Deep learning

2.2. Over and under fitting

François Fleuret

https://fleuret.org/dlc/

UNIVERSITÉ DE GENÈVE

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

With

$$Q_k^n \sim \mathscr{B}(0.5), \;\; n = 1, \dots, 1000, \;\; k = 1, \dots, 10,$$

independent standing for "candidate n answers question k correctly", we have

$$\forall n, \;\; P(\forall k, Q_k^n = 1) = \frac{1}{1024}$$

and

$$P(\exists n, \forall k, Q_k^n = 1) \simeq 0.62.$$

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So there is 62% chance that among $1,000$ candidates answering completely at random, at least one will score perfectly.

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."

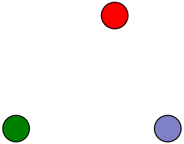
Given

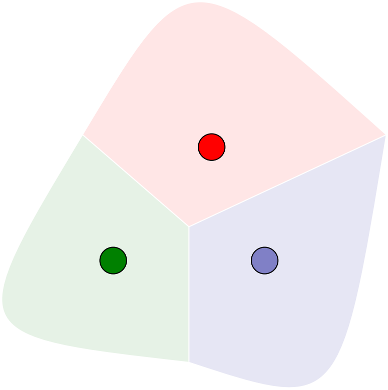
$$(x_n, y_n) \in \mathbb{R}^D \times \{1, \dots, C\}, \ n = 1, \dots, N$$

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

$$\begin{aligned} n^*(x) &= \operatorname*{argmin}_n \|x_n - x\| \\ f^*(x) &= y_{n^*(x)}. \end{aligned}$$

This recipe corresponds to $K = 1$, and makes the empirical training error zero.





$K = 1$

Under mild assumptions of regularities of $\mu_{X,Y}$, for $N \rightarrow \infty$ the asymptotic error rate of the 1-NN is less than twice the (optimal!) Bayes' Error rate.

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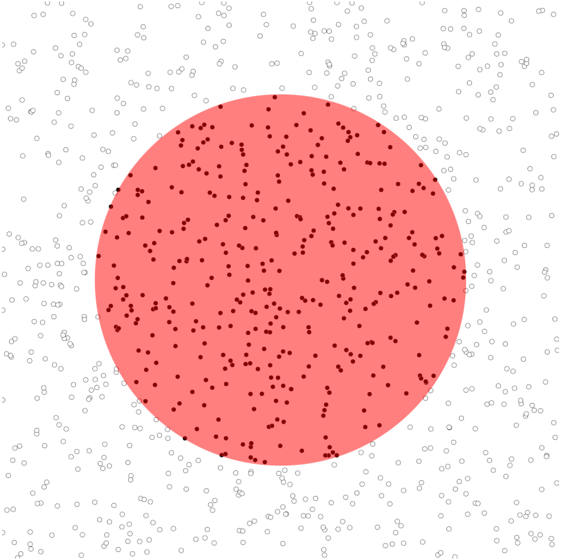
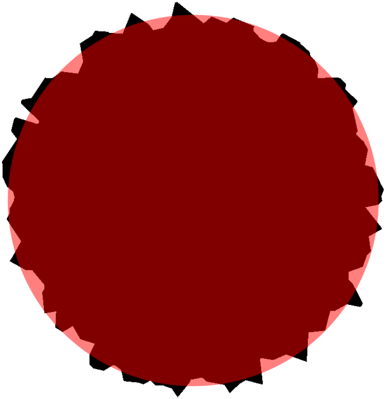
It can be made more stable by looking at the $K > 1$ closest training points, and taking the majority vote.

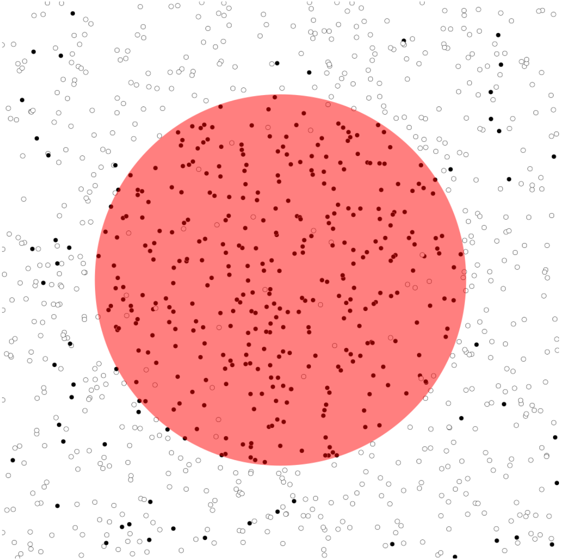
If we let also $K \rightarrow \infty$ "not too fast", the error rate is the (optimal!) Bayes' Error rate.



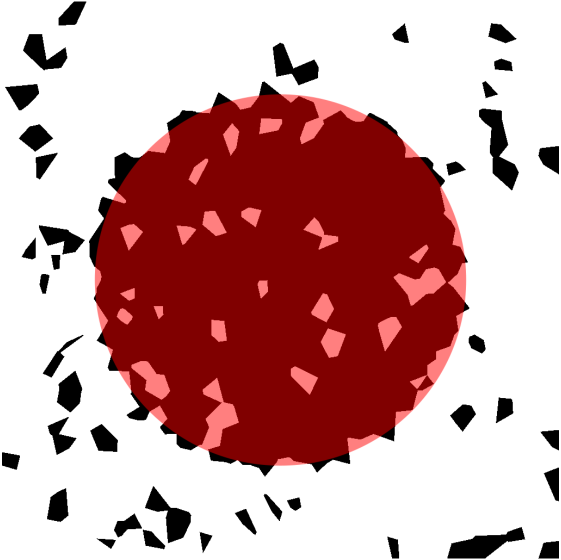
Training set



Prediction (K=1)



Training set



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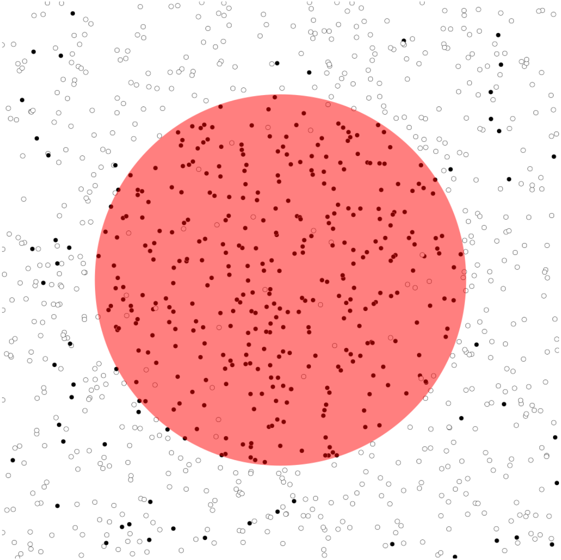
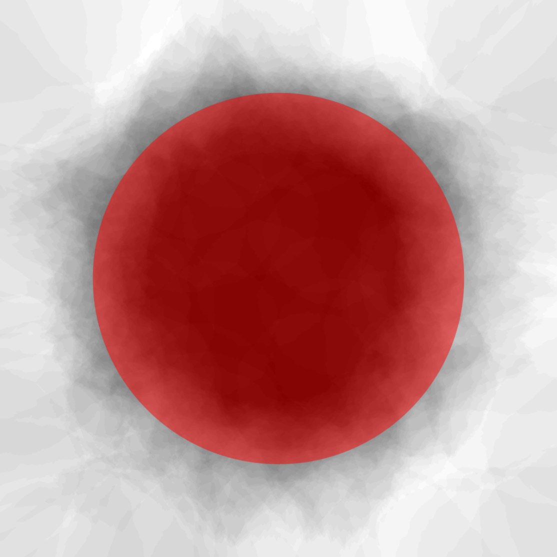
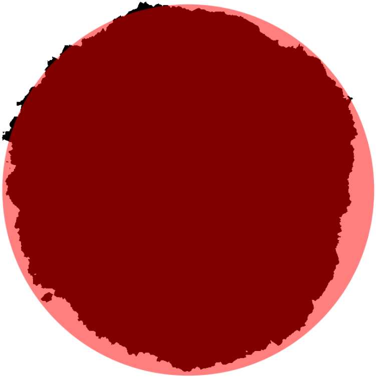


