2.2. Over and under fitting

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Here the candidates are our models and the questions are the training examples used to pick the best one.
With

\[ Q^n_k \sim \mathcal{B}(0.5), \; n = 1, \ldots, 1000, \; k = 1, \ldots, 10, \]

independent standing for “candidate \( n \) answere question \( k \) correctly”, we have

\[ \forall n, \; P(\forall k, Q^n_k = 1) = \frac{1}{1024} \]

and

\[ P(\exists n, \forall k, Q^n_k = 1) \approx 0.62. \]
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Selecting a candidate based on a statistical estimator biases the said estimator for that candidate. And you need a greater number of “competence checks” if you have a larger pool of candidates.
Over and under-fitting, capacity. $K$-nearest-neighbors
A simple classification procedure is the “$K$-nearest neighbors.”

Given

$$(x_n, y_n) \in \mathbb{R}^D \times \{1, \ldots, C\}, \ n = 1, \ldots, N$$

to predict the $y$ associated to a new $x$, take the $y_n$ of the closest $x_n$:

$$n^*(x) = \arg\min_n \|x_n - x\|$$

$$f^*(x) = y_{n^*(x)}.$$

This recipe corresponds to $K = 1$, and makes the empirical training error zero.
$K = 1$
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If we let also $K \to \infty$ “not too fast”, the error rate is the (optimal!) Bayes’ Error rate.
Training set
Prediction (K=1)
Training set
Prediction (K=1)
Training set
Votes ($K=51$)
Prediction (K=51)
Training set
Votes (K=51)
Prediction (K=51)
Underfitting Overfitting

Error

K

Train
Test

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Over and under-fitting, capacity, polynomials
Given a polynomial model

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$$\mathcal{L}(\alpha) = \sum_{n} (f(x_n; \alpha) - y_n)^2$$
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$$= \sum_n \left( \sum_{d=0}^{D} \alpha_d x_n^d - y_n \right)^2$$

$$= \left\| \begin{pmatrix} x_0^0 & \ldots & x_1^D \\ x_1^0 & \ldots & x_1^D \\ \vdots & \ddots & \vdots \\ x_N^0 & \ldots & x_N^D \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_D \end{pmatrix} - \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \right\|^2.$$
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\[ = \left\| \begin{pmatrix} x_1^0 & \cdots & x_1^D \\ \vdots & \ddots & \vdots \\ x_N^0 & \cdots & x_N^D \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_D \end{pmatrix} - \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \right\|^2. \]

Hence, minimizing this loss is a standard quadratic problem, for which we have efficient algorithms.
def fit_polynomial(D, x, y):
    X = torch.empty(x.size(0), D + 1)
    for d in range(D + 1):
        X[:, d] = x**d

    # lstsq expects a matrix for target
    Y = y.view(-1, 1)

    # Least square solution
    alpha, _ = torch.lstsq(Y, X)

    return alpha[:D+1, 0]
D, N = 4, 100
x = torch.linspace(-math.pi, math.pi, N)
y = x.sin()
alpha = fit_polynomial(D, x, y)

X = torch.empty(N, D + 1)
for d in range(D + 1):
    X[:, d] = x.pow(d)

y_hat = X.mv(alpha)

for k in range(N):
    print(x[k].item(), y[k].item(), y_hat[k].item())
We can use this model to illustrate how the prediction changes when we increase the degree or the regularization.
Data
Degree D=2

Data

\[ f^* \]
Degree D=6

Data

Degree D=6

Data

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Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data

Degree D=7

Data
Degree D=8

Data

f*
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We can visualize the influence of the noise by generating multiple training sets $\mathcal{D}_1, \ldots, \mathcal{D}_M$ with different noise, and training one model on each.
Degree D=4
Degree D=5
Degree D=7

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Degree D=8

\[ \text{f} \quad \text{f}^* \]
We can reformulate this control of the degree with a penalty

\[ \mathcal{L}(\alpha) = \sum_n (f(x_n; \alpha) - y_n)^2 + \sum_d l_d(\alpha_d) \]

where

\[ l_d(\alpha) = \begin{cases} 
0 & \text{if } d \leq D \text{ or } \alpha = 0 \\
+\infty & \text{otherwise.} 
\end{cases} \]

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Such a penalty kills any term of degree \( > D \).

This suggests more subtle variants. For instance, to keep all this quadratic

\[ \mathcal{L}(\alpha) = \sum_n (f(x_n; \alpha) - y_n)^2 + \rho \sum_d \alpha_d^2. \]
$D=9, \rho=1e0$
D=9, \rho=1e-2

Graph showing the relationship between \( f \) and \( f^* \) with \( D=9, \rho=1e-2 \).
D=9, \rho=1e^{-3}
D=9, $\rho=1\times10^{-4}$

The graph shows multiple curves labeled as $f^*$ and $f$. The y-axis ranges from -0.5 to 1.5, and the x-axis ranges from 0 to 1. The curves converge as the x-value increases.
D=9, \rho=1e-5

\begin{center}
\includegraphics[width=\textwidth]{figure.png}
\end{center}
D=9, \( \rho=1e^{-7} \)
D=9, \rho=1e-8

![Graph showing the relationship between D=9 and \rho=1e-8 with two functions f^* and f.](image)
D=9, ρ=1e-9

The diagram shows a comparison between the true function $f^*$ and the learned function $f$. The graph plots the functions over a range of input values, with $f^*$ represented by a blue line and $f$ by a red line. The $f^*$ line is smooth and follows the data more closely, indicating a better fit to the underlying function.
D=9, ρ=1e-10
D=9, \( \rho=1e^{-12} \)
D=9, ρ=1e-13
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![Graph showing error (MSE) vs. \( \rho \)](image)

- **Train**
- **Test**

- Error (MSE)
  - 10^{-3}
  - 10^{-2}
  - 10^{-14}
  - 10^{-12}
  - 10^{-10}
  - 10^{-8}
  - 10^{-6}
  - 10^{-4}
  - 10^{-2}
  - 10^0

- **\( \rho \)**
We define the **capacity** of a set of predictors as its ability to model an arbitrary functional. This is a vague definition, difficult to make formal.
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A mathematically precise notion is the Vapnik–Chervonenkis dimension of a set of functions, which, in the Binary classification case, is the cardinality of the largest set that can be labeled arbitrarily (Vapnik, 1995).

It is a very powerful concept, but is poorly adapted to neural networks. We will not say more about it in this course.
Although the capacity is hard to define precisely, it is quite clear in practice how to modulate it for a given class of models.

In particular one can control over-fitting either by

- Reducing the space $\mathcal{F}$ (less functionals, constrained or degraded optimization), or

- Making the choice of $f^*$ less dependent on data (penalty on coefficients, margin maximization, ensemble methods).
The end
References