

EE-559 – Deep learning

2.3. Bias-variance dilemma

François Fleuret

<https://fleuret.org/ee559/>

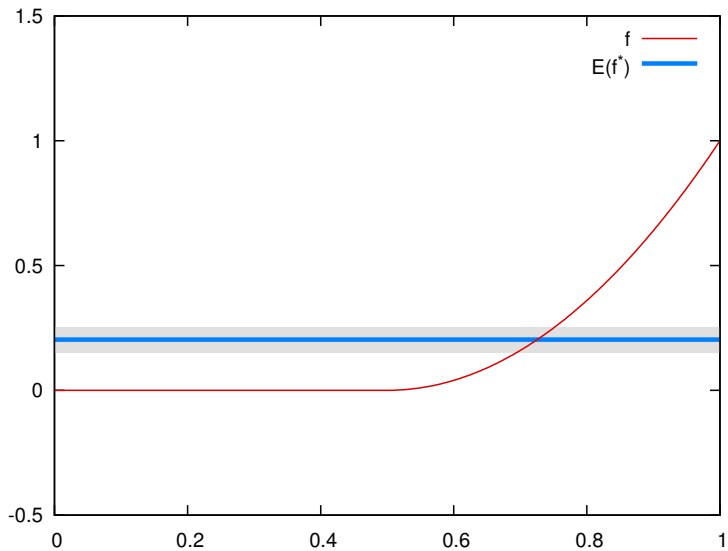
Feb 9, 2020

We can visualize over-fitting for our polynomial regression by generating multiple training sets $\mathcal{D}_1, \dots, \mathcal{D}_M$, training as many models f_1, \dots, f_M , and computing empirically the mean and standard deviation of the prediction at every point.

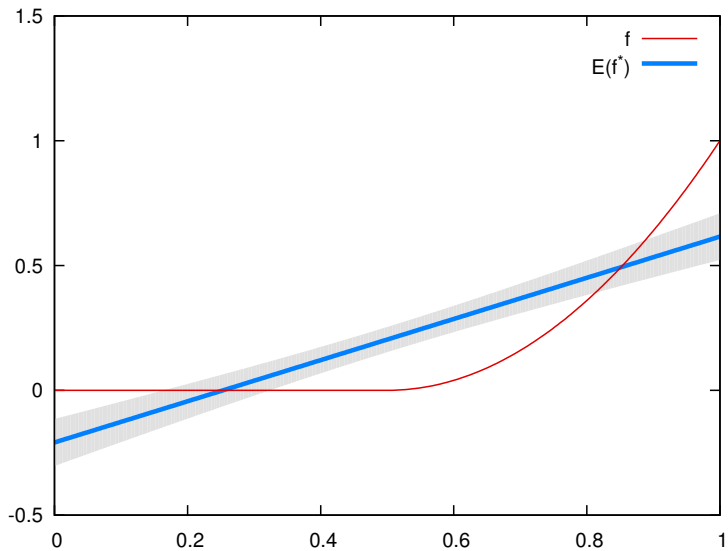
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When the capacity increases or regularization decreases, the mean of the predicted value gets right on target, but the prediction varies more across runs.

