Deep Learning

2.2 Over and Under fitting

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Aug-Dec 2021

Generalization

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2. Goal of good ML model is to generalize well from training data to any data from the task domain

Fit

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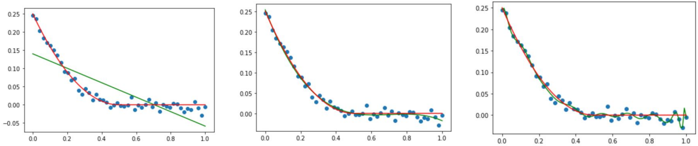

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2. Goodness of the fit refers to measures used to estimate how well the approximation matches the target
3. In ML we don't know the target function under approximation

Over and under fitting

1. Cause of poor performance in ML is either overfitting or underfitting to the data

Overfitting

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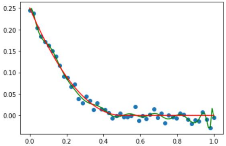

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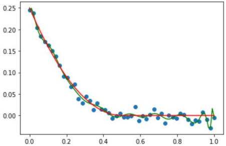

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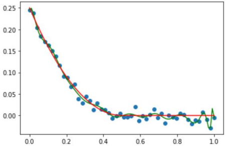

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3. More likely to occur in case of nonparametric and nonlinear models with more flexibility

Example

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2. Flexible and prone to overfitting training data
3. Can be addressed by pruning the tree after learning (removes some of the detail picked up)

Underfitting

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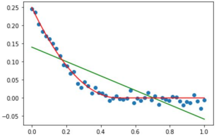

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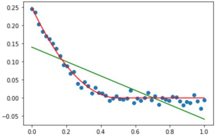

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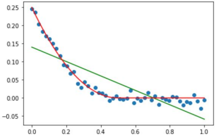

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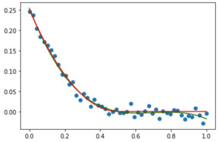
3. Can be alleviated by trying alternate ML algorithms (e.g. relatively complex)

Good fit in ML

1. Ideally, one should select a model at the sweet spot between over and underfitting



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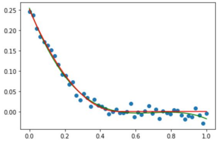

2. Very difficult in practice

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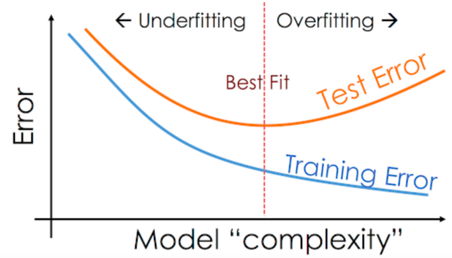

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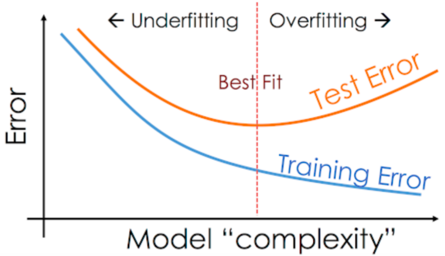

3. Cross validation is often used for estimating the generalization (hence limit overfitting)

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2. More rigorous notion is VC dimension

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1. Although it is difficult to define precisely, in practice it is not very hard to manipulate it for a given class of models
2. In general overfitting can be controlled by
   - Restricting the space of functions $\mathcal{F}$ (regularization, constrained optimization)
   - Making the choice of optimal function f^* less dependent on the data (e.g. ensemble methods)

Polynomial Model

1. Given a polynomial model
$\forall x, \alpha_0, \ldots, \alpha_D \in \mathcal{R}, f(x, \alpha) = \sum_{\mathbf{d=0}}^{\mathbf{D}} \alpha_{\mathbf{d}} \mathbf{x}^{\mathbf{d}}$,
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2.

$$
\begin{aligned}
\mathcal{L}(\alpha) &= \sum_n (f(x_n; \alpha) - y_n)^2 \\
&= \sum_n (\sum_{d=0}^{D} \alpha_d x^d - y_n)^2 \\
&= \left\| \begin{bmatrix} x_1^0 & \ldots & x_1^D \\ \vdots & \ddots & \vdots \\ x_N^0 & \ldots & x_N^D \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_D \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \right\|^2
\end{aligned}
$$

Polynomial Model

- $\underset{\alpha}{\operatorname{argmin}} \left\| \begin{bmatrix} x_1^0 & \dots & x_1^D \\ \vdots & \ddots & \vdots \\ x_N^0 & \dots & x_N^D \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_D \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \right\|^2$ is a standard least squares problem

Polynomial Model- Prediction with degree