Introduction to Artificial Intelligence (ENSIMAG) Intelligent Systems (MOSIG)

Regularization

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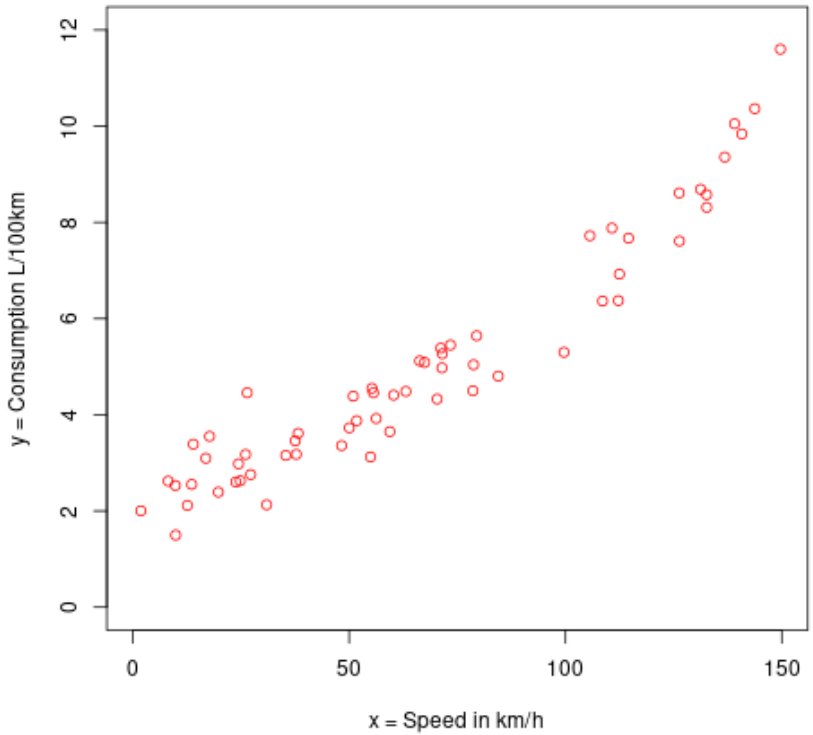
Worked-out example

You want to model the fuel consumption (L/100km) with respect to the speed (km/h).

Worked-out example: the training data

Your neighbor, gives you her home-made measurements.

It consists in $(x_i, y_i), i = 1, ..60$



Worked-out example: choose the model

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What is the associated loss?

Loss

Write the negative log-likelihood:

$$\mathcal{L}(\theta, x, y) = \frac{1}{2\sigma^2} \sum_i [y_i - (\theta_0 + \theta_1.x_i)]^2$$

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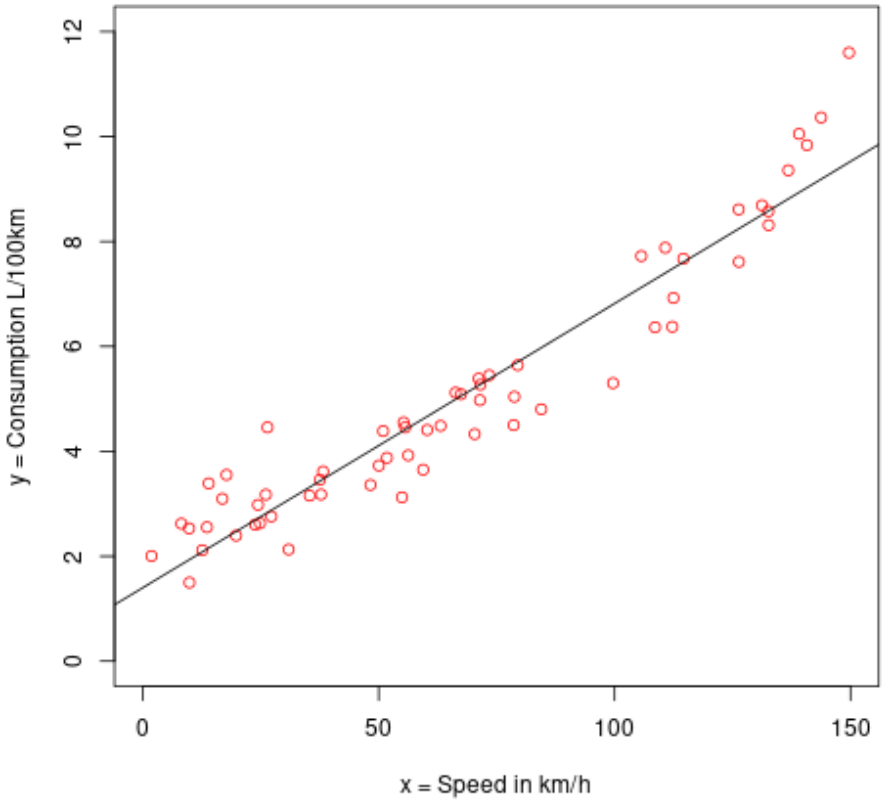