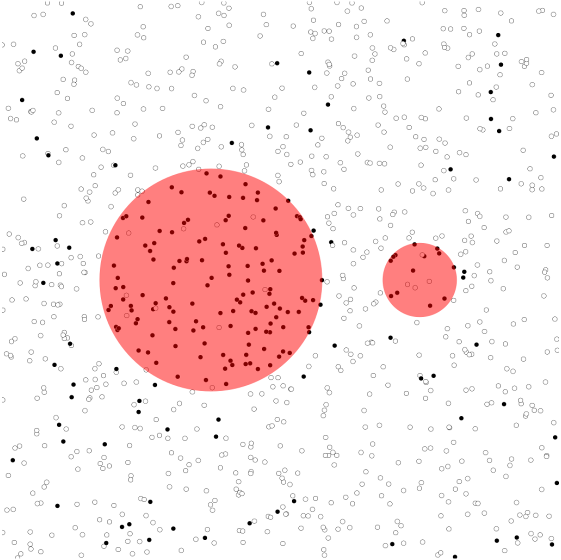
Training set



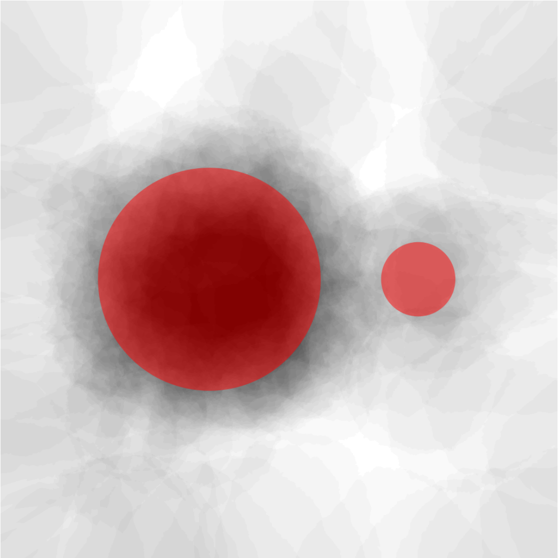
Votes (K=51)



Prediction (K=51)



Training set



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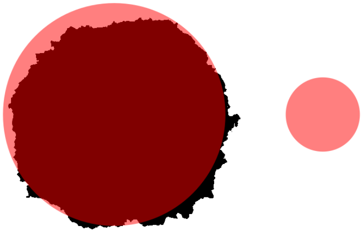

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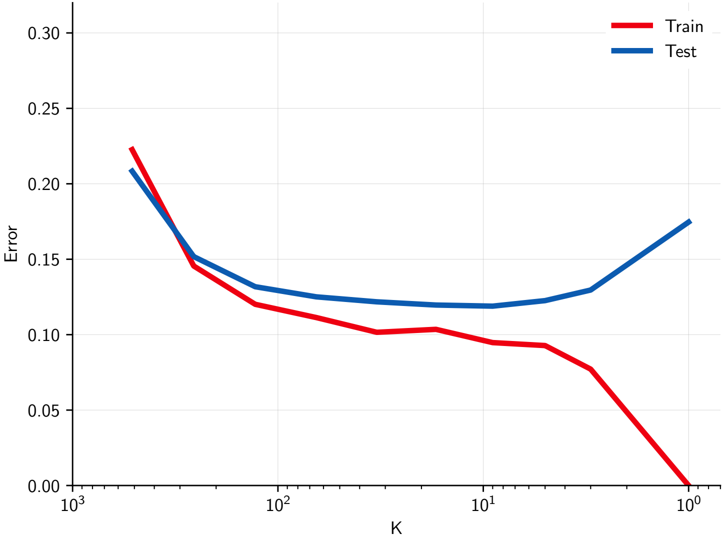
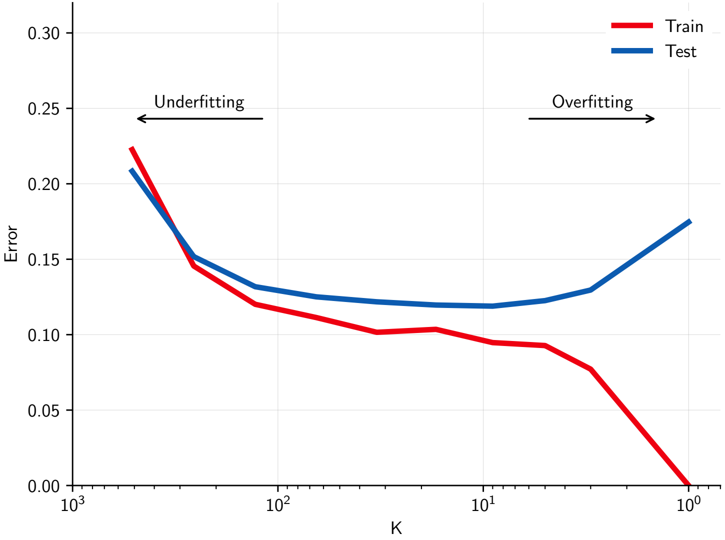


Train
Test
Error
0.30
0.25
0.20
0.15
0.10
0.05
0.00
10^3
10^2
10^1
10^0
K


Train
Test
Underfitting
Overfitting
Error
0.30
0.25
0.20
0.15
0.10
0.05
0.00
K
10^3
10^2
10^1
10^0

Over and under-fitting, capacity, polynomials

Given a polynomial model

$$\forall x, \alpha_0, \dots, \alpha_D \in \mathbb{R},\ f(x; \alpha) = \sum_{d=0}^{D} \alpha_d x^d.$$

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

$$\mathscr{L}(\alpha) = \sum_n \left(f(x_n;\alpha) - y_n\right)^2$$

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\mathscr{L}(\alpha) &= \sum_n (f(x_n;\alpha) - y_n)^2 \\
&= \sum_n \left(\sum_{d=0}^{D} \alpha_d x_n^d - y_n \right)^2 \\
&= \left\| \begin{pmatrix} x_1^0 & \dots & x_1^D \\ \vdots & & \vdots \\ x_N^0 & \dots & 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.
\end{aligned}$$

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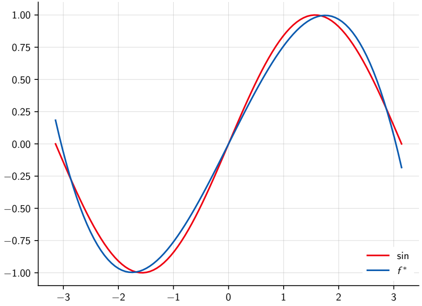
\end{aligned}$$

Hence, minimizing this loss is a standard quadratic problem, for which we have efficient algorithms.

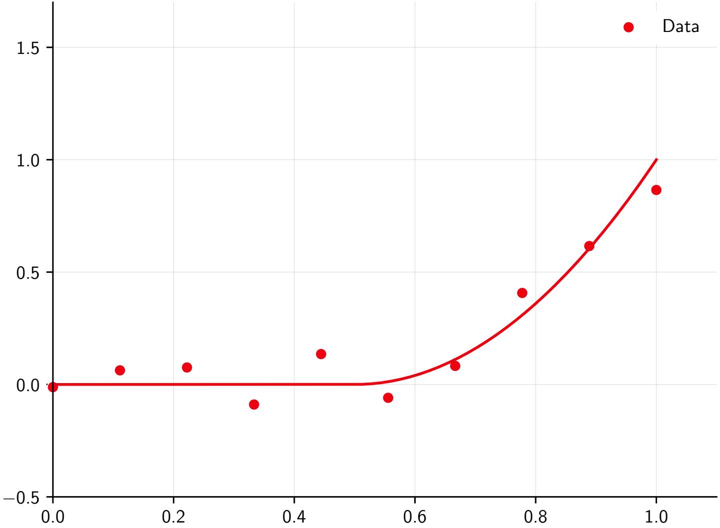
$$\underset{\alpha}{\operatorname{argmin}} \left\| \begin{pmatrix} x_1^0 & \dots & x_1^D \\ \vdots & & \vdots \\ x_N^0 & \dots & x_N^D \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_D \end{pmatrix} - \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} \right\|^2$$

