Deep Learning & Applied AI

Going nonlinear, overfitting, and regularization

Emanuele Rodolà
rodola@di.uniroma1.it

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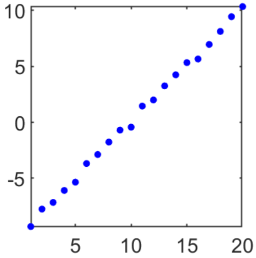
A glimpse into neural networks

In deep learning, we deal with highly parametrized models called deep neural networks:

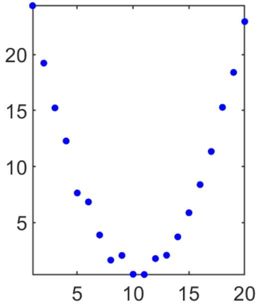
$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

Parametrized models

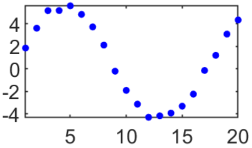
The parameters describe the behavior of the network, and must be solved for.



$$y = ax + b$$



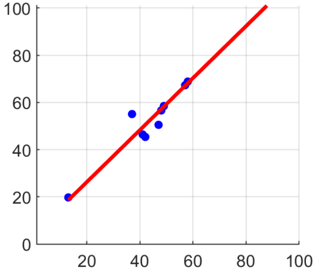
$$y = ax^2 + bx + c$$



$$y = a\sin(x) + bx + c$$

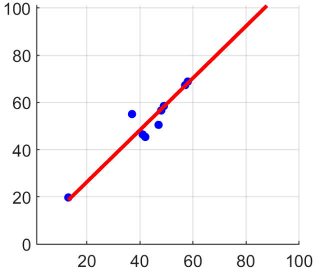
From a technical standpoint, our task is to determine the parameters Θ.

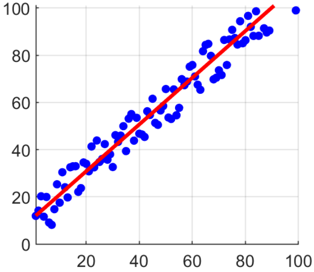
Data distribution



Assumption: linear model

Data distribution





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More data allows us to improve our prediction

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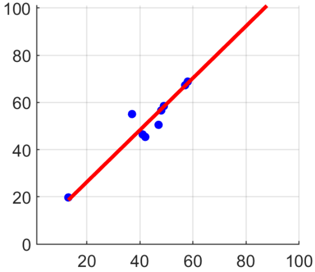

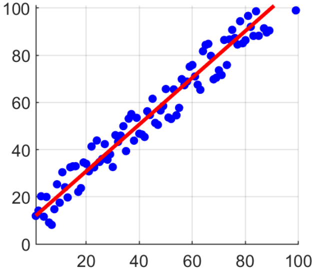

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What if the assumption (i.e. linear prior here) is **wrong**?

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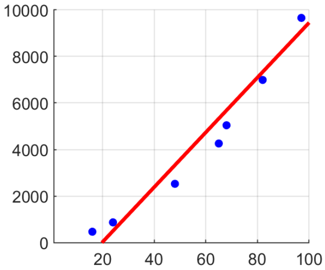

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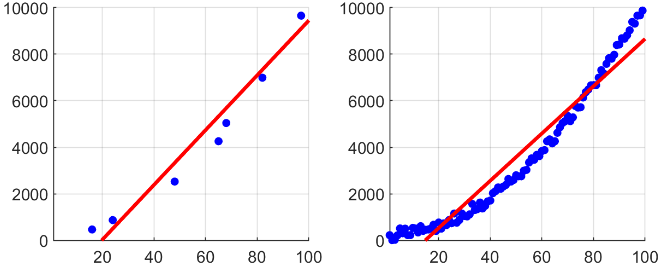

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More data confutes our assumptions

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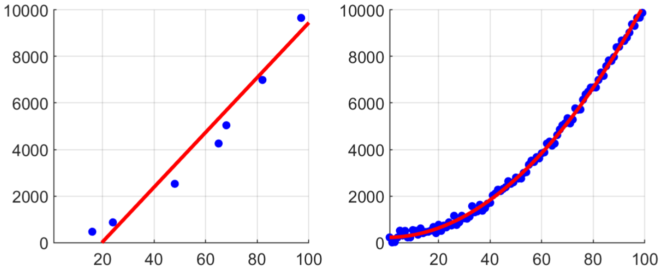