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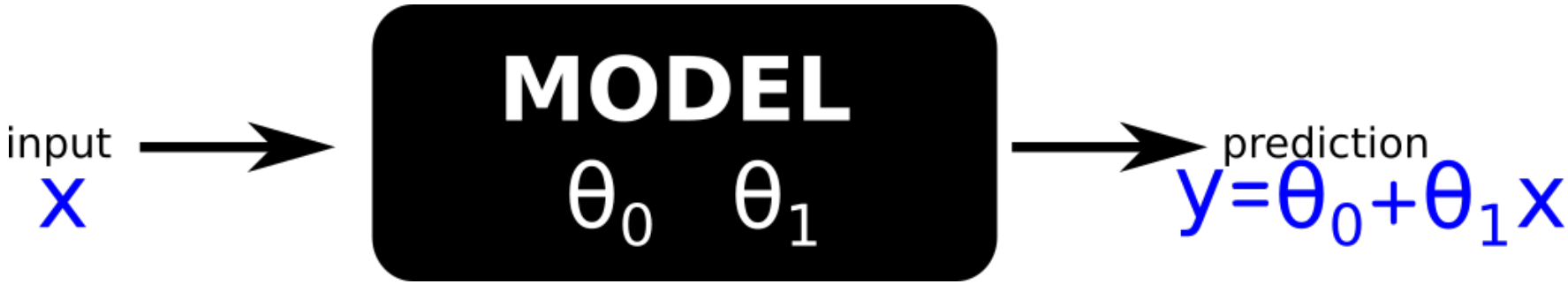