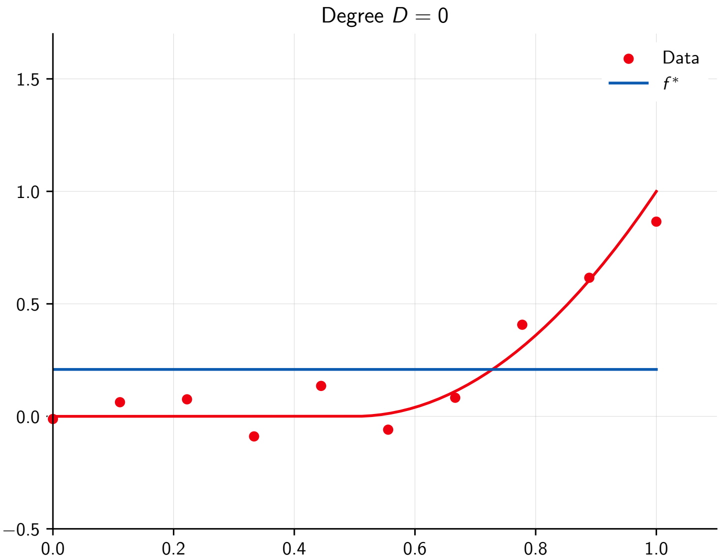
```
def fit_polynomial(D, x, y):
    # Broadcasting magic
    X = x[:, None] ** torch.arange(0, D + 1)[None]

    # Least square solution
    return torch.linalg.lstsq(X, y).solution
```

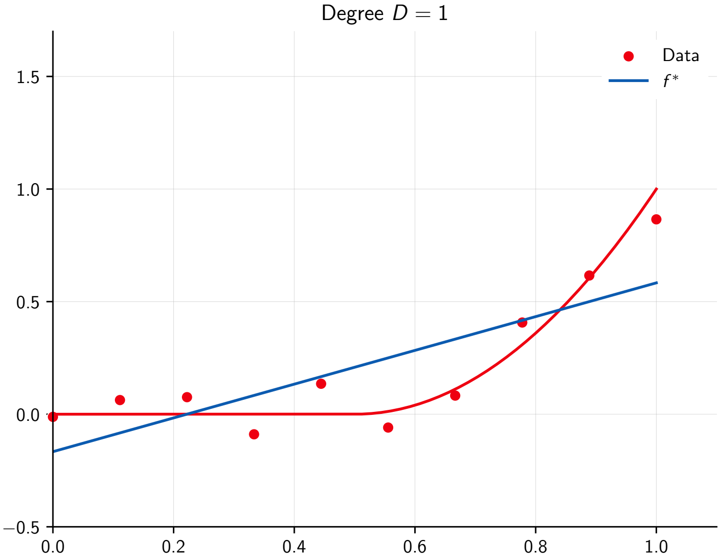
```
D, N = 4, 100
x = torch.linspace(-math.pi, math.pi, N)
y = x.sin()
alpha = fit_polynomial(D, x, y)

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())
```

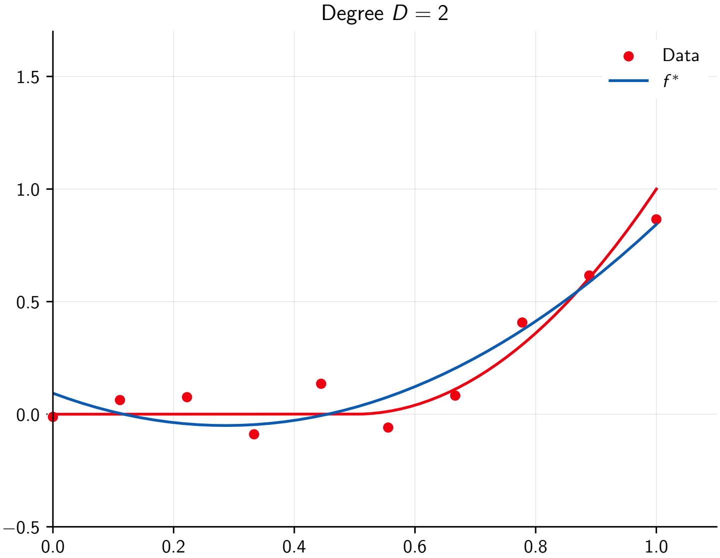


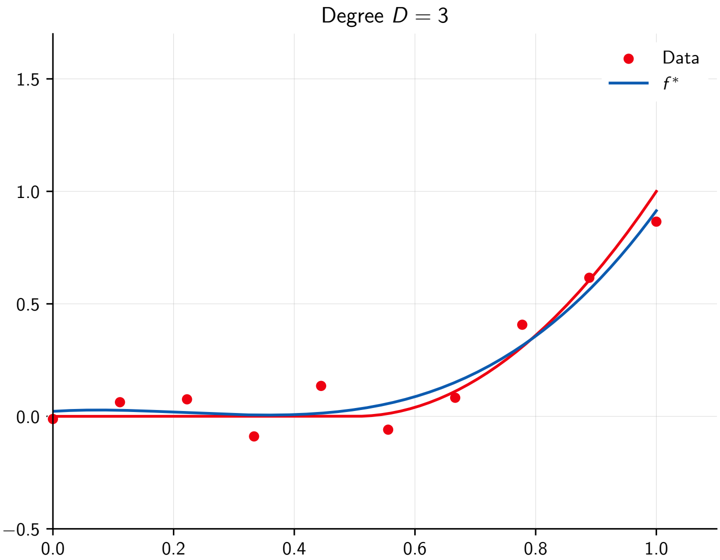
We can use this model to illustrate how the prediction changes when we increase the degree or the regularization.


Data
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

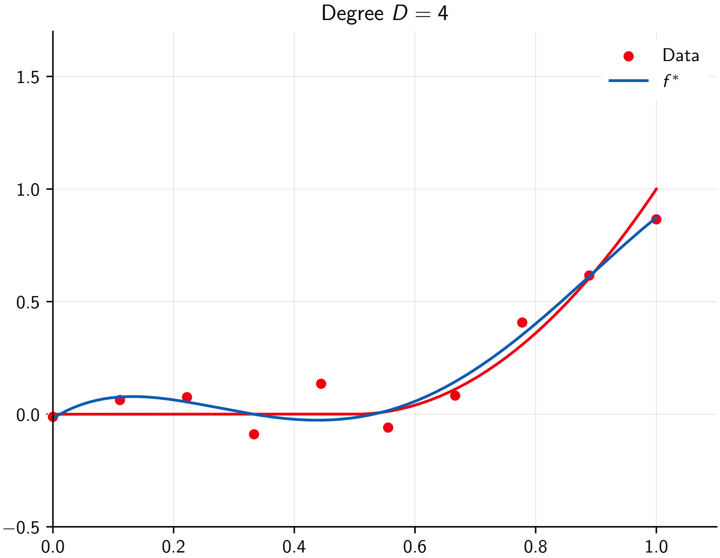

Degree $D = 0$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


Degree $D = 1$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

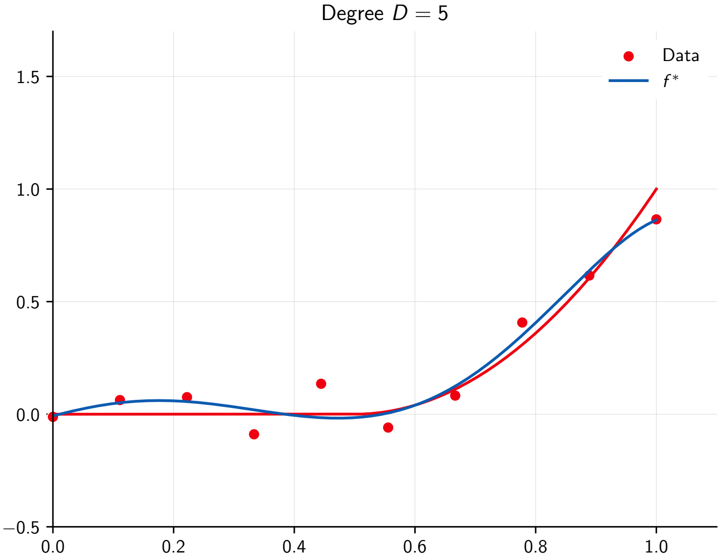

Degree $D = 2$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0



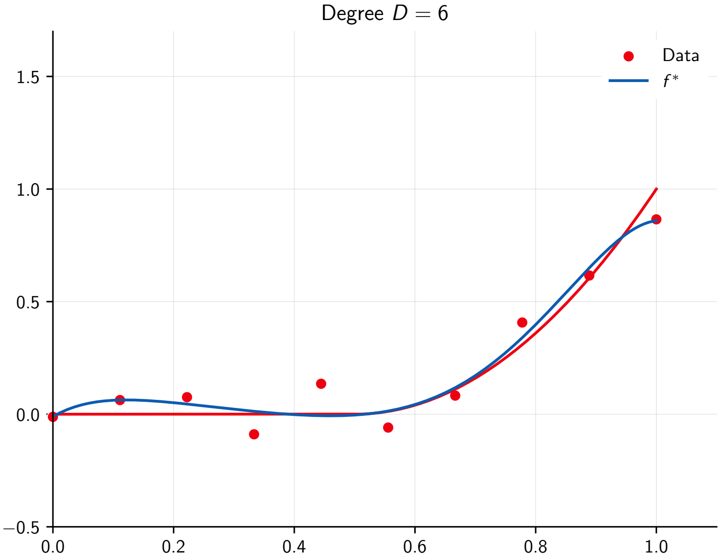
Degree $D = 3$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

