Machine Learning

Empirical and Structural Risk. Error Decomposition. Model Selection. Underfitting and overfitting

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ML Research

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Content

Content

1. Structural Risk and its Minimization
2. Overfittning and underfitting

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2. Overfittning and underfitting
3. Model Selection overview
4. Bias-variance tradeoff

Content

Instance-based learning

- X – set of objects descriptions, Y – set of objects labels
- Unknown target dependency: mapping $y : X \to Y$
- Finite training set: $X^m = \{(x_1, y_1), \ldots, (x_m, y_m)\}$, so as $y_i = y(x_i)$

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- **Empirical Risk Minimization** (ERM) – the common approach to solve the broad range of tasks of inductive learning (e.g., classification / regression tasks)

Empirical risk: definitions

Loss function $L(\hat{y}, y)$

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Empirical Risk (ER)

Performance metric reflecting the average error made by an algorithm a upon the set X^m: $R(a, X^m) = \frac{1}{m}\sum_{i=1}^{m} L(a(x_i), y(x_i))$

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ERM cons

Overfitting on the training set X^m. Happens almost always when using ERM, because the performance criteria is the error **on the very same set** (solution: to measure the performance it makes sense to change the set)

Loss functions examples

Classification task

- Classification error: $L(a, x) = L(\hat{y}, y) = [\hat{y} \neq y] = 1 - \delta_y(\hat{y})$
- The function is discontinuous $\Rightarrow$ ERM is a task of combinatorial optimization $\Rightarrow$ in many practical applications can be reduced to the search of maximal consistent subsystem of inequality system (number of inequalities is equal to the number of training examples m) $\Rightarrow$ NP-hard

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Regression task

- Squared error: $L(\hat{y}, y) = (\hat{y} - y)^2$

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SRM cons

Hard to guess in advance what is the right form of the regularization term $C(a)$ and what should be the regularization weight λ

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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Train vs Test (Validation) error discrepancy (can be seen via cross-validation)

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Handling methods

Regularization + decreasing model complexity

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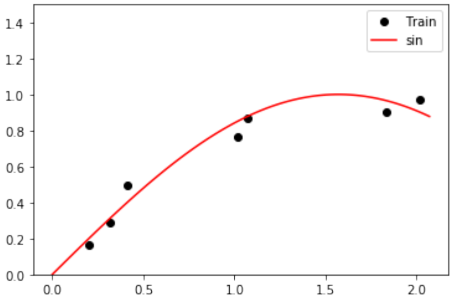
Handling method

Better / bigger model

Overfitting and Underfitting: examples



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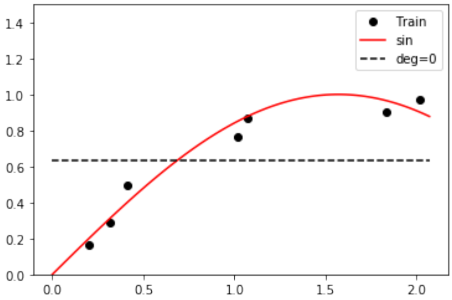

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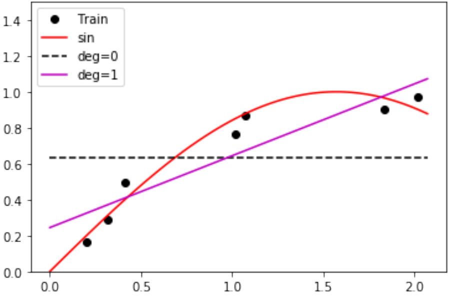

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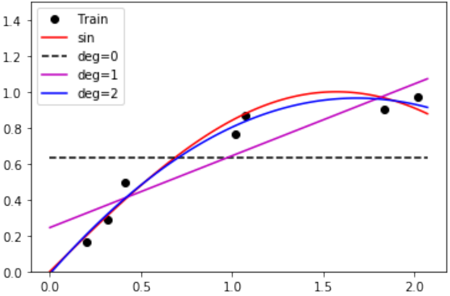

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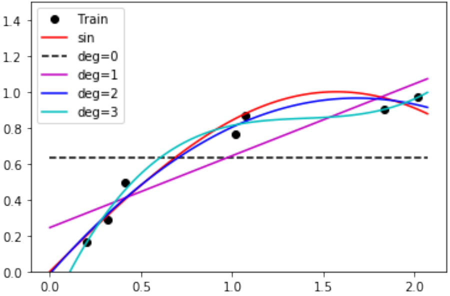

