Deep learning

2.2. Over and under fitting

François Fleuret

https://fleuret.org/dlc/
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What about interviewing ten candidates and picking the best? What about interviewing one thousand?

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 \( n \) answers 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.
$K = 1$
Under mild assumptions of regularities of $\mu_X, \gamma$, for $N \to \infty$ the asymptotic error rate of the 1-NN is less than twice the (optimal!) Bayes’ Error rate.
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It can be made more stable by looking at the $K > 1$ closest training points, and taking the majority vote.

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)
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```plaintext
K
0.00
0.05
0.10
0.15
0.20
0.25
0.30
```

![Graph showing error over K for Train and Test sets]
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Error

Underfitting

Overfitting

Train

Test

K

0.00

0.05

0.10

0.15

0.20

0.25

0.30

0.00

10^3

10^2

10^1

10^0
Over and under-fitting, capacity, polynomials
Given a polynomial model

\[ \forall x, \alpha_0, \ldots, \alpha_D \in \mathbb{R}, \quad f(x; \alpha) = \sum_{d=0}^{D} \alpha_d x^d. \]
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and training points \((x_n, y_n) \in \mathbb{R}^2, n = 1, \ldots, N\), the quadratic loss is

\[ \mathcal{L}(\alpha) = \sum_{n} (f(x_n; \alpha) - y_n)^2 \]
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\]

\[
= \sum_n \left( \sum_{d=0}^{D} \alpha_d x_n^d - y_n \right)^2
\]

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

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and training points \((x_n, y_n) \in \mathbb{R}^2, n = 1, \ldots, N\), the quadratic loss is

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

Hence, minimizing this loss is a standard quadratic problem, for which we have efficient algorithms.
def fit_polynomial(D, x, y):
    # Broadcasting magic
    X = x[:, None] ** torch.arange(0, D + 1)[None]

    # lstsq expects a matrix for target
    Y = y[:, None]

    # Least square solution, we ignore the second returned value which
    # contains information about the used QR factorization
    alpha, _ = torch.lstsq(Y, X)

    # We get rid of the last coefficients that contain residuals
    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 = x[:, None] ** torch.arange(0, D + 1)[None]
y_hat = X @ 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.
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Degree $D = 0$

$\text{Data}$

$\text{f}^*$
Degree $D = 1$
Degree $D = 2$

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Degree $D = 3$

$\text{Data}$

$f^*$
Degree $D = 4$
Degree $D = 5$
Degree $D = 6$

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Degree $D = 7$

$\mathbf{f}^*$

Data
Degree $D = 8$

$\deg D = 8$
Degree $D = 9$
Over and under fitting

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Deep learning / 2.2. Over and under fitting
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 $D = 0$
Degree $D = 1$

$\frac{\text{Degree}}{D} = 1$

$f^*$

$f$
Degree $D = 2$
Degree $D = 3$
Degree $D = 4$
Degree $D = 5$

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Deep learning / 2.2. Over and under fitting
Degree $D = 6$
Degree $D = 7$
Degree $D = 8$
Degree $D = 9$
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

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

Such a penalty kills any term of degree $> D$. 

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

$$\mathcal{L}(\alpha) = \sum_n (f(x_n; \alpha) - y_n)^2 + \rho \sum_d \alpha_d^2.$$
\[
D = 9, \rho = 1 \times 10^1
\]
$D = 9, \rho = 1 \times 10^0$
\[ D = 9, \rho = 1 \times 10^{-1} \]
\[ D = 9, \rho = 1 \times 10^{-2} \]
\[ D = 9, \rho = 1 \times 10^{-3} \]
$D = 9, \rho = 1 \times 10^{-4}$
$D = 9, \rho = 1 \times 10^{-5}$
$D = 9, \rho = 1 \times 10^{-6}$
\[ D = 9, \rho = 1 \times 10^{-7} \]
$D = 9, \rho = 1 \times 10^{-8}$
$D = 9, \rho = 1 \times 10^{-9}$
$D = 9, \rho = 1 \times 10^{-10}$
\[ D = 9, \rho = 1 \times 10^{-11} \]
$D = 9, \rho = 1 \times 10^{-12}$
\[ D = 9, \rho = 1 \times 10^{-13} \]
$D = 9, \rho = 0$
Error (MSE)
Train
Test

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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