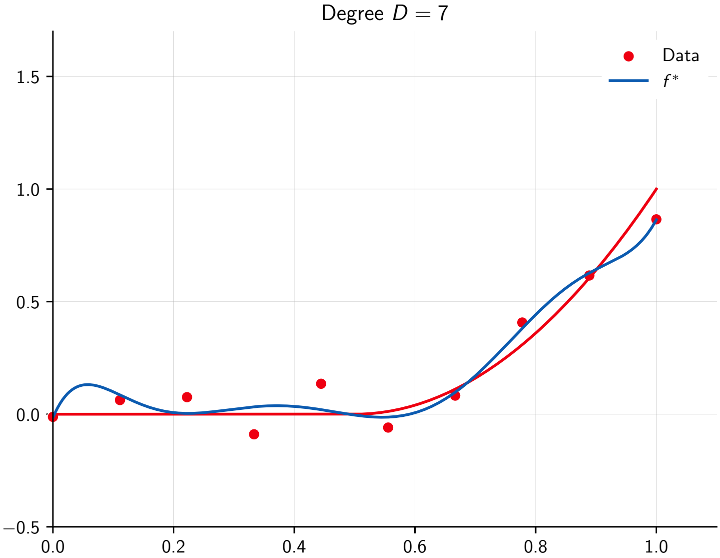


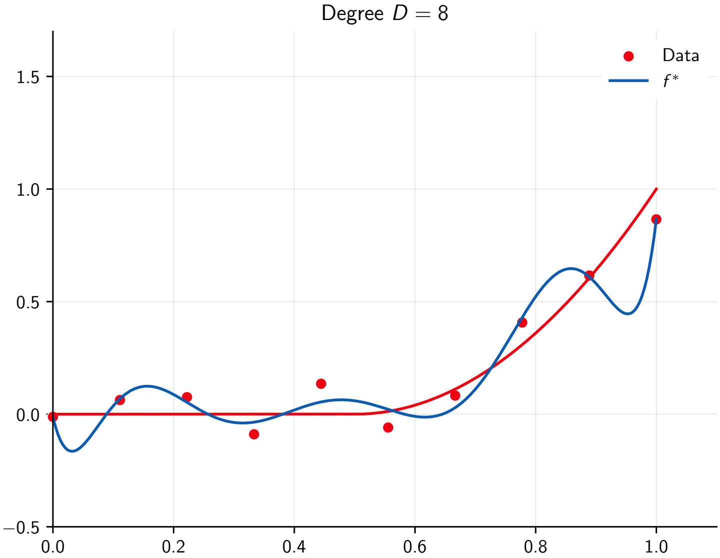
Degree $D = 4$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

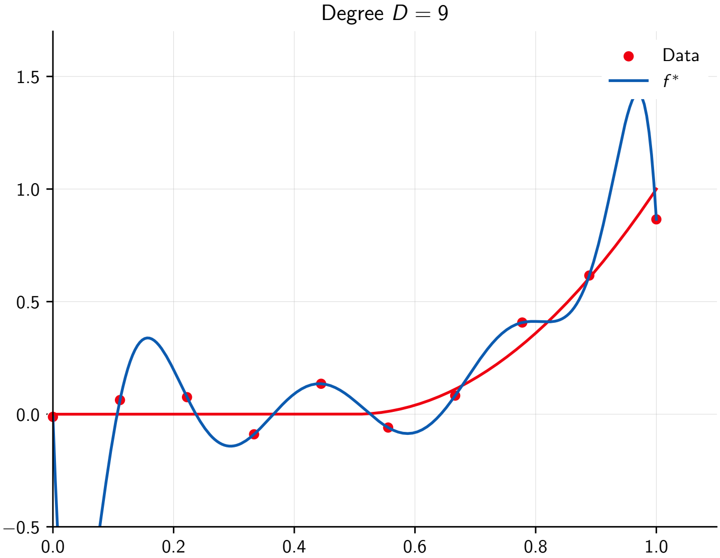


Degree $D = 5$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

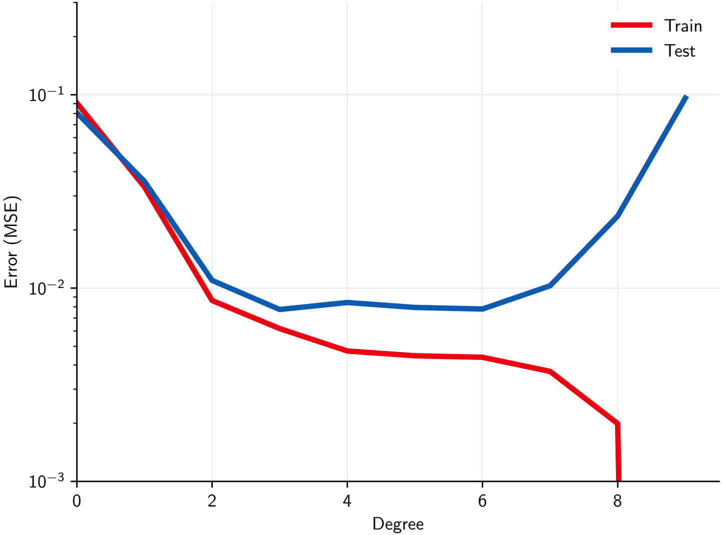

Degree $D = 6$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


Degree $D = 7$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

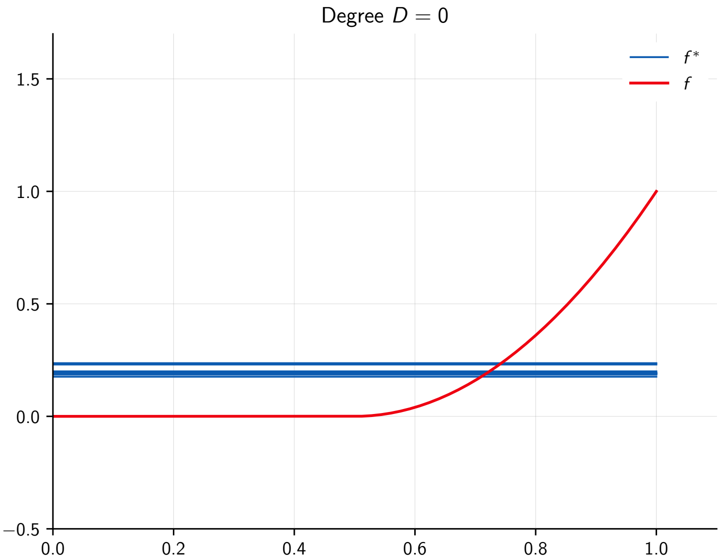

Degree $D = 8$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0



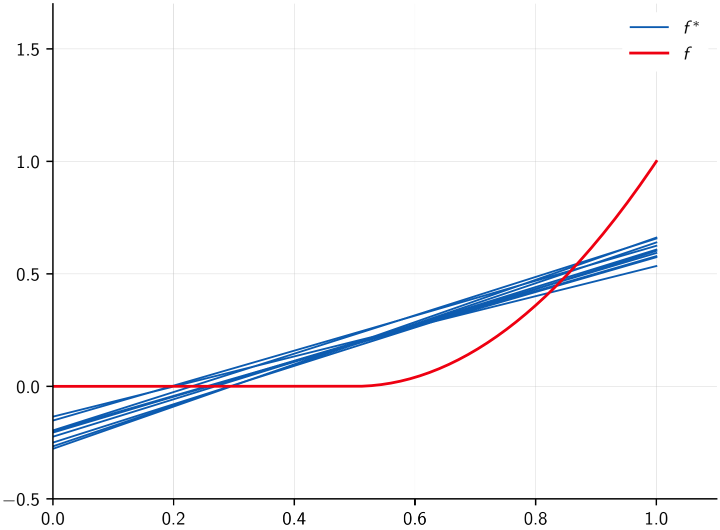
Degree $D = 9$
Data
f^*
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

