Machine Learning

Introduction, Supervised Learning, and Overfitting

Aleksandr Petiushko

ML Research

July 22nd, 2023

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1. Introduction
2. Course logistics and syllabus

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1. Introduction
2. Course logistics and syllabus
3. Historical reference
4. Setting of basic machine learning tasks

Content

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Intro

About the lecturer[1]

- Aleksandr Petiushko, PhD in theoretical CS (2016)
- Lecturer in Lomonosov MSU / MIPT for Machine Learning, Computer Vision, Deep Learning Theory, Python for an ML Researcher since 2019
- Former Huawei Chief Scientist (Scientific Expert), AIRI Director of Key Research Programs (Leading Scientific Researcher)
- Currently at Nuro, leading the ML Research

[1] Homepage: `https://petiushko.info/`

Intro

Time to introduce yourselves: what are your hobbies, motivation in ML, etc

Sofia Plagiarism Policy[2]

- It covers parts "*sourced from AI*"
  - **First offense**: students need to rewrite assignment
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  - And *probably* some others, but not so obvious
  - Grades for them: 0

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- Current situation: one full assignment + one discussion were written by using xGPTx (plus some specific questions inside assignments)
  - And *probably* some others, but not so obvious
  - Grades for them: 0
- Current approach: to check your text via OpenAI tool: `https://platform.openai.com/ai-text-classifier` and get the answer "**very unlikely**", "**unlikely**", or "**unclear if it is**"
  - Answers "**possibly**", or "**likely**" will be treated as plagiarism

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  - It can really hallucinate some things which are just untrue
  - It can produce very different information in comparison to the source used to ask question (e.g., book chapter)

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- Since **Module 4** your discussion answer like "I agree because of bla-bla-bla" won't be graded — they do not provide any value

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- Only the answers with some non-trivial arguments that contradict the initial post will be considered as graded ones

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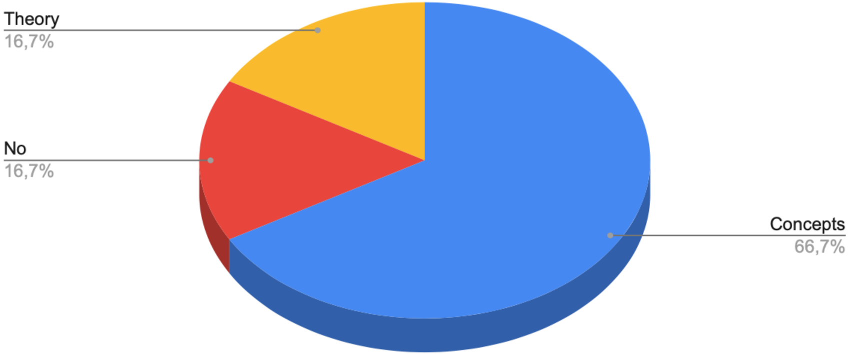
- Preliminary grading scale:

Grade	Percent accumulated
A	90-100 %
B	75-89 %
C	60-74 %

Results of Survey: Level of Math



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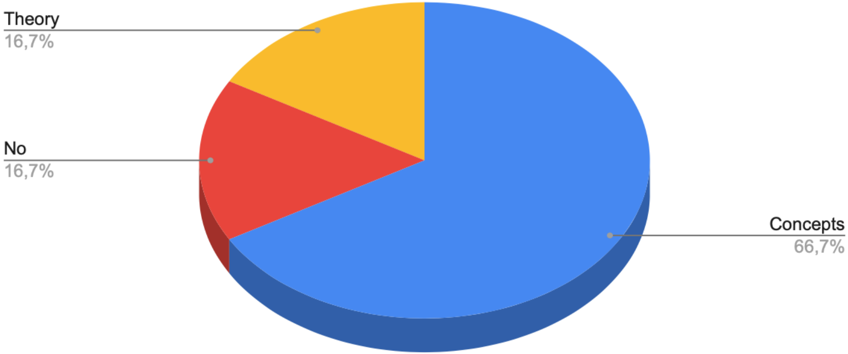

<u>Conclusion</u>:

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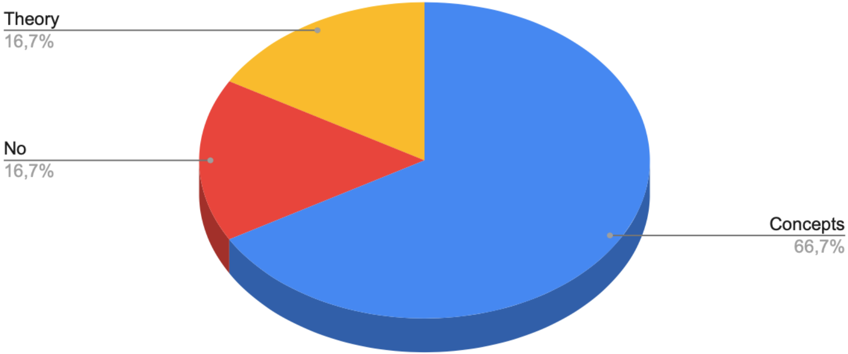

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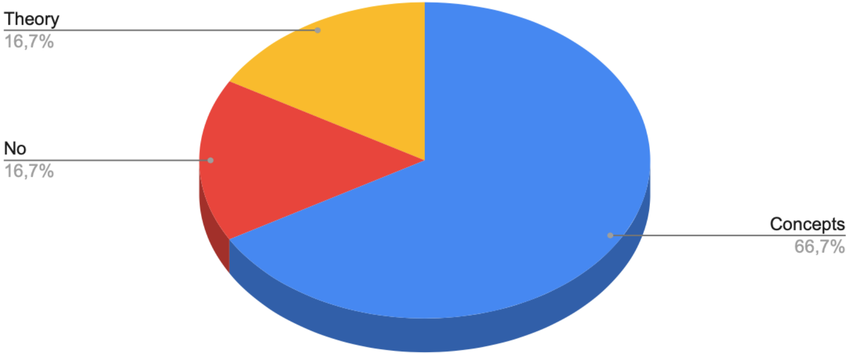

<u>Conclusion</u>:

- Will be some math inside covering the basics
- Will be links to more advanced stuff

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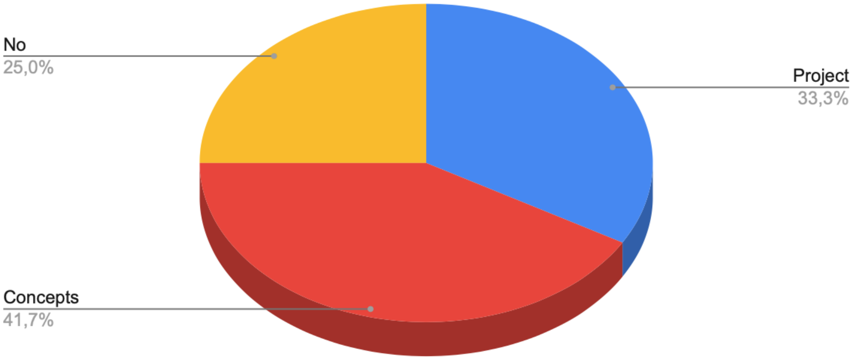

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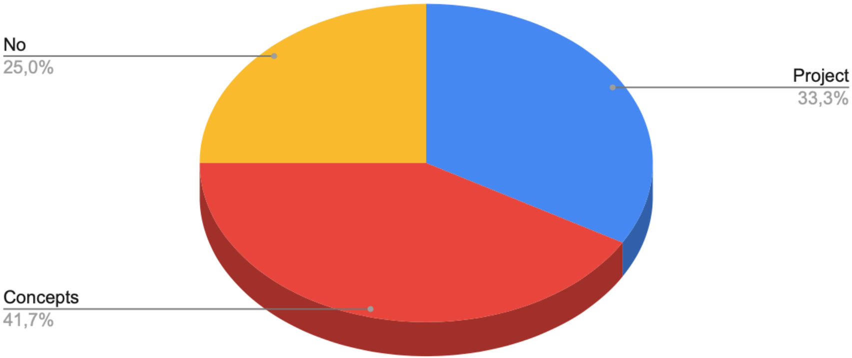

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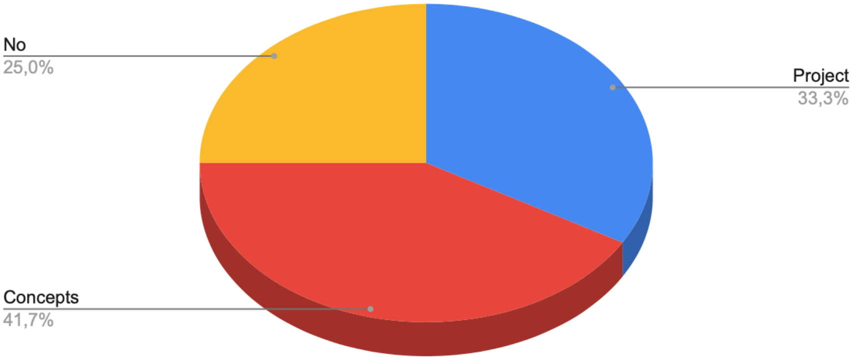

