Machine Learning

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

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ML Research

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SOFIA UNIVERSITY

Content

1. Structural Risk and its Minimization

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2. Overfittning and underfitting

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3. Model Selection overview

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4. Bias-variance tradeoff

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5. Recent results: Double Descent

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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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

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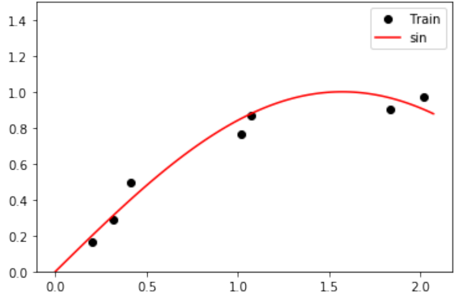
Train error observation

Overfitting and Underfitting: examples



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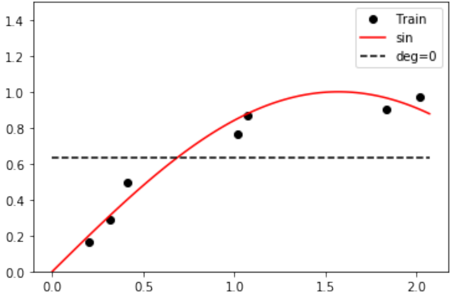

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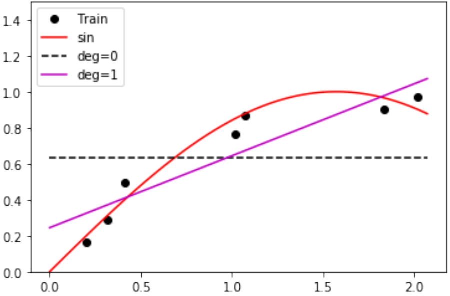

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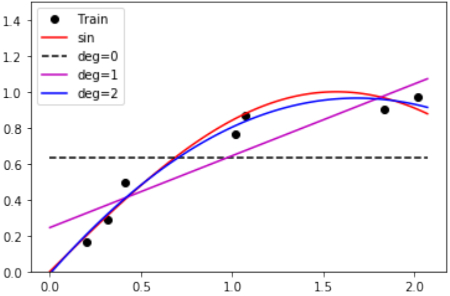

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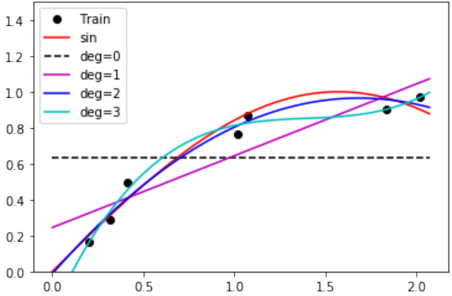

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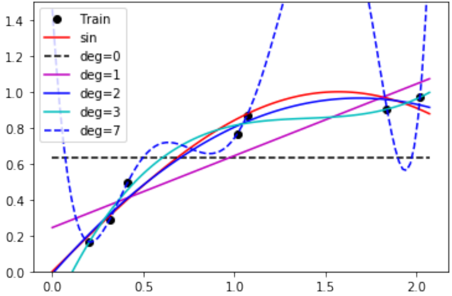

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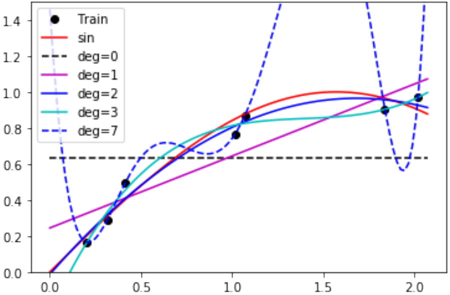

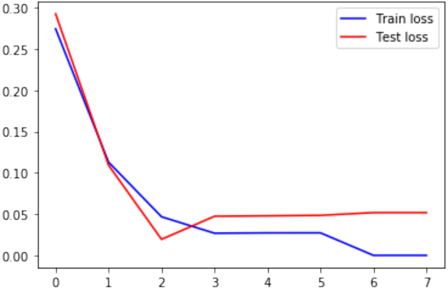

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- **Hyperparameters**: the degree of the polynomial n, which is chosen before training starts; then chosen from the set of hyperparameters tested on the validation set

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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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= Dy + Da + (E(f-a))^2 = \sigma^2 + variance(a) + bias^2(f, a)
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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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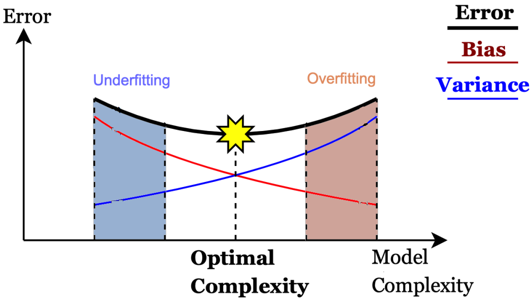
- The optimal complexity of the model is somewhere between



Model of Optimal Complexity: Recent Empirical Evidence

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- This behavior is called **double descent**

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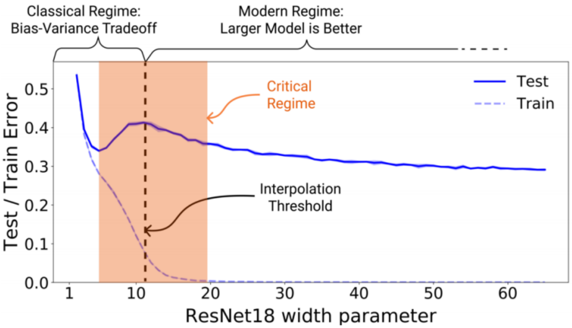
Model of Optimal Complexity: Double Descent

- Example of double descent in practice[2]:



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

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5. In case of a huge amount of data and parameters ($\approx$billions), classical estimates stop working

Thank you!