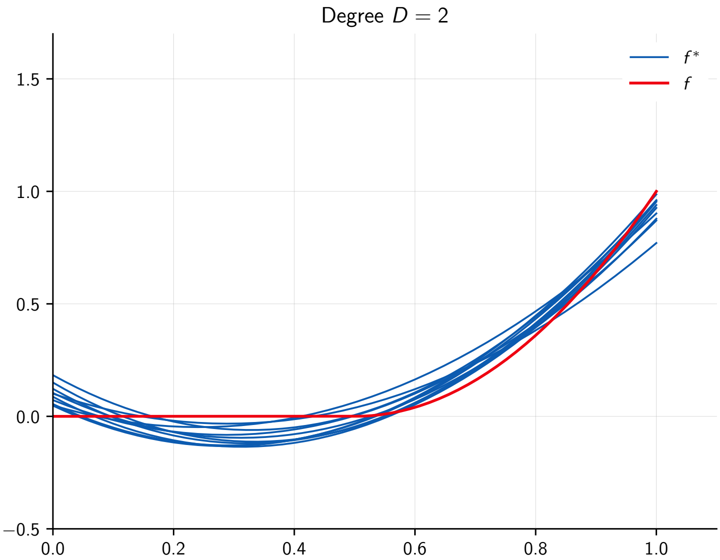

Train
Test
10^{-1}
10^{-2}
10^{-3}
Error (MSE)
0
2
4
6
8
Degree

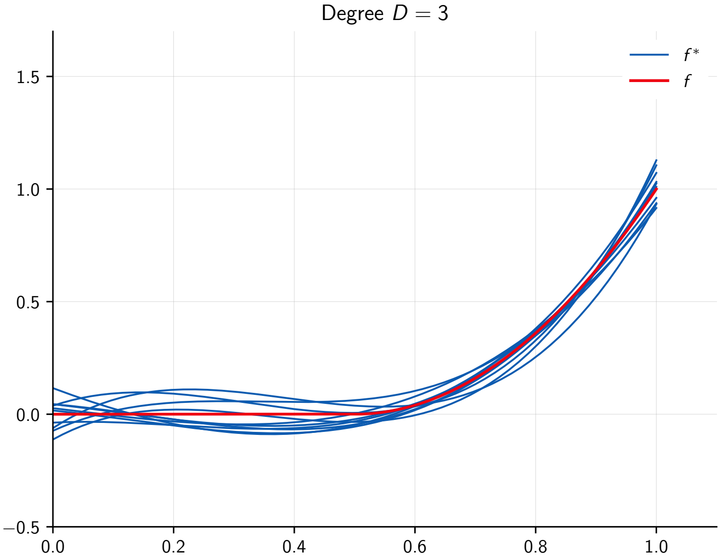
We can visualize the influence of the noise by generating multiple training sets $\mathscr{D}_1, \dots, \mathscr{D}_M$ with different noise, and training one model on each.

