paper/2011/file/86e8f7ab32cfd12577bc2619bc635690-Paper.pdf) [86e8f7ab32cfd12577bc2619bc635690-Paper.pdf](https://proceedings.neurips.cc/paper/2011/file/86e8f7ab32cfd12577bc2619bc635690-Paper.pdf).

Ian J. Goodfellow, Yaroslav Bulatov, Julian Ibarz, Sacha Arnoud, and Vinay Shet. Multi-digit number recognition from street view imagery using deep convolutional neural networks, 2014.

Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In Carlos A. Coello Coello, editor, *Learning and Intelligent Optimization*, pages 507–523, Berlin, Heidelberg, 2011. Springer Berlin Heidelberg. ISBN 978-3-642-25566-3. Andrew NG. Machine learning yearning. *URL¡*

https://www.deeplearning.ai/programs/, 1, 2018.

Jasper Snoek, Hugo Larochelle, and Ryan Adams. Practical bayesian optimization of machine learning algorithms. *Advances in Neural Information Processing* Baraa Hassan and Keanu Buschbacher **2012.** Baraa Hassan and Keanu Buscher Practical Methodology 46/47

Thank You for Listening!