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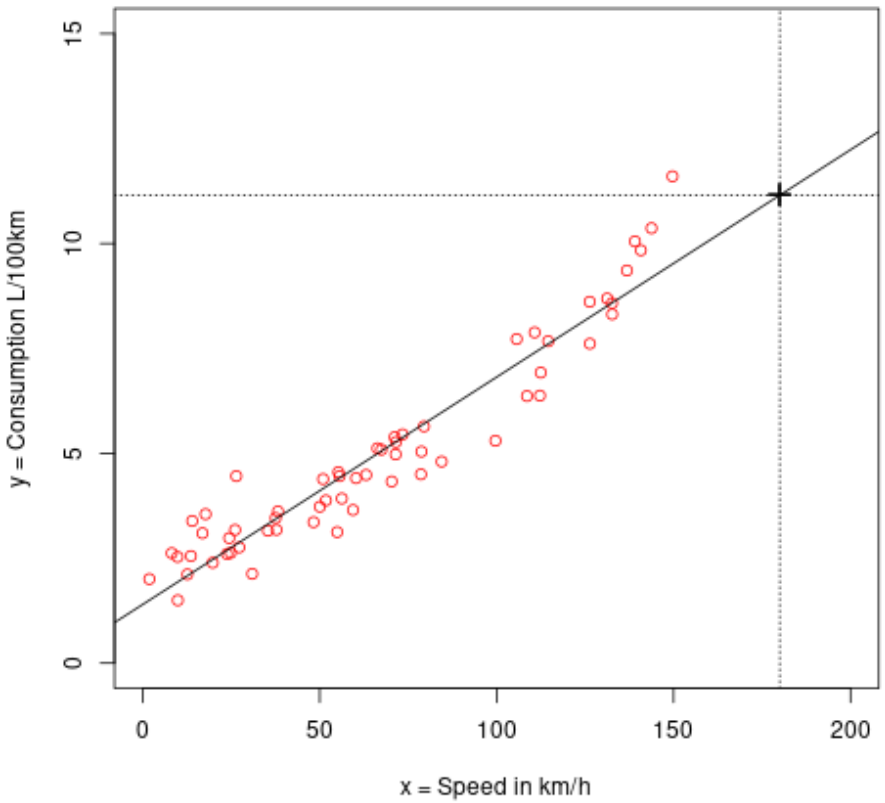
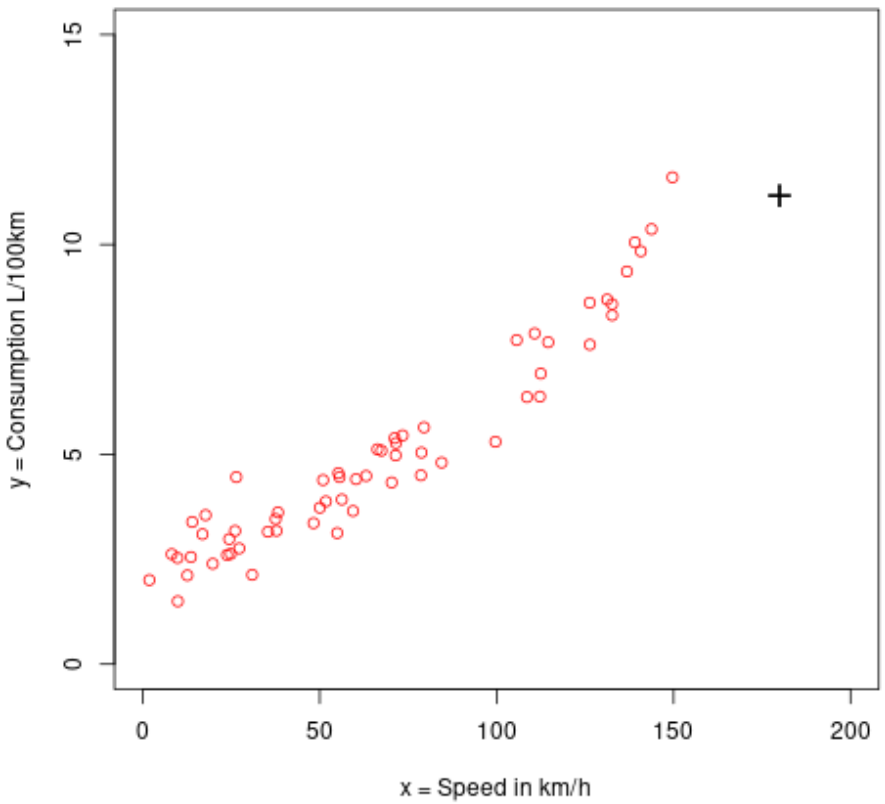