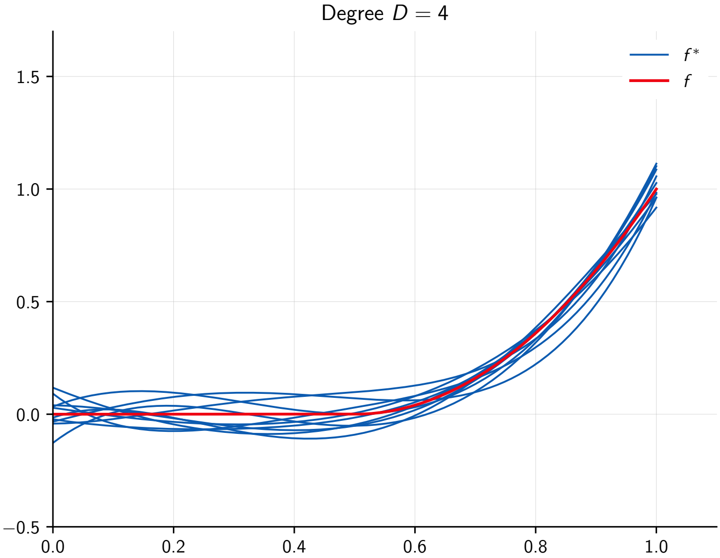

Degree $D = 0$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

Degree $D = 1$

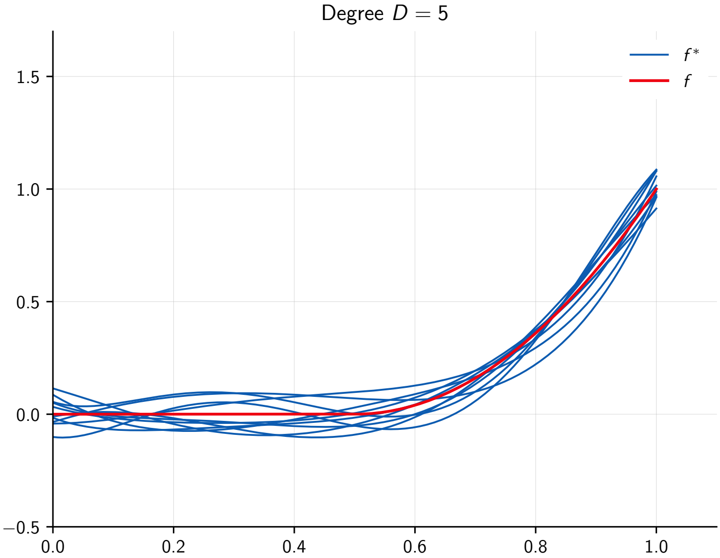


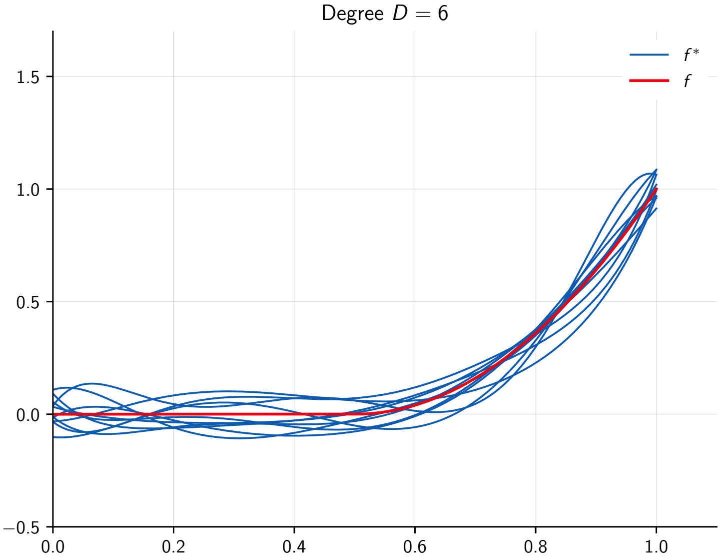

Degree $D = 2$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

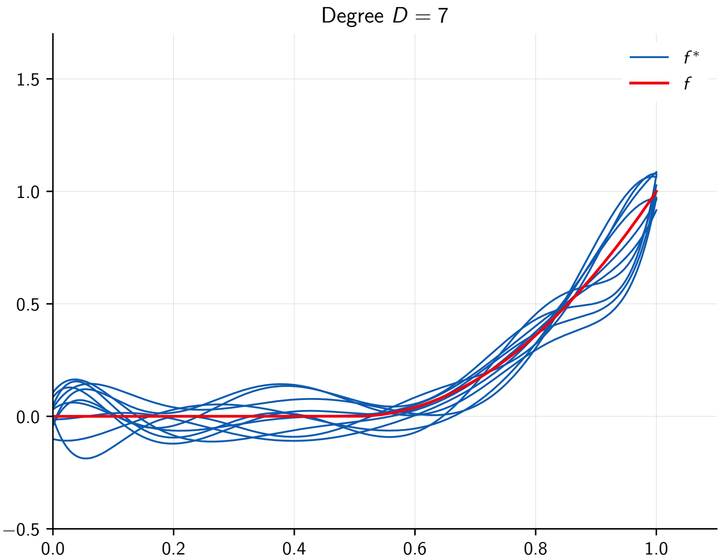

Degree $D = 3$
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
f^*
f



Degree $D = 4$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

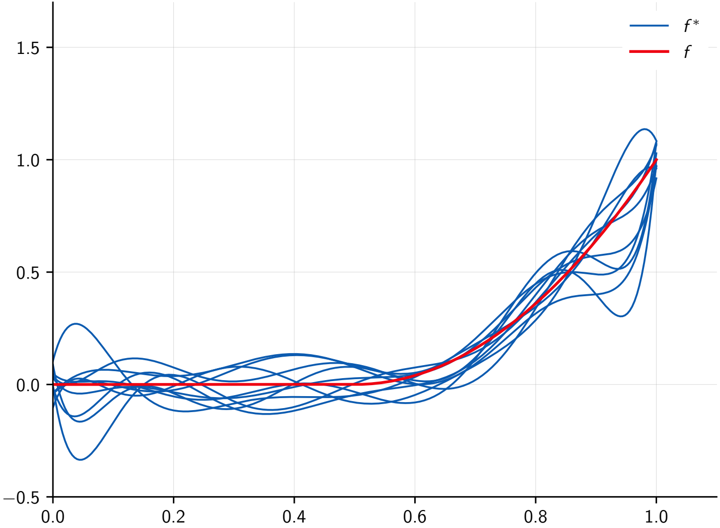

Degree $D = 5$
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
f^*
f

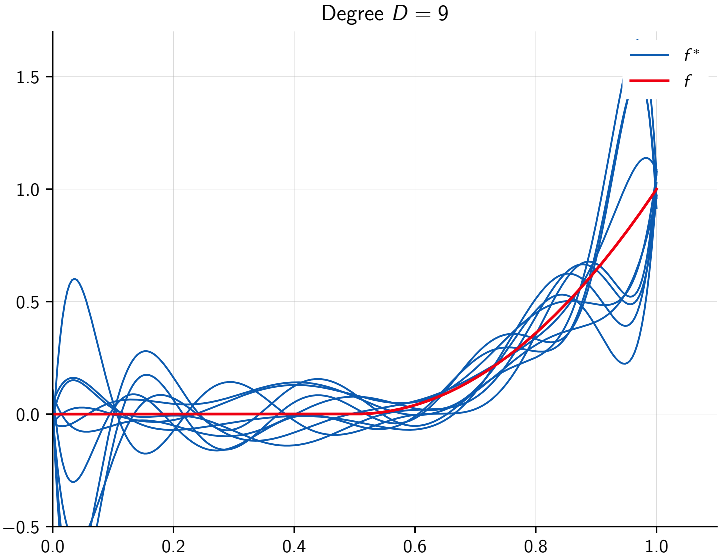

Degree $D = 6$
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
f^*
f



Degree $D = 7$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

Degree $D = 8$




Degree $D = 9$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

We can reformulate this control of the degree with a penalty

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

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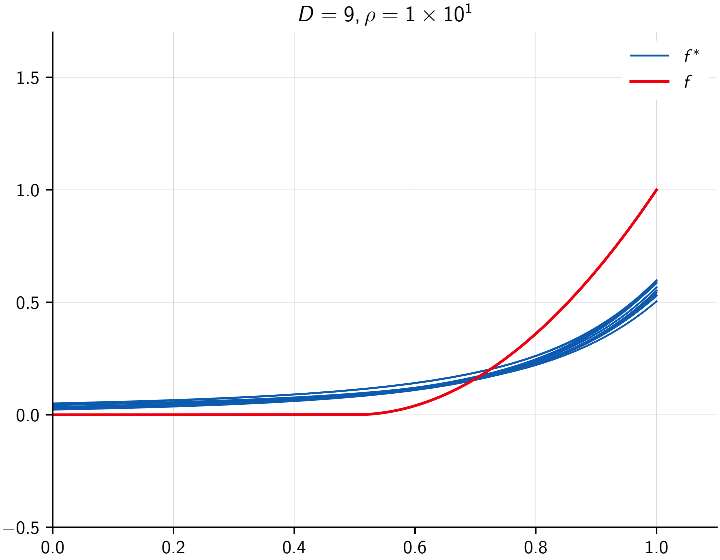
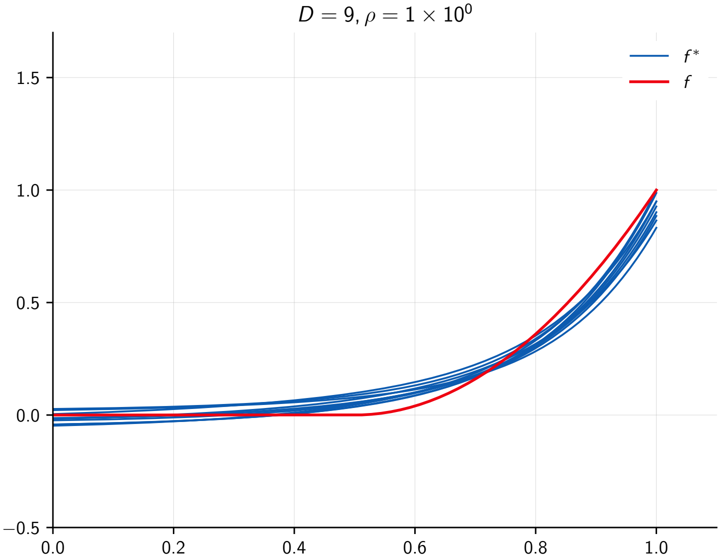
Such a penalty kills any term of degree $> D$.

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

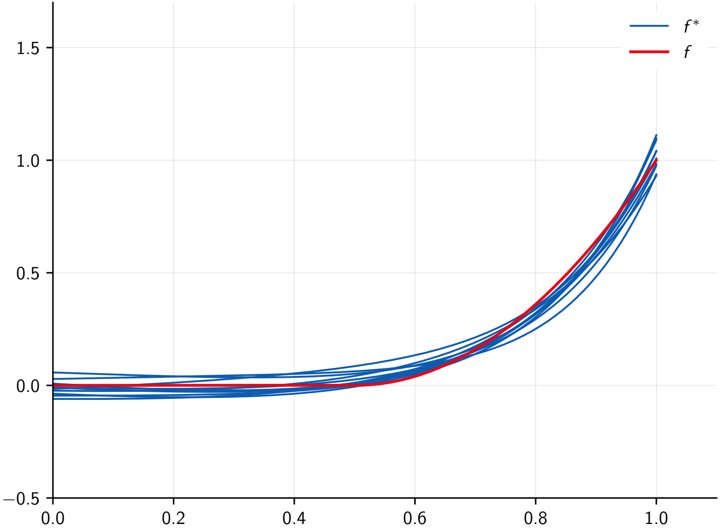
$$\mathscr{L}(\alpha) = \sum_n (f(x_n; \alpha) - y_n)^2 + \rho \sum_d \alpha_d^2.$$



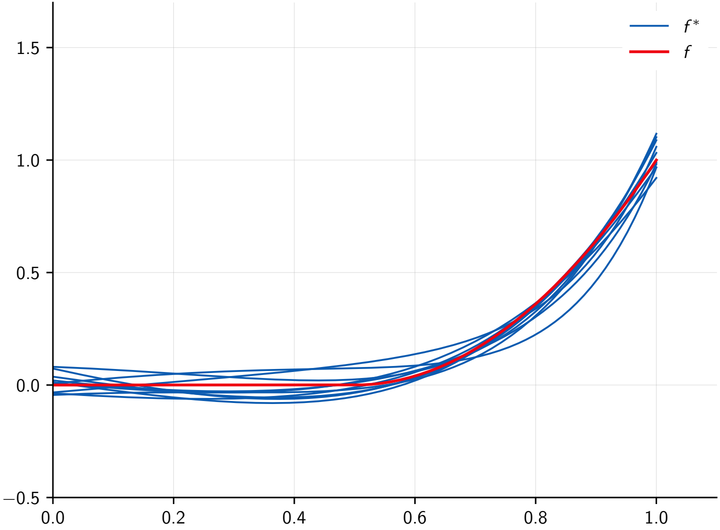
$D = 9, \rho = 1 \times 10^1$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

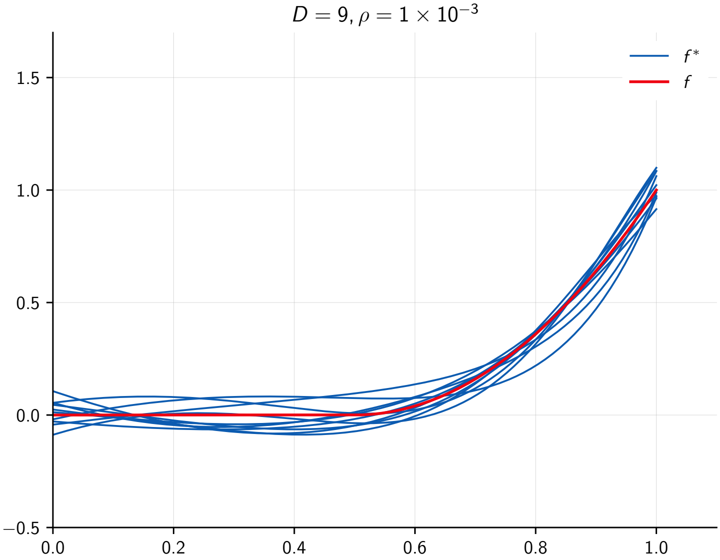

$D = 9, \rho = 1 \times 10^0$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