Assumption: quadratic model

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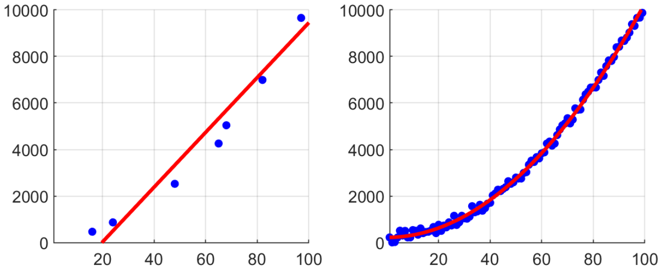

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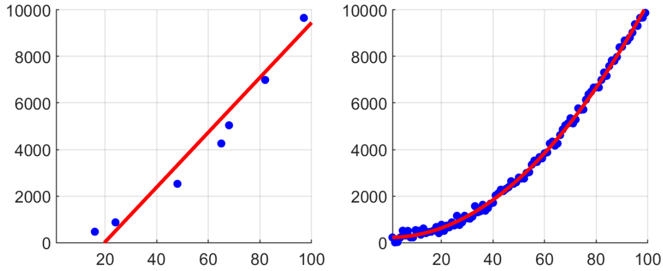

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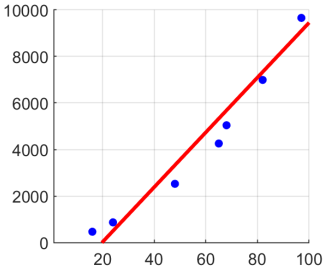

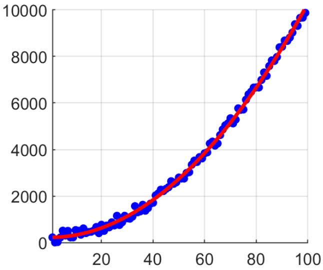

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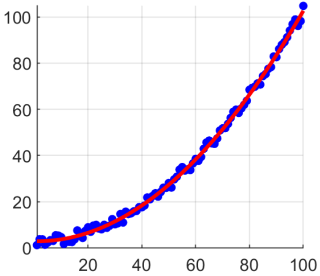
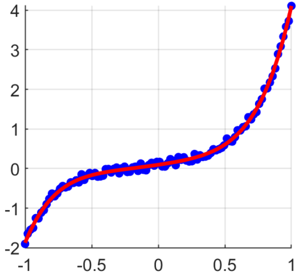
- How much data do we need?
- What if the correct distribution does not admit a simple expression?

Polynomial regression

After the linear model, the simplest thing is a polynomial model.



2nd-order



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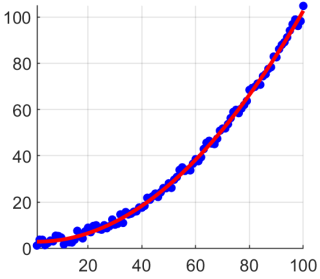

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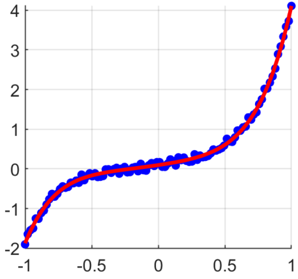

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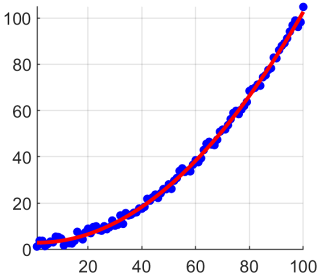

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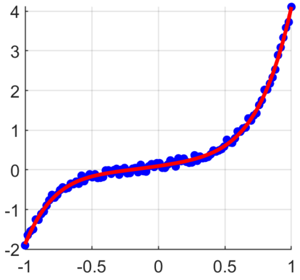

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More data are needed to make an informed decision on the order.

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The same exact least-squares solution as with linear regression applies, with the requirement that $k < n$.

Polynomial fitting

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If f is continuous on the interval $[a, b]$, then for every $\epsilon > 0$ there exists a polynomial p such that $|f(x) - p(x)| < \epsilon$ for all x.

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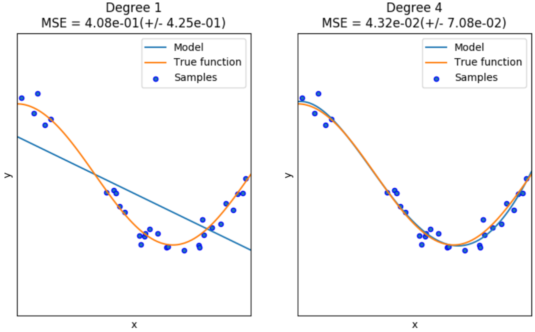