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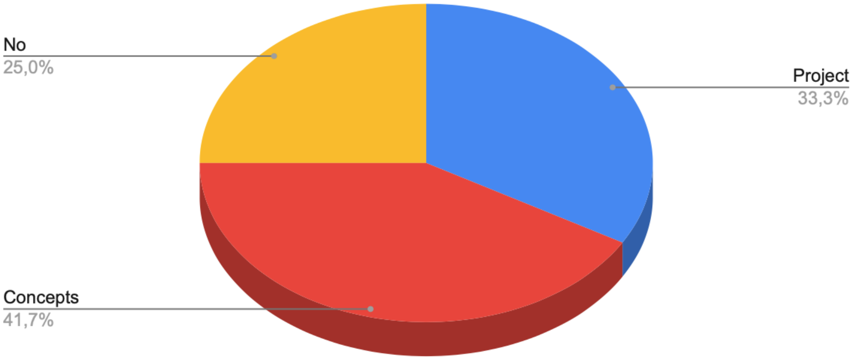

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- Project will be discussed on the personal basis / wish

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  - **Math**: for research and design of ML algorithms
  - **Programming**: usage and tuning of ML algorithms
- Hope we could touch a little both

Github

- Course page: `https://github.com/fatheral/sofia-ml-2023-1`
- The on ground lectures will be uploaded there

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- Able to perceive the information, analyze it, make decisions based on this analysis

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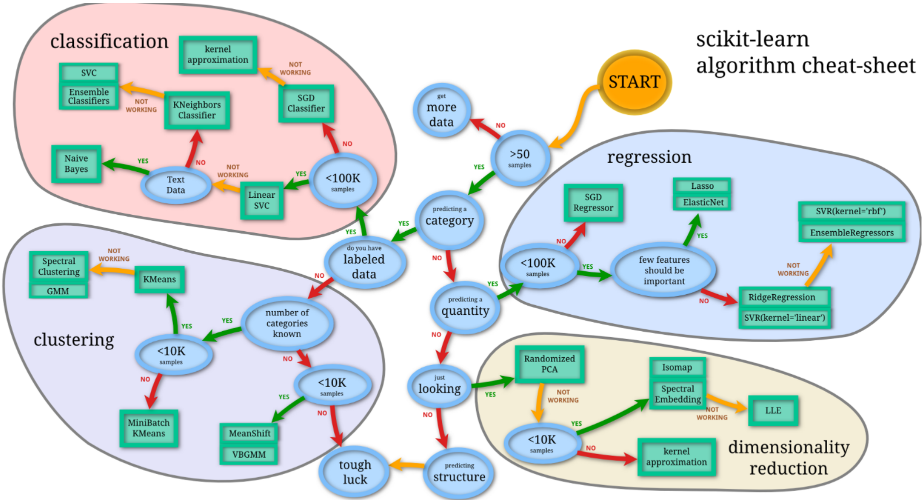
Artificial Intelligence

- (Strong) The same as natural intelligence, but computer is instead of human
- (**Weak**) Algorithm which is able to train using the input data in order to do tasks afterward — instead of human

Scikit-Learn[3] Roadmap



[3] https://scikit-learn.org/stable/tutorial/machine_learning_map/

(Tentative) future content

Theoretic part

- Quality metrics
  - Precision / Recall, TPR / FPR, ROC, AUC, Cross-Validation, . . .

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- Ensembles
  - Bootstrapping, Bagging, Boosting, ...

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Practice part

- Data processing and analysis by Python
  - Scikit-Learn, Numpy, ...

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General definition

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In 1997 Tom M. Mitchell introduced more formal definition of a machine learning algorithm.

Formal definition

A **computer program** is said **to learn** from examples E for some set of problems T and a quality metric P if its performance on problems from T, as measured by P, is improved by using examples E.

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- **1906**: Andrey Andreyevich Markov develops the apparatus of Markov chains, which in **1913** he uses to study the text “Eugene Onegin”. Markov chains are used to generate and recognize signals.

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- **2022**: OpenAI, a (not so) non-profit research company, provided the breakthrough in LLMs: ChatGPT.