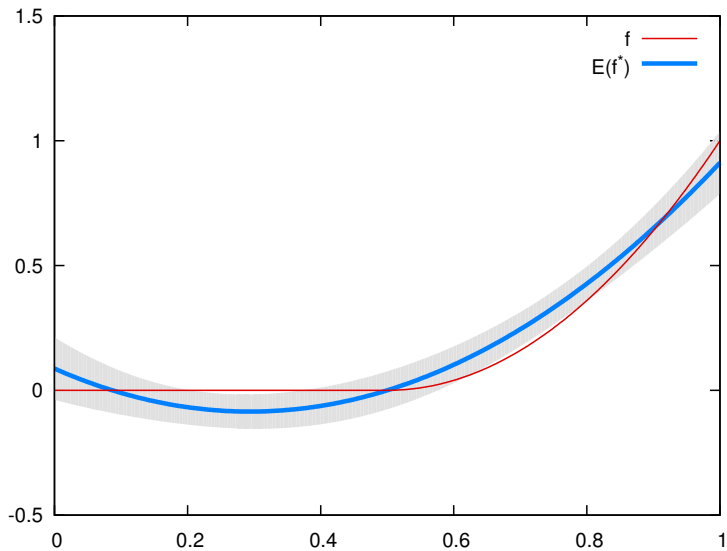
Degree D=0



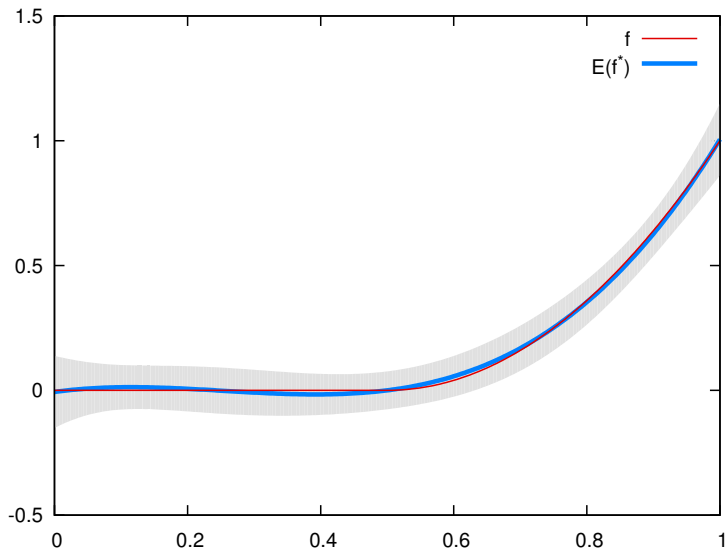
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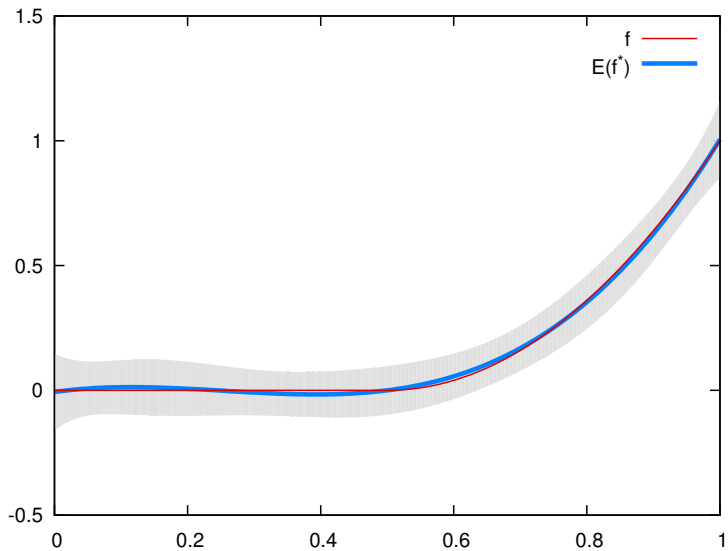
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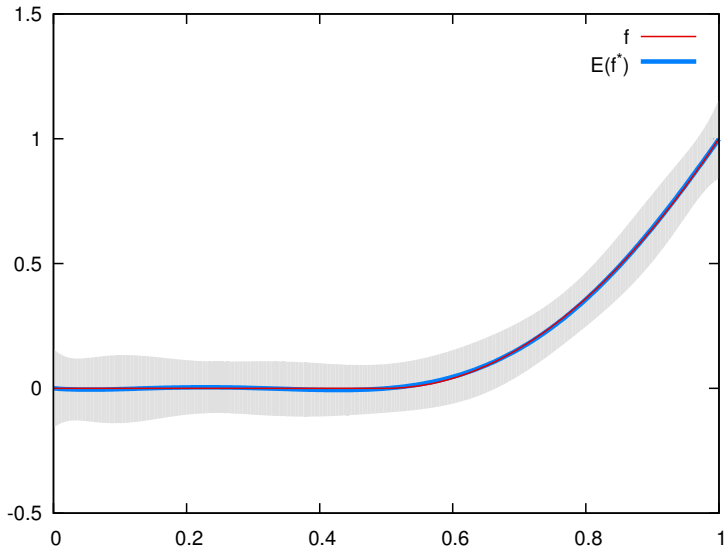
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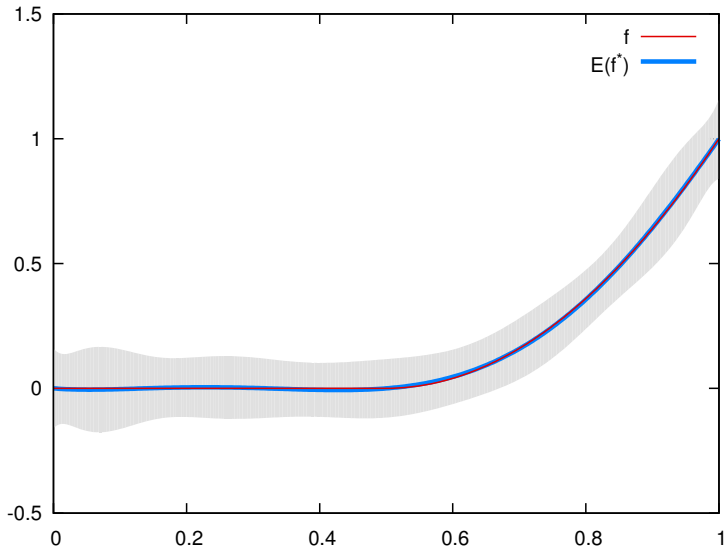
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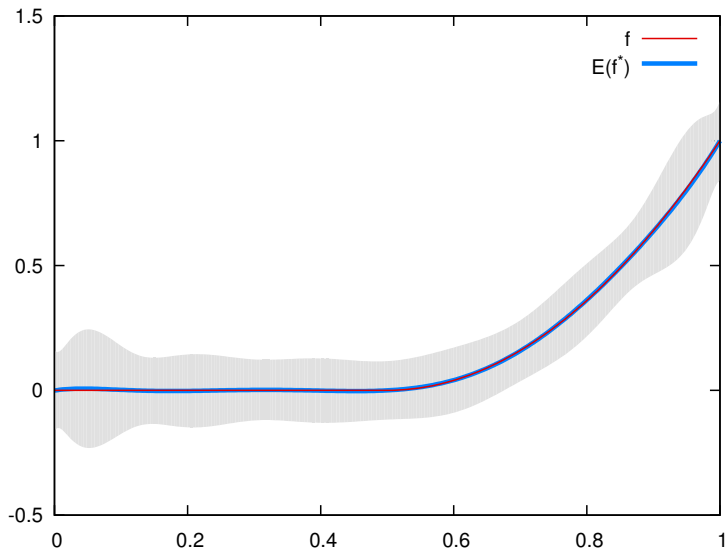
