Machine learning from scratch

Lecture 6: Non-linear models, parameter selection

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Course outline

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This lecture will go a bit further by introducing:

- Regularization
- Non linear models (polynomial kernels)
- Model evaluation
- Parameter selection

Regularizing models

Outliers and overfitting

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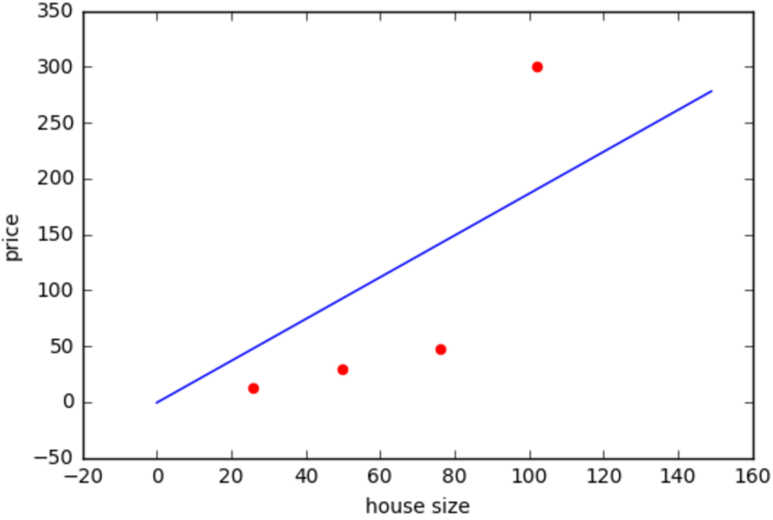

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where λ is a **hyper-parameter** that quantifies how much we want to penalize big values of θ.

Outliers and overfitting

In the end, $J(\theta)$ is as follows:

$$J(\theta) = L(\theta) + \lambda R(\theta)$$

where

- L is the **loss term**
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A commonly used regularization term is often the squared ℓ_2-norm, given by:

$$R(\theta) = \|\theta\|_2^2 = \sum_{j=1}^{d} \theta_j^2$$

ℓ_2-regularized OLS

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Exercice: Recall

$$R(\theta) = \|\theta\|_2^2 = \sum_{j=1}^{d} \theta_j^2$$

What is $\nabla R(\theta)$?

ℓ_2-regularized OLS

Hint: Recall the definition of the gradient:

$$\nabla R(\theta) = \left[\frac{\partial}{\partial \theta_1} R(\theta), \ldots, \frac{\partial}{\partial \theta_d} R(\theta) \right]$$

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Hint: Recall the definition of the gradient:

$$\nabla R(\theta) = \left[\frac{\partial}{\partial \theta_1} R(\theta), \ldots, \frac{\partial}{\partial \theta_d} R(\theta)\right]$$

Solution:

$$\begin{aligned}
\frac{\partial}{\partial \theta_k} R(\theta) &= \frac{\partial}{\partial \theta_k} \sum_{j=1}^{d} \theta_j^2 \\
&= \sum_{j=1}^{d} \frac{\partial}{\partial \theta_k} \theta_j^2 \\
&= 2\theta_j
\end{aligned}$$

Conclusion:

$$\nabla R(\theta) = [2\theta_1, \ldots, 2\theta_d]$$

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Question: Given

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Hint: Recall the gradient descent update rule:

$$\theta_k := \theta_k - \alpha \frac{\partial}{\partial \theta_k} J(\theta)$$

Solution: We have

$$\frac{\partial}{\partial \theta_k} L(\theta) = (y - h(\boldsymbol{x}))\, x_k \qquad \text{and} \qquad \frac{\partial}{\partial \theta_k} R(\theta) = 2\theta_k$$

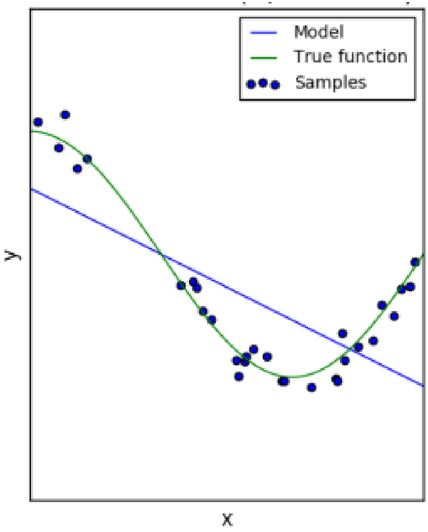
so

$$\theta_k := \theta_k - \alpha((y - h(\boldsymbol{x}))\, x_k - 2\lambda\theta_k)$$

More sophisticated models

Non-linearity

We might want to apply OLS to this data:



Non-linearity

We'd rather try to fit **a polynomial** on the data:

$$\hat{y} = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d = \sum_{k=0}^{d} \theta_d x^d$$