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Time for questions

Machine Learning Paradigms

Definitions

- X — set of objects
- Y — set of (correct) answers/labels
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- Reinforced
  - Action generation based on interaction with the environment

Problem setting for supervised learning

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  - How answers are given
  - What does it mean that one dependency approximates another

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Regression Tasks

$Y = \mathbb{R}$ or $Y = \mathbb{R}^n$

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Definition

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Loss functions for regression problems

$L(a, x) = (a(x) - y)^2$ — squared error

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Why even bother with this?

- There are many machine learning algorithms and it is important to understand which one is more applicable to a particular task
- Even within the same model, there can be many (hyper)parameters to choose from

How to choose the best model

Naive approach

Train models with different parameters and choose the best one on the test

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Disadvantages of the naive approach

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So... what to do?

In order not to implicitly learn from test data — you need to use **cross-validation**

Cross Validation

General idea

The main idea of cross-validation is to split the training set into two non-overlapping sets (possibly multiple times):

$$X^{learn} = X^{train} \sqcup X^{val}$$

On one of them, training takes place, and on the other, the model is validated.

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Why validate?

Usually, any machine learning algorithm contains a whole set of so-called "**hyperparameters**" (i.e. parameters that are not learned, but set initially): dimension, various weighting factors, etc.
And in order to select these parameters "fairly", without using any test data at all, a validation procedure is carried out.

Cross Validation

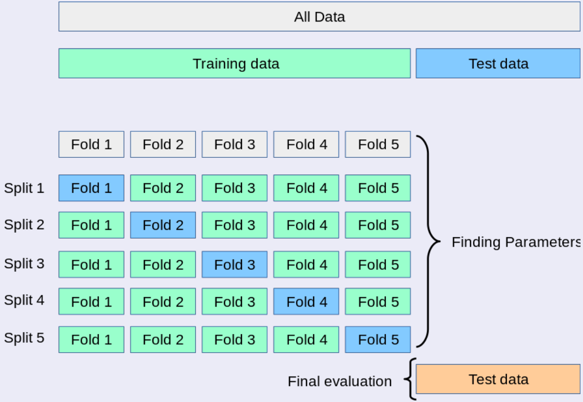
Special cases

1. The simplest cross-validation is **hold-out** control, in which the set is split once:

Cross Validation

Special cases

2. k block control (**k-fold** validation)[5]:



[5] Image source: `https://scikit-learn.org/`

Cross Validation

Special cases

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4. **Multiple k-fold** validation — repeat k-fold validation several times with different splits.

Time for questions

Overfitting

Definition

Overfitting is an undesirable phenomenon that occurs when solving problems of learning by precedents, when the probability of the error of the trained algorithm on the objects of the test sample is significantly higher than the average error on the training sample.
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Using Cross Validation

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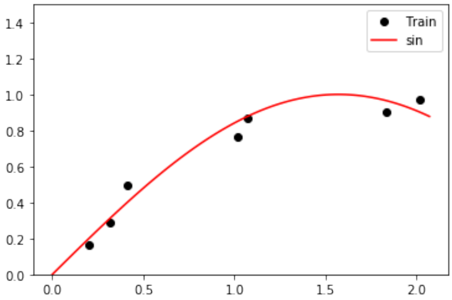
Train error observation

Overfitting and Underfitting: examples



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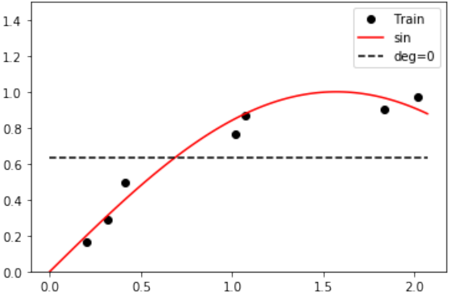

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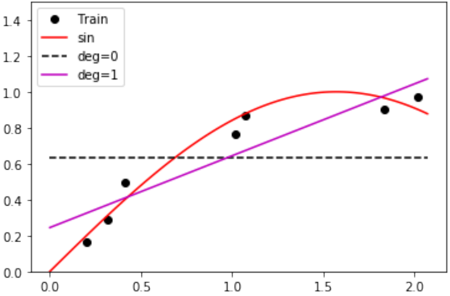

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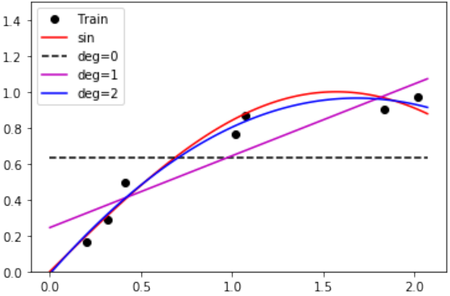