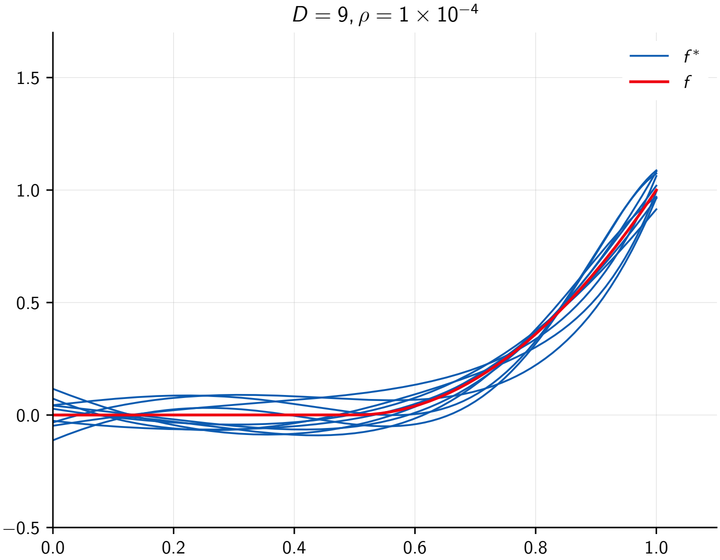
$D = 9, \rho = 1 \times 10^{-1}$



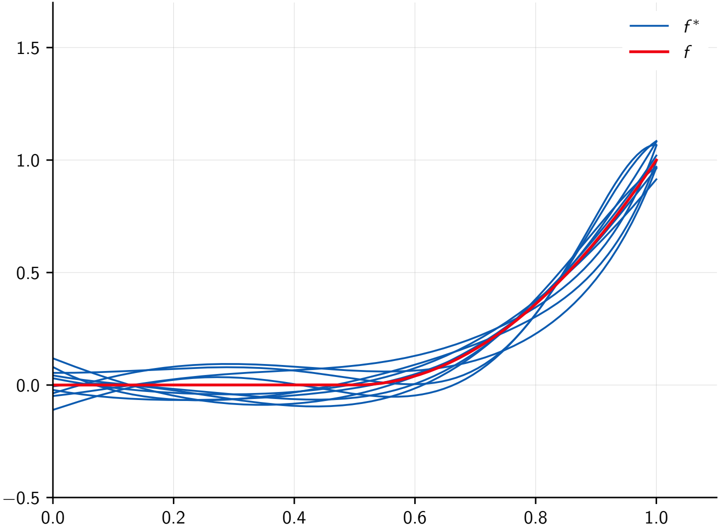
$D = 9, \rho = 1 \times 10^{-2}$

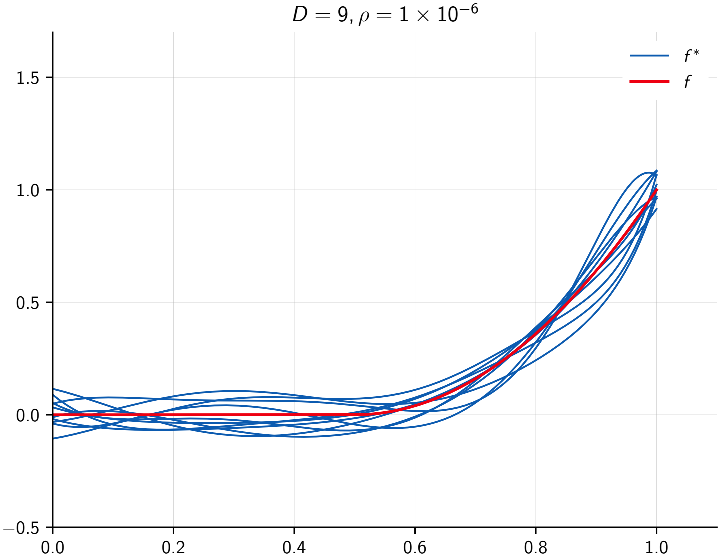


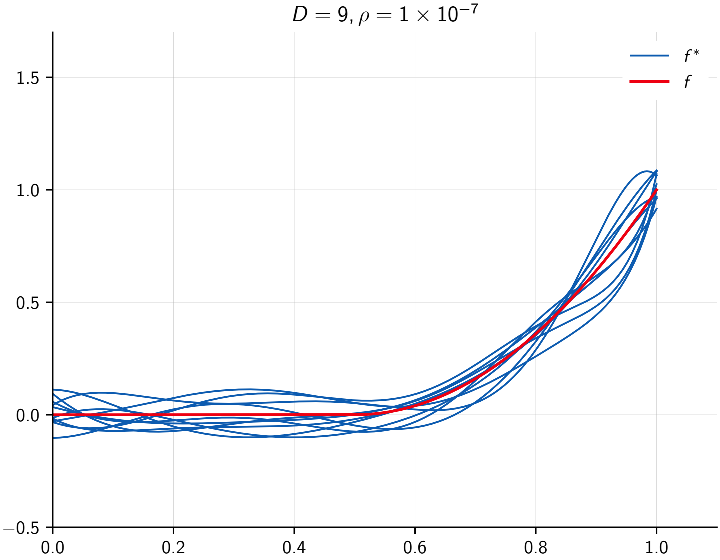

$D = 9, \rho = 1 \times 10^{-3}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

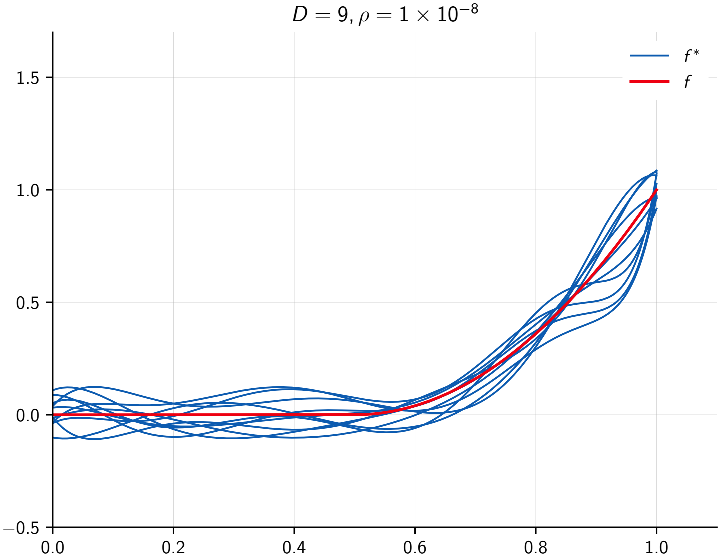

$D = 9, \rho = 1 \times 10^{-4}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