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Se need to find $\theta_0, \theta_1, \ldots, \theta_d$, which can be achieved by defining a new feature vector $\phi(x) = [1, x, x^2, \ldots, x^d]$ and define the prediction model

$$\hat{y} = \theta^T h(\phi(x)) = \sum_{k=0}^{d} \theta_d x^d$$

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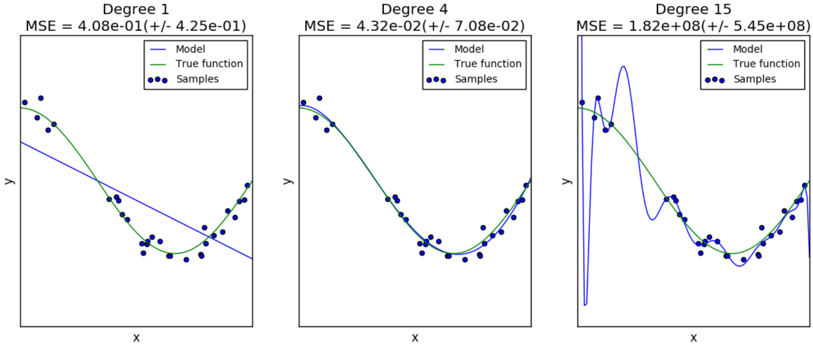
OLS can train θ and we have a **polynomial model**. The trick is to apply a **non-linearity mapping** ϕ.

Non-linearity

Problem: We would need to find an appropriate value for the degree d, because:



Hyperparameters

This is a **more general problem**: **Tuning hyperparameters**. The current version of OLS we have has several parameters:

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As we've seen, all these 3 parameters can have a **dramatic impact** on the quality of our prediction model! Hence, we need to **tune them** properly.

Model evaluation
Parameter selection

Train-test split

As we saw with OLS, ML algorithms usually rely on **many parameters**. How to **tune** them properly given a data set?

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This is often referred to as **cross-validation**.

Cross-validation

Standard technique: Hold-out cross-validation:

- Train on a part of the data (e.g. 70%)
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Another standard technique: k-**fold cross-validation**

- Split the data into k (equally-sized) folds
- Remove 1 fold (= test fold)
- Train on the other folds
- Test on the removed fold
- Do it for all the folds

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- **Remove 1 sample** from the data set
- Train on **all the other samples**
- Test on the sample you've removed
- **Evaluate** the prediction
- Do it **for each sample of the data set**
- **Aggregate** the evaluations

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Alternative: Leave-p-out (LPO). LOO is LPO with $p = 1$.

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- For each parameter combination, train/test the model
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Important note: Hyper-parameter ranges vary a lot from an application to another. It is **data-dependent**.

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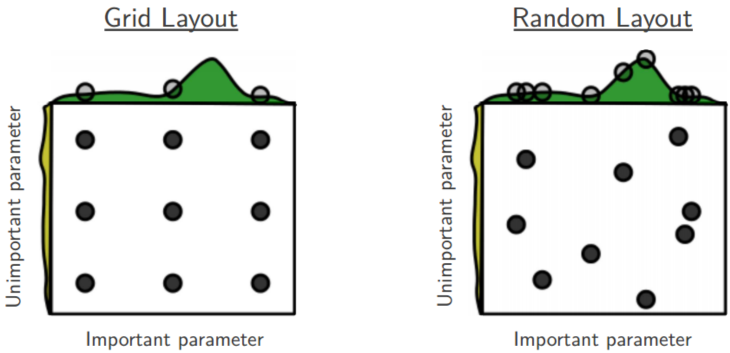

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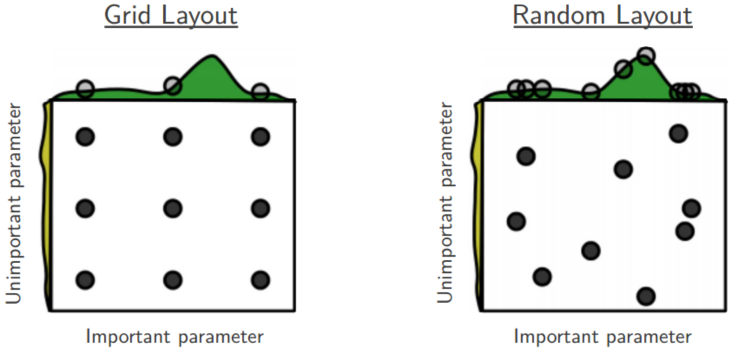

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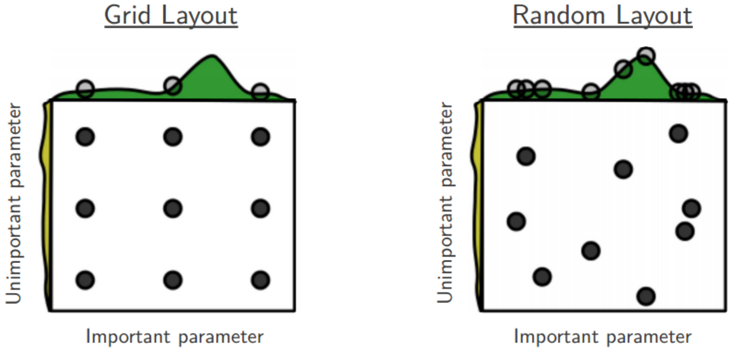

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Practical note: Each parameter combination can be trained/tested separately => possibility to distribute the tasks

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- How to evaluate models
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During the next lecture, we will work on implementing regularization to the OLS algorithm and cross-validating it and switch to classification if the time allows it.

Thank you! Questions?