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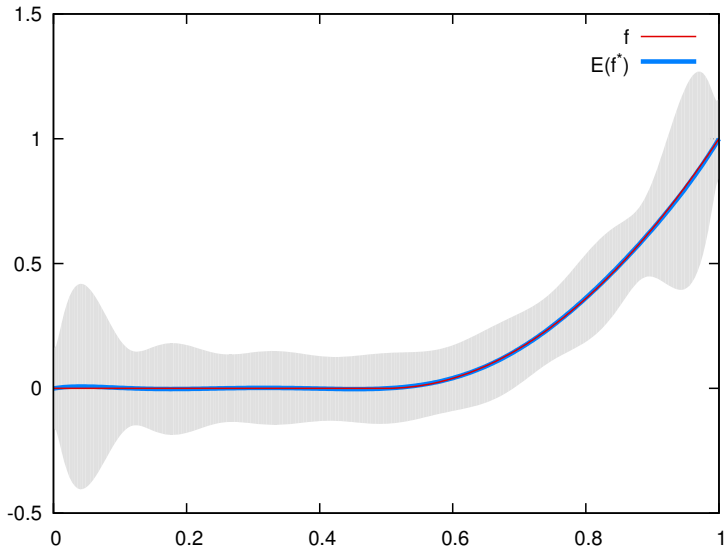
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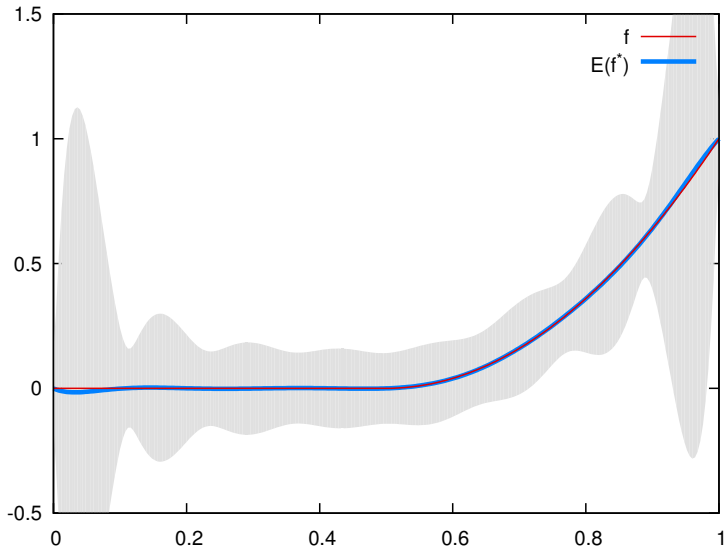
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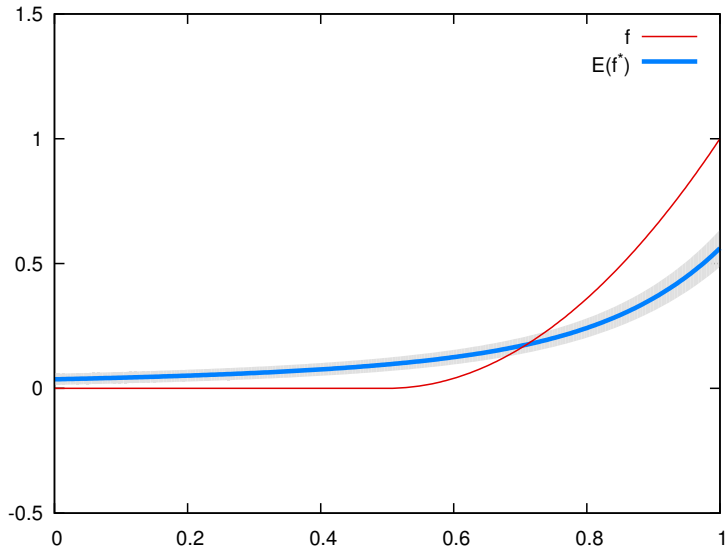
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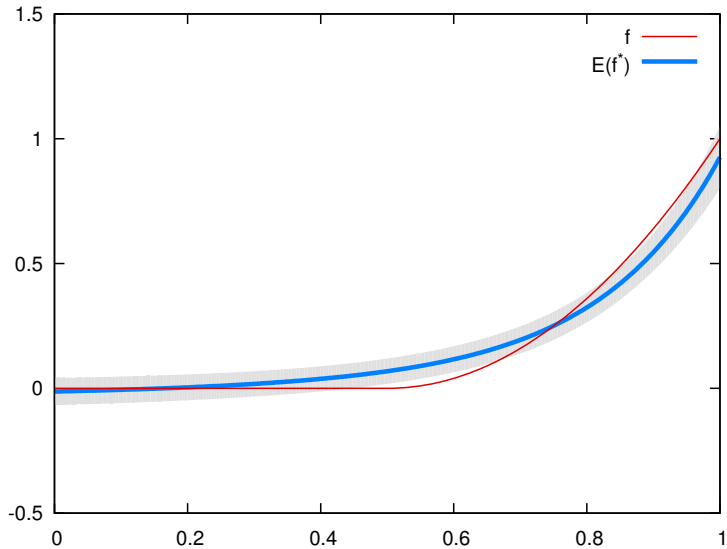
Degree D=9