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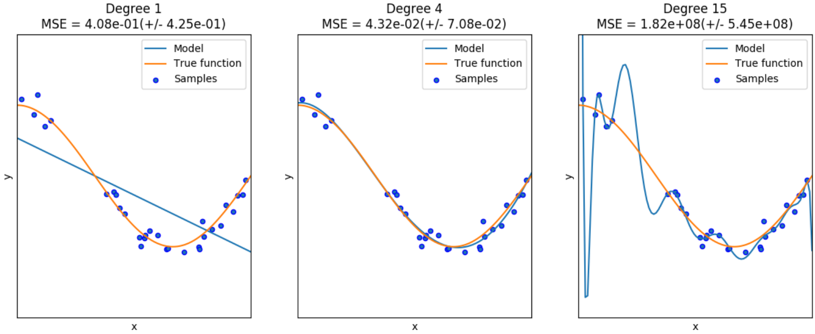

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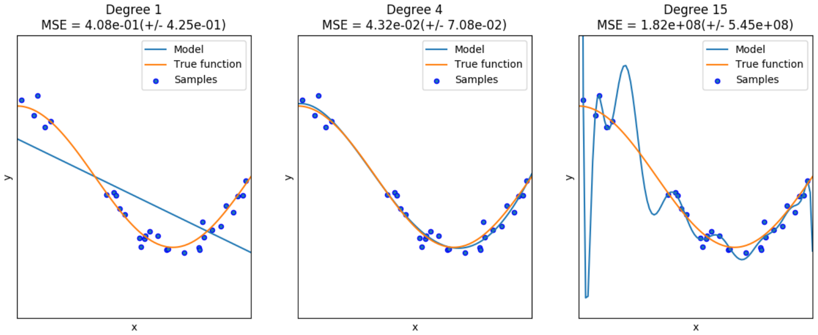

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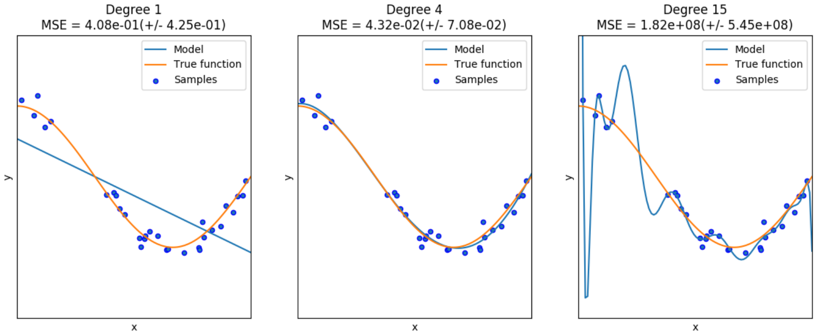

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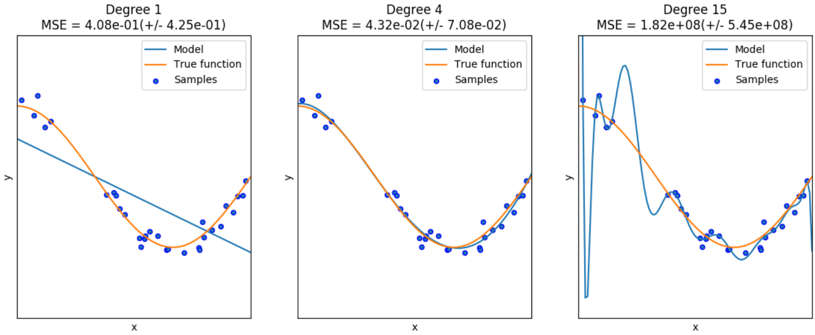

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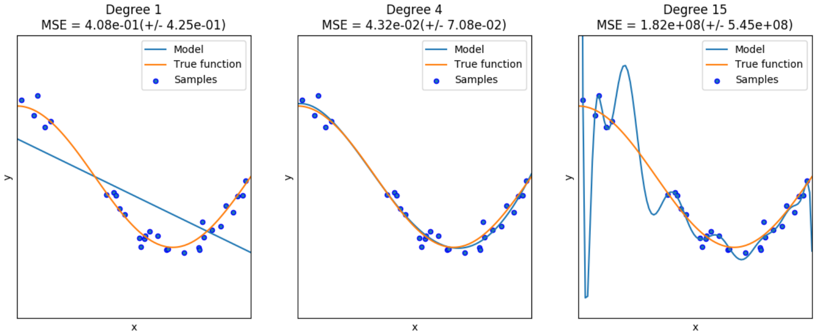

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Adding complexity can lead to overfitting and thus worse generalization.