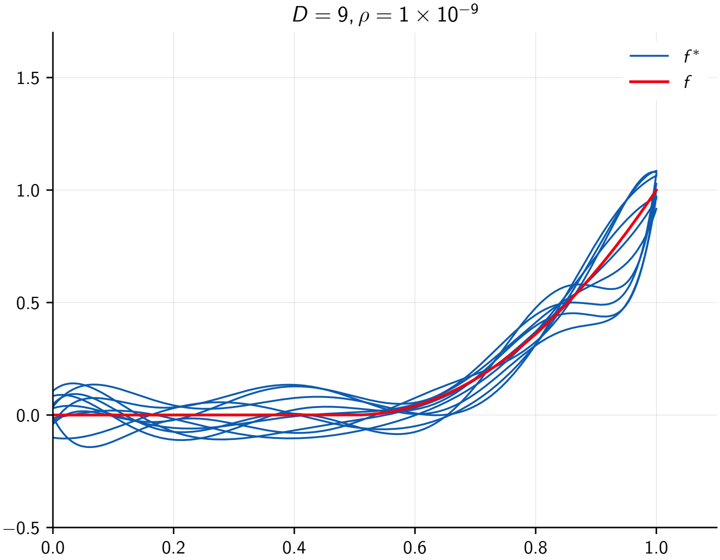
$D = 9, \rho = 1 \times 10^{-5}$



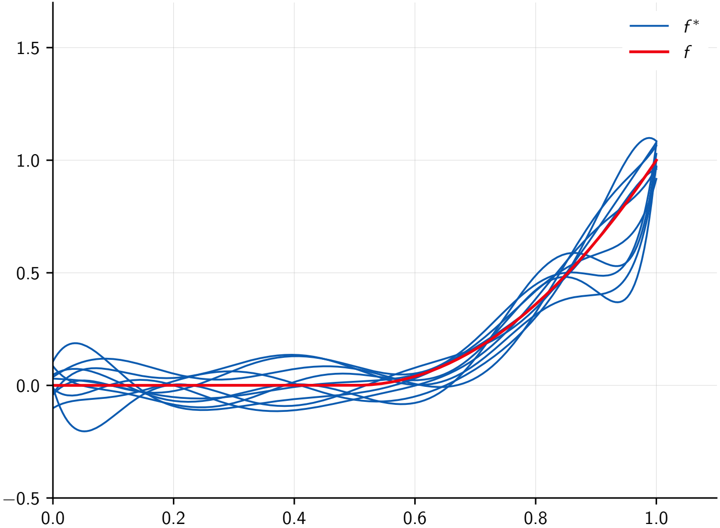

$D = 9, \rho = 1 \times 10^{-6}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


$D = 9, \rho = 1 \times 10^{-7}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

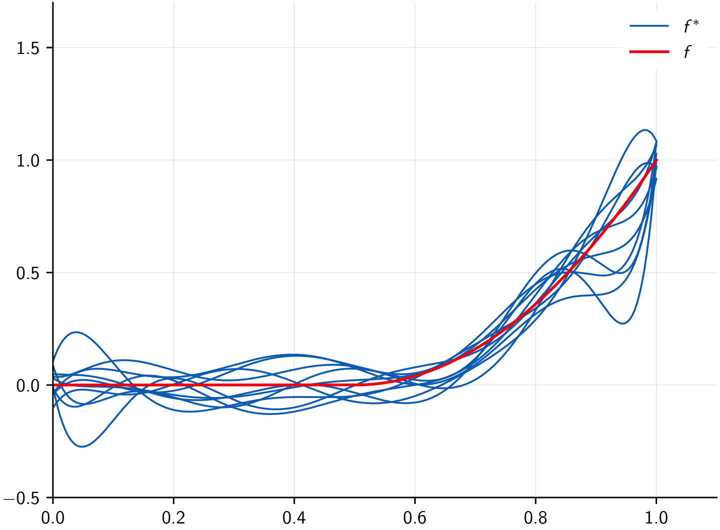

$D = 9, \rho = 1 \times 10^{-8}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


$D = 9, \rho = 1 \times 10^{-9}$
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
f^*
f

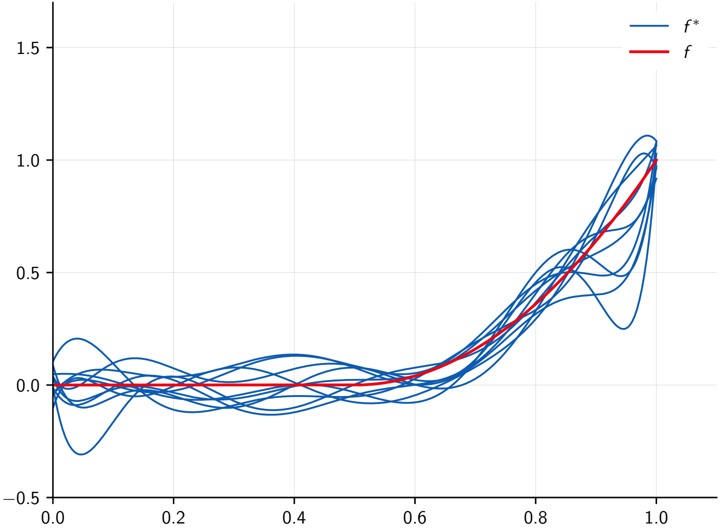
$D = 9, \rho = 1 \times 10^{-10}$

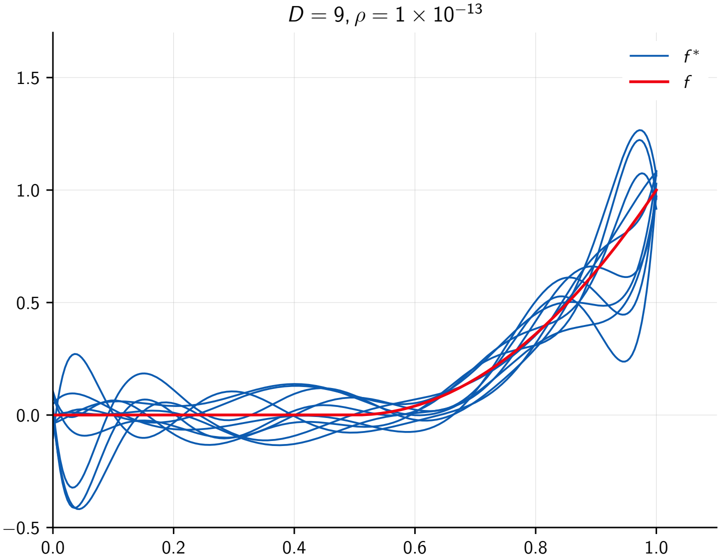


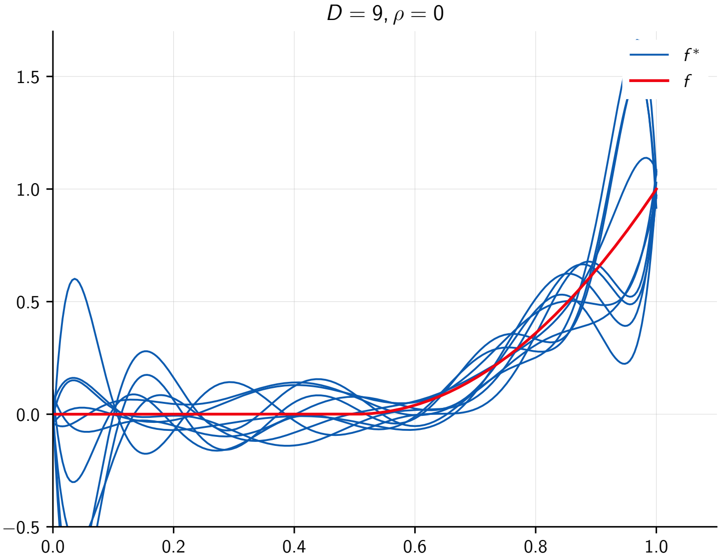
$D = 9, \rho = 1 \times 10^{-11}$

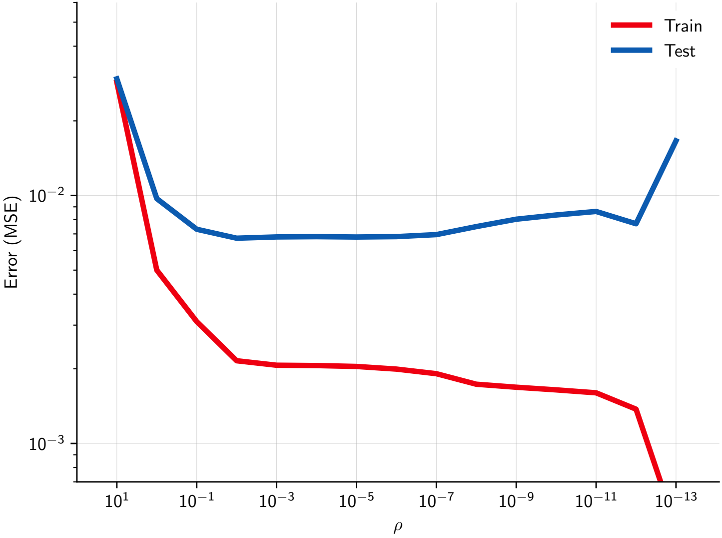


$D = 9, \rho = 1 \times 10^{-12}$




$D = 9, \rho = 1 \times 10^{-13}$
f^*
f
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0


$D = 9, \rho = 0$
1.5
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
f^*
f


Train
Test
Error (MSE)
10^{-2}
10^{-3}
10^{1}
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
ρ

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.

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.

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 $\mathscr{F}$ (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

V. N. Vapnik. The Nature of Statistical Learning Theory. Springer-Verlag, New York, 1995.