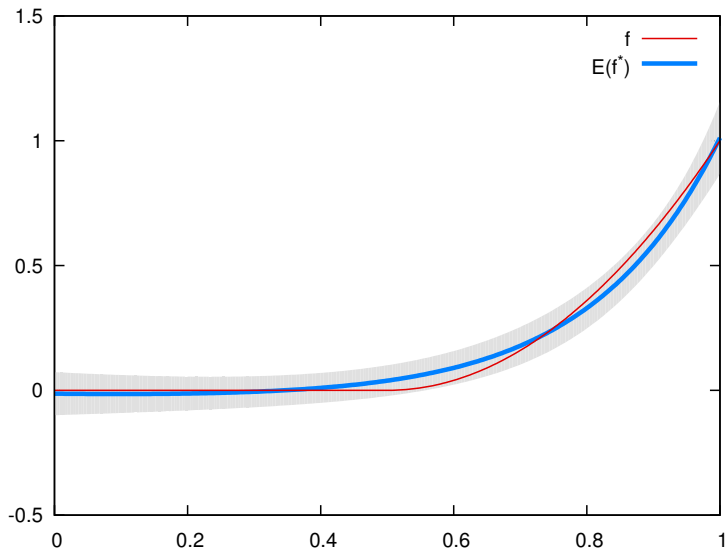
D=9, $\rho=1e1$



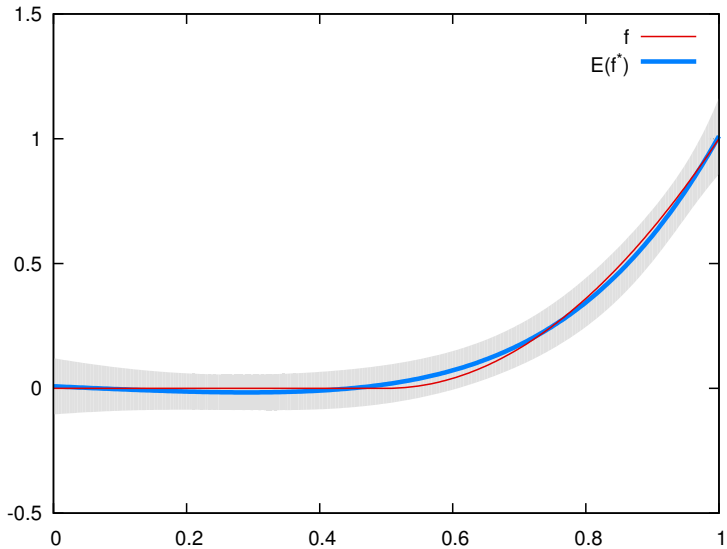
$D=9, \rho=1e0$



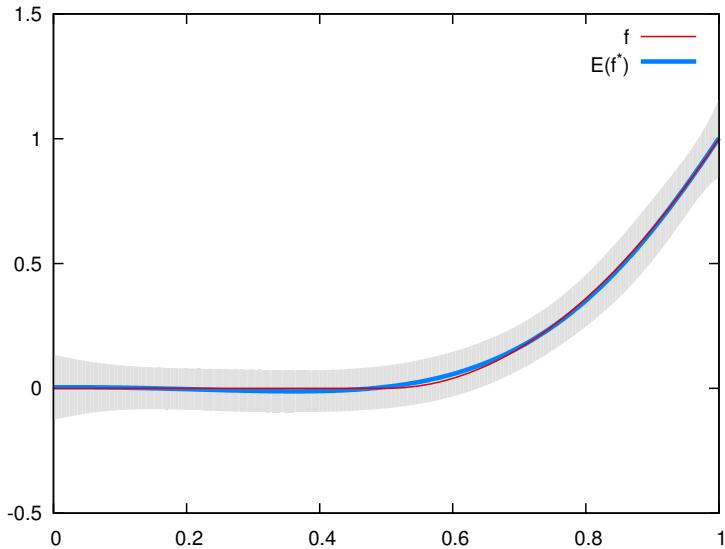
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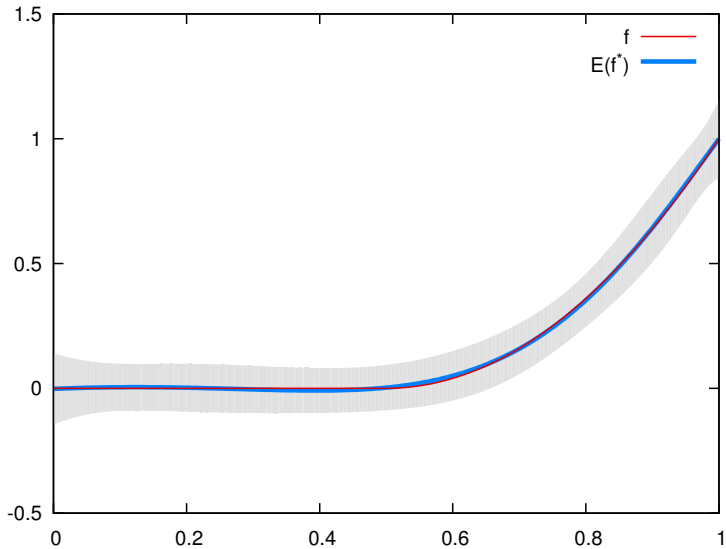
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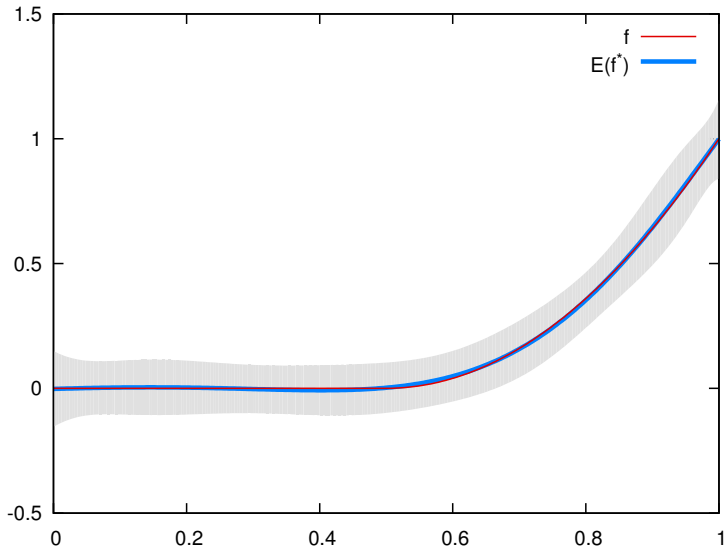
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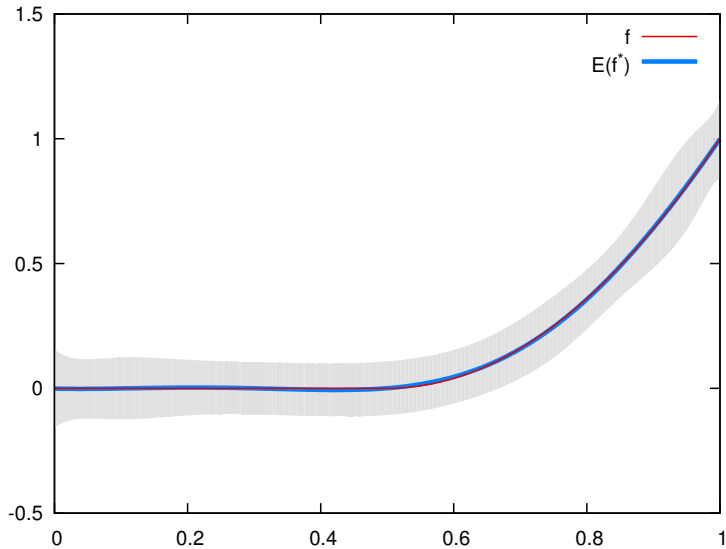