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Underfitting:
large training error, large validation error

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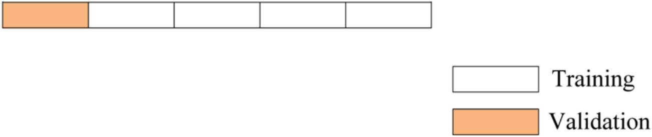

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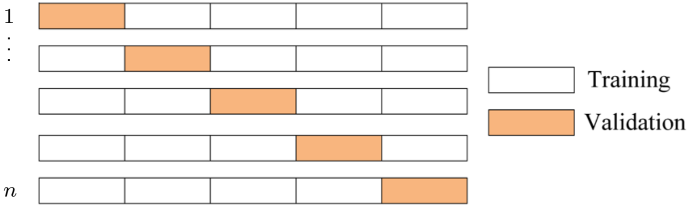

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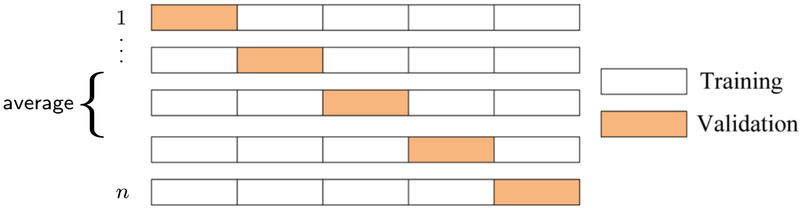

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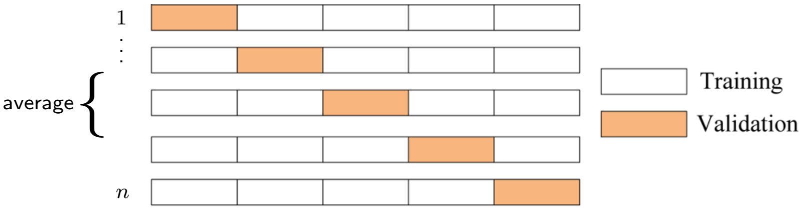

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Example: For polynomial regression, do the above many times with different degrees, choose the run with the smallest average MSE.

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- Regularization
- Additional priors
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From now on, we embrace the idea that many natural phenomena of interest are nonlinear.

Regularization penalties

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For example, avoid large parameters to counteract overfitting and thus control the complexity of our learning model:

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Other forms include the choice of a representation, early stopping, dropout, etc. (we'll see them in the future lectures)

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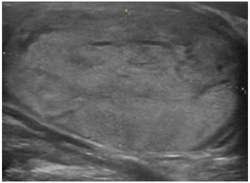
Classification

What if we want to predict a category instead of a value?

$f_\Theta($  $) = \{0, 1\}$

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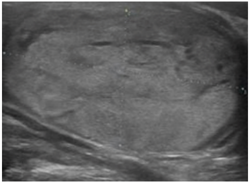
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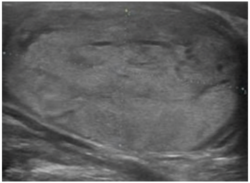
$f_{\Theta}($  $) = \{0, 1\}$

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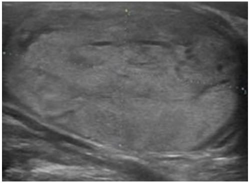
$$f_\Theta($$  $$) = \{0, 1\}$$

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Instead: Modify the loss to minimize over categorical values directly.

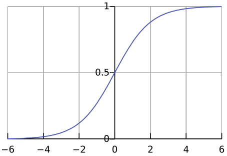
Logistic regression

New loss:

$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} (y_i - \sigma(\underbrace{ax_i + b}_{\text{linear}}))^2$$

Here, σ is the nonlinear logistic sigmoid:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



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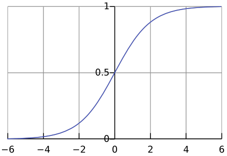

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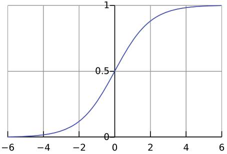

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$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} c(x_i, y_i)\,, \quad \text{with}$$

$$c(x_i, y_i) = \begin{cases} -\ln(\sigma(ax_i + b)) & y_i = 1 \\ -\ln(1 - \sigma(ax_i + b)) & y_i = 0 \end{cases} \qquad \text{convex}$$

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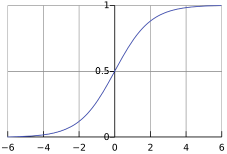

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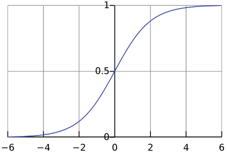

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$$\ell_\Theta(\{x_i, y_i\}) = -\sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b))$$

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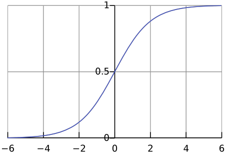

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With neural networks, the number of parameters will be very high, so the risk of overfitting is always behind the corner.

Suggested reading

On polynomial regression vs. neural nets:
https://arxiv.org/pdf/1806.06850

Proof that the logistic loss is convex:
https://math.stackexchange.com/questions/1582452/logistic-regression-prove-that-the-cost-function-is-convex