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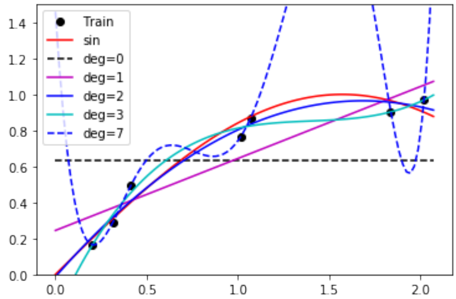

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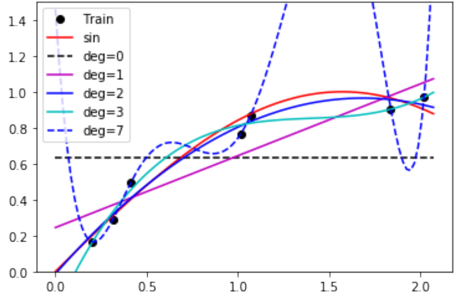

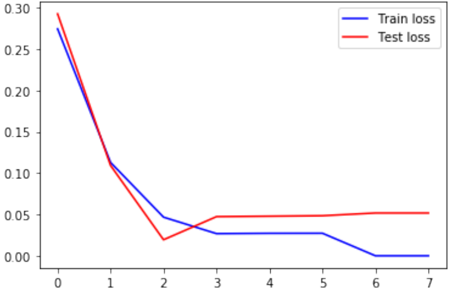

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- **Hyperparameters**: the degree of the polynomial n, which is chosen before training starts; then chosen from the set of hyperparameters tested on the validation set

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- Explainability (tradeoff between good and interpretable model)

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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Remark. x: test point; expectation E is done over all possible training datasets

Additional definitions

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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

- Simple models tend to be underfit

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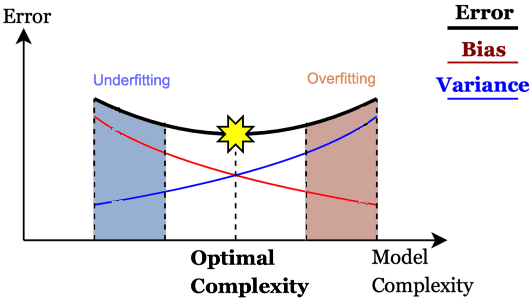
- Complex models tend to overfit

Model of Optimal Complexity: Classic View

- Simple models tend to be underfit
- Complex models tend to overfit
- The optimal complexity of the model is somewhere between



Model of Optimal Complexity: Recent Empirical Evidence

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- Tipping point — the point at which the complexity of the model is comparable to the cardinality of the training set (interpolation threshold)
- This behavior is called **double descent**

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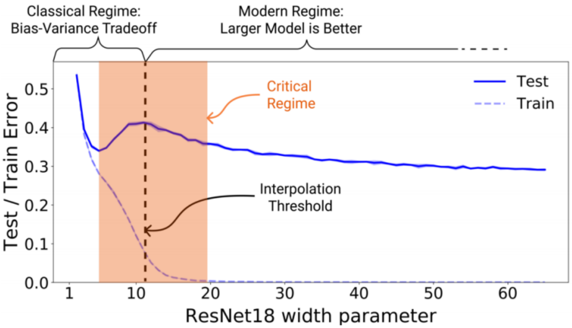
Model of Optimal Complexity: Double Descent

- Example of double descent in practice[2]:



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

Mandatory external links to read

1. Read the sections 5.2 and 5.4 from "**The Hundred-Page Machine Learning Book**"(see "*References*" course page)
2. Re-read the section about How Supervised Learning algorithms work paying more attention to the *Empirical* and *Structural Risk* subsections
3. Read the sections "*Introduction* "*Motivation* and "*Bias–variance decomposition of mean squared error*"of the Bias-Variance Tradeoff page
4. Read the material about Overfitting and Underfitting

Takeaway notes

1. Structural Risk is needed to avoid overfitting doing Empirical Risk Minimization

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2. There is a tradeoff between bias and variance for any ML model

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2. There is a tradeoff between bias and variance for any ML model
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5. In case of a huge amount of data and parameters (≈billions), classical estimates stop working

Thank you!