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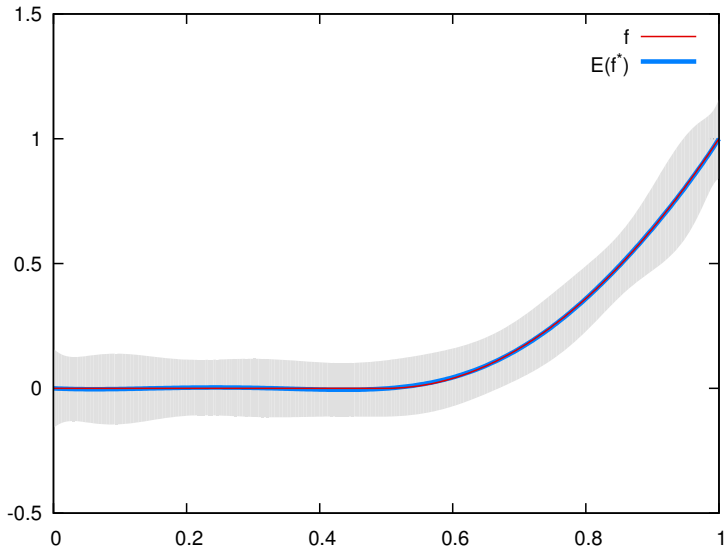
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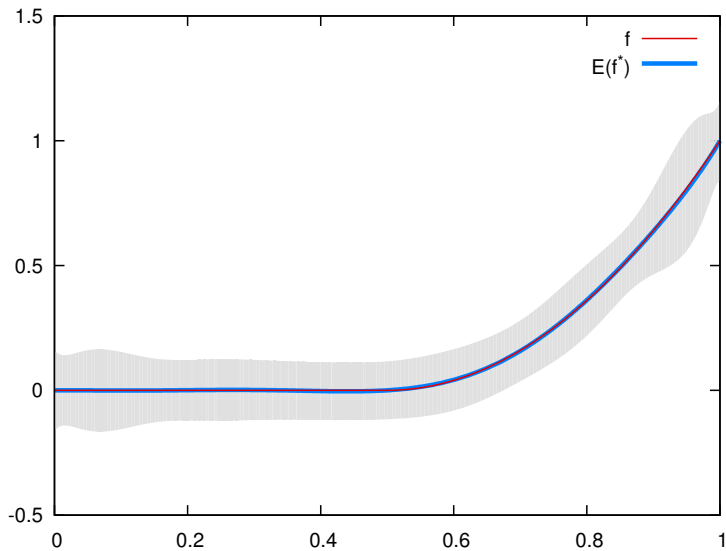
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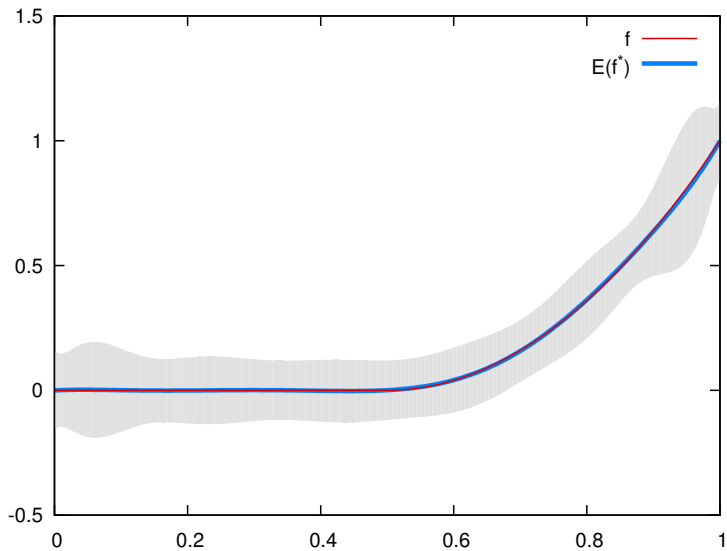
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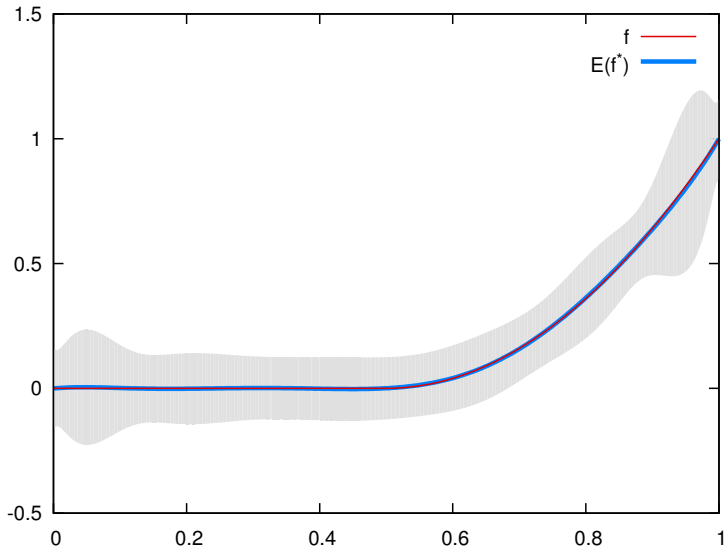
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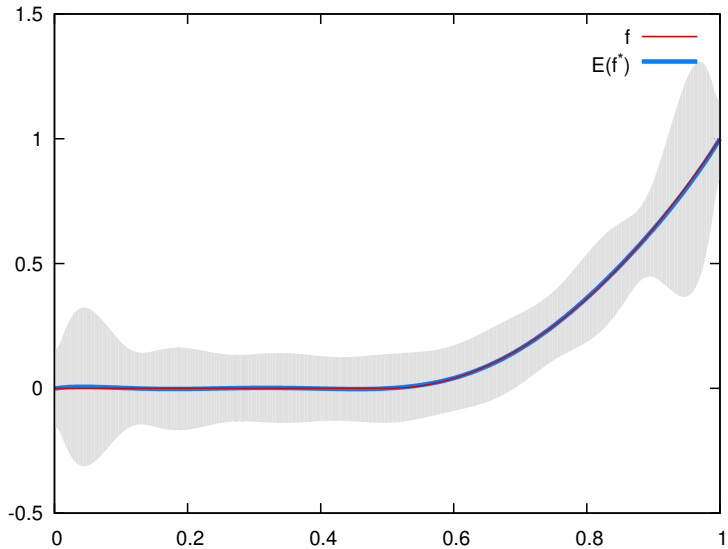
$D=9, \rho=1e-9$