Worked-out example: toward more complex models



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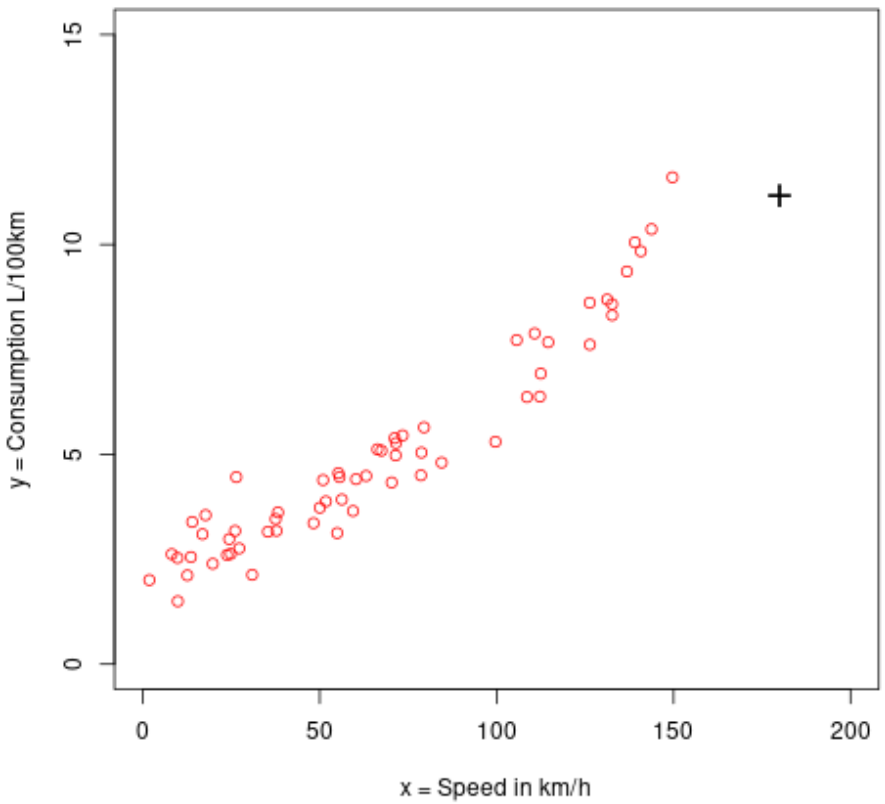

Any comment?

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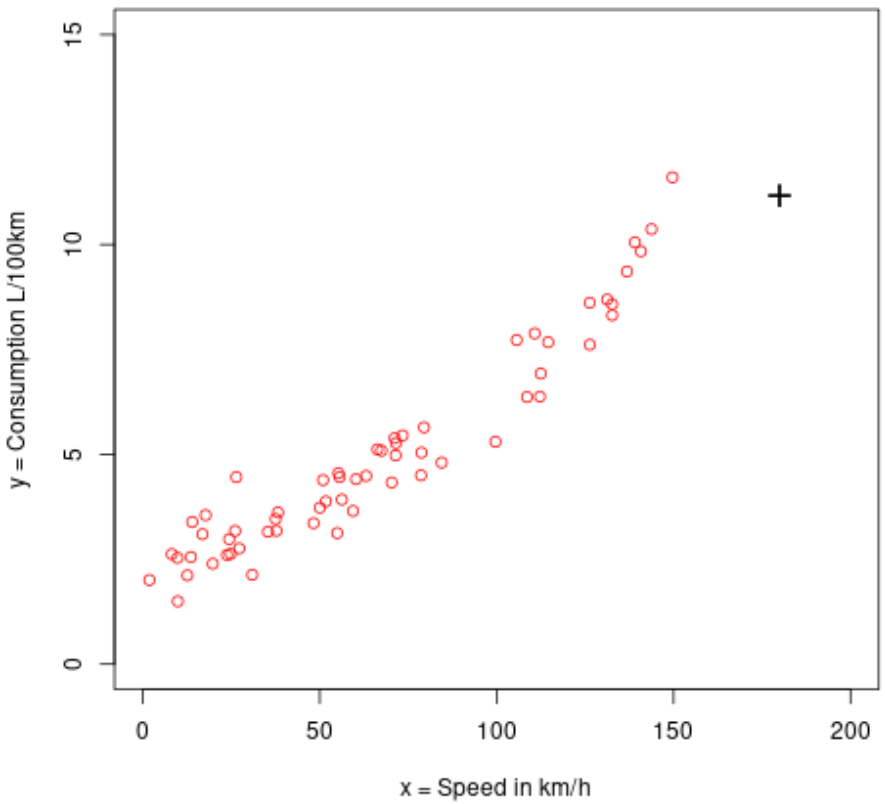

Any comment?