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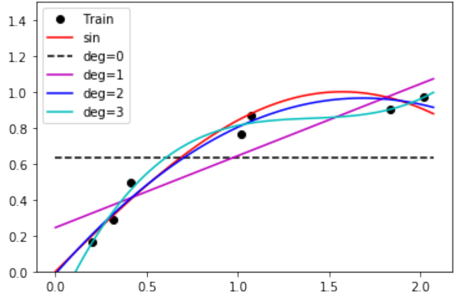

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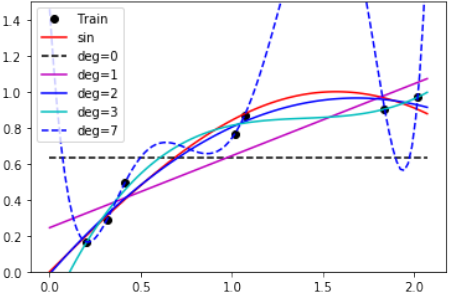

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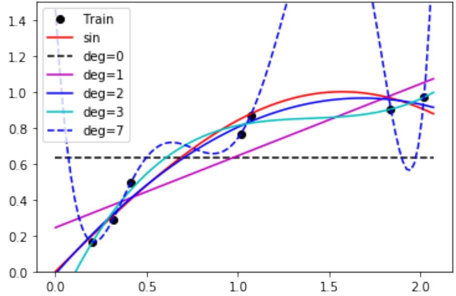

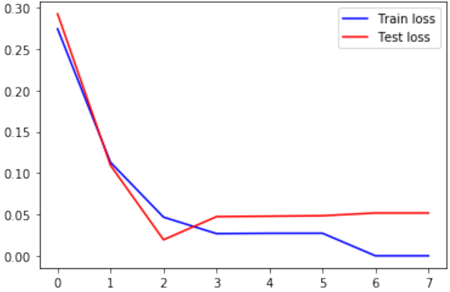

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On parameters and hyperparameters

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- **Hyperparameters**: the degree of the polynomial n, which is chosen before training starts; then chosen from the set of hyperparameters tested on the validation set

Derivation of mean squared error expression

Definitions

Let $y = y(x) = f(x) + \varepsilon$ be the target dependence, where $f(x)$ is the deterministic function, $\varepsilon \sim N(0, \sigma^2)$ and $a(x)$ is the machine learning algorithm.

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= Dy + Da + (E(f-a))^2 = \sigma^2 + variance(a) + bias^2(f,a)
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Additional definitions

Definition

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The mean squared error decomposition in the example above is called the **bias-variance tradeoff**

Model of Optimal Complexity: Classic View

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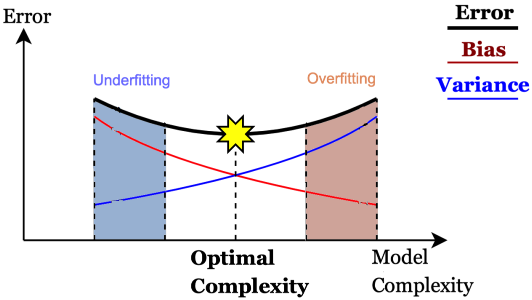

Model of Optimal Complexity: Recent Empirical Evidence

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- This behavior is called **double descent**

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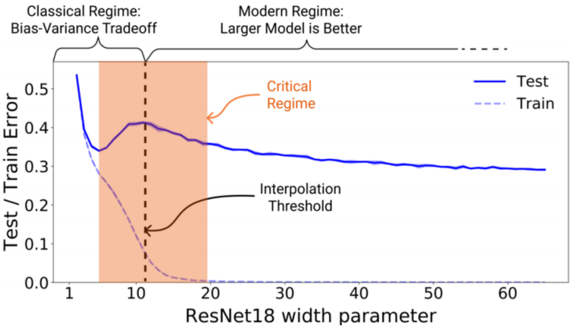
Model of Optimal Complexity: Double Descent

- Example of double descent in practice[7]:



[7] Image source: `https://arxiv.org/pdf/1912.02292.pdf`

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2. It is necessary to monitor the complexity of the model — too large will lead to overfitting, too small — to underfitting.
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3. In the case of a huge amount of data and parameters ($\approx$billions), classical estimates stop working

Time for questions

Thank you!