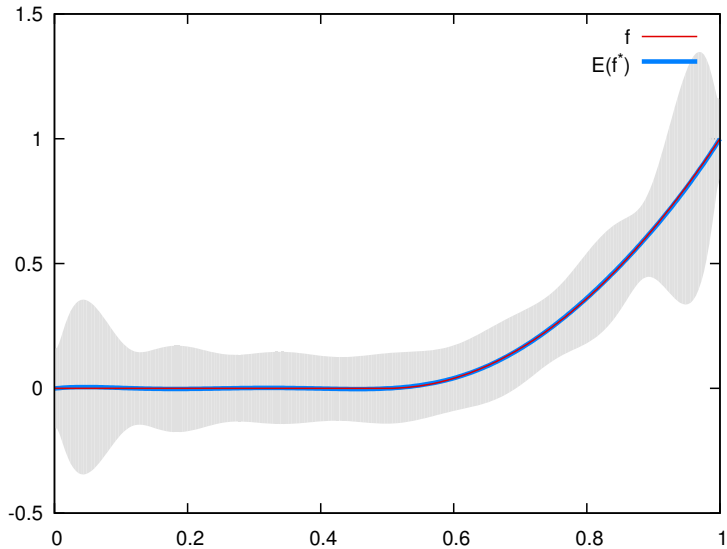
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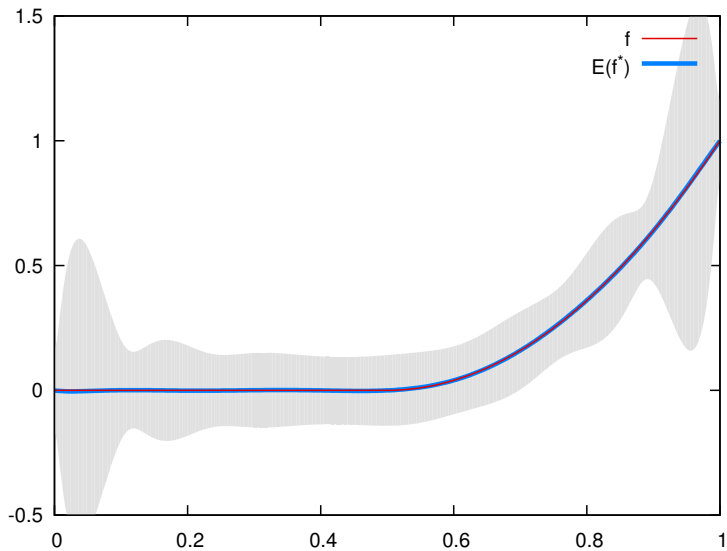
$D=9, \rho=1e-11$