This phenomenon is known as **underfitting**

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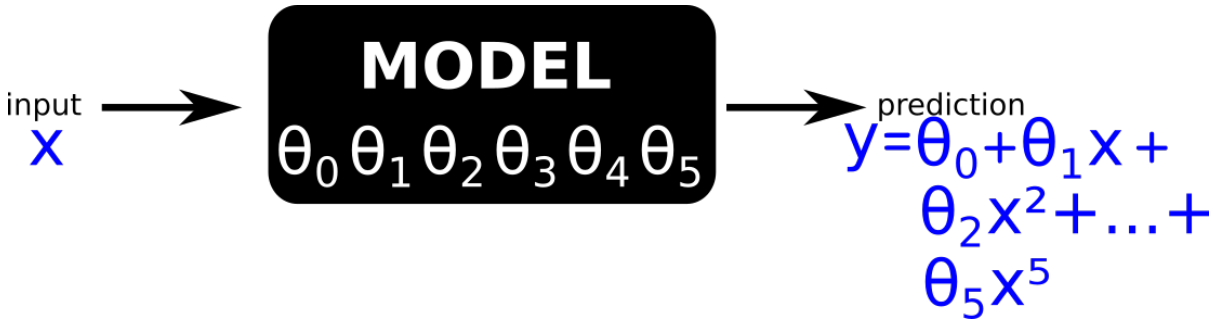

Worked-out example: toward more complex models

$\theta_0, \theta_1 ..., \theta_5$ such that

$$\mathcal{L}(\theta_0, ..., \theta_5) = \sum_{i=1}^{N} [y_i - (\sum_{j=0}^{5} \theta_j . x_i^j)]^2 \quad (1)$$

is **minimal**.

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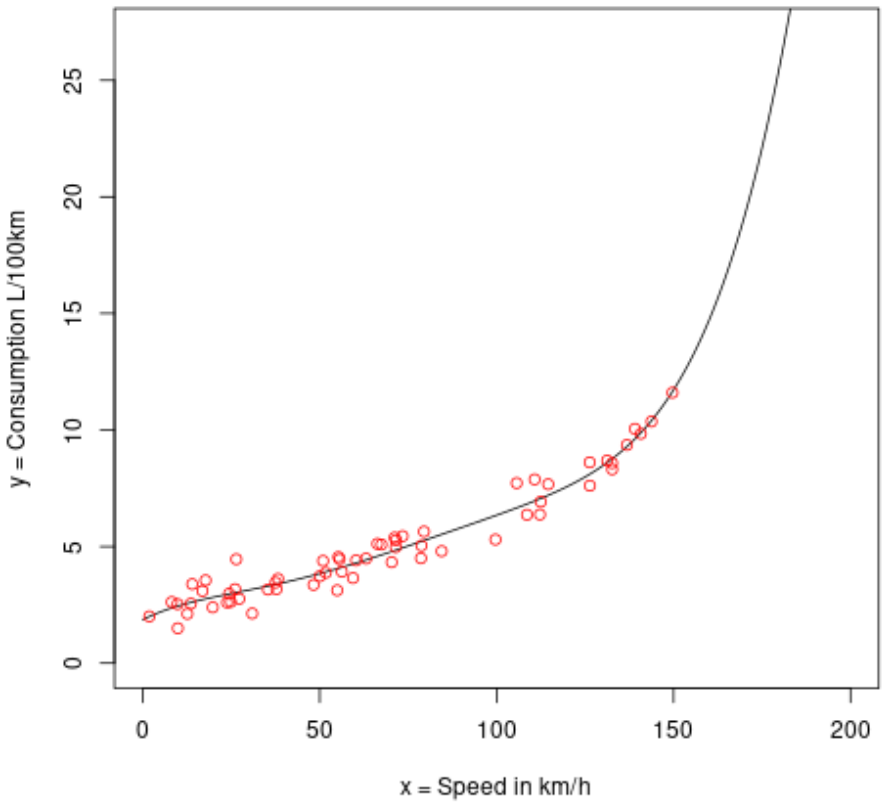

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