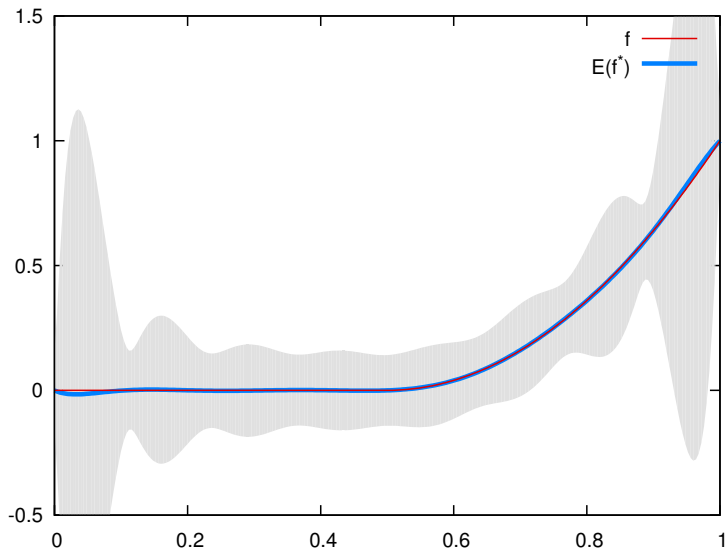
$D=9, \rho=1e-12$



$D=9, \rho=1e-13$



$D=9, \rho=0.0$



We can formalize these observations as follows:

Let x be fixed, y the “true” value associated to it, f^* the predictor we learned from the data-set \mathcal{D} , and $Y = f^*(x)$ be the value we predict at x .

If we consider that the training set \mathcal{D} is a random quantity, then f^* is random, and consequently Y is.

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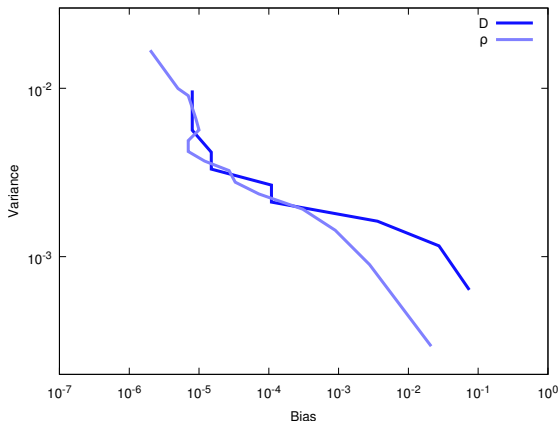
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This is the **bias-variance decomposition**:

- the bias term quantifies how much the model fits the data on average,
- the variance term quantifies how much the model changes across data-sets.

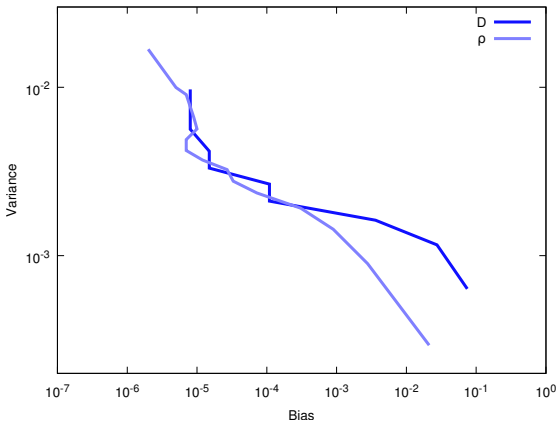
(Geman and Bienenstock, 1992)

From this comes the **bias-variance tradeoff**:



Reducing the capacity makes f^* fit the data less on average, which increases the bias term.

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Reducing the capacity makes f^* fit the data less on average, which increases the bias term. Increasing the capacity makes f^* vary a lot with the training data, which increases the variance term.

Is all this probabilistic?

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By looking at the data \mathcal{D} , we can estimate a posterior distribution for the said parameters,

$$\mu_A(\alpha \mid \mathcal{D} = \mathbf{d}) \propto \mu_{\mathcal{D}}(\mathbf{d} \mid A = \alpha) \mu_A(\alpha),$$

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and from that their most likely values.

So instead of a penalty term, we define a prior distribution, which is usually more intellectually satisfying.

For instance, consider a polynomial model with Gaussian prior, that is

$$\forall n, Y_n = \sum_{d=0}^D A_d X_n^d + \Delta_n,$$

where

$$\forall d, A_d \sim \mathcal{N}(0, \xi), \forall n, X_n \sim \mu_X, \Delta_n \sim \mathcal{N}(0, \sigma)$$

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For clarity, let $A = (A_0, \dots, A_D)$ and $\alpha = (\alpha_0, \dots, \alpha_D)$.

Remember that $\mathcal{D} = \{(X_1, Y_1), \dots, (X_N, Y_N)\}$ is the (random) training set and $\mathbf{d} = \{(x_1, y_1), \dots, (x_N, y_N)\}$ is a realization.

$$\log \mu_A(\alpha \mid \mathcal{D} = \mathbf{d})$$

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&= \log \frac{\mu_{\mathcal{D}}(\mathbf{d} \mid A = \alpha) \mu_A(\alpha)}{\mu_{\mathcal{D}}(\mathbf{d})} \\
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&= \log \prod_n \mu(x_n, y_n \mid A = \alpha) + \log \mu_A(\alpha) - \log Z \\
&= \log \prod_n \mu(y_n \mid X_n = x_n, A = \alpha) \underbrace{\mu(x_n \mid A = \alpha)}_{= \mu(x_n)} + \log \mu_A(\alpha) - \log Z
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&= \log \prod_n \mu(y_n \mid X_n = x_n, A = \alpha) + \log \mu_A(\alpha) - \log Z' \\
&= - \underbrace{\frac{1}{2\sigma^2} \sum_n \left(y_n - \sum_d \alpha_d x_n^d \right)^2}_{\text{Gaussian noise on } Y} - \underbrace{\frac{1}{2\xi^2} \sum_d \alpha_d^2}_{\text{Gaussian prior on } A} - \log Z'' .
\end{aligned}$$

Taking $\rho = \sigma^2/\xi^2$ gives the penalty term of the previous slides.

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Regularization seen through that prism is intuitive: The stronger the prior, the more evidence you need to deviate from it.

The end

References

- S. Geman and E. Bienenstock. **Neural networks and the bias/variance dilemma.** Neural Computation, 4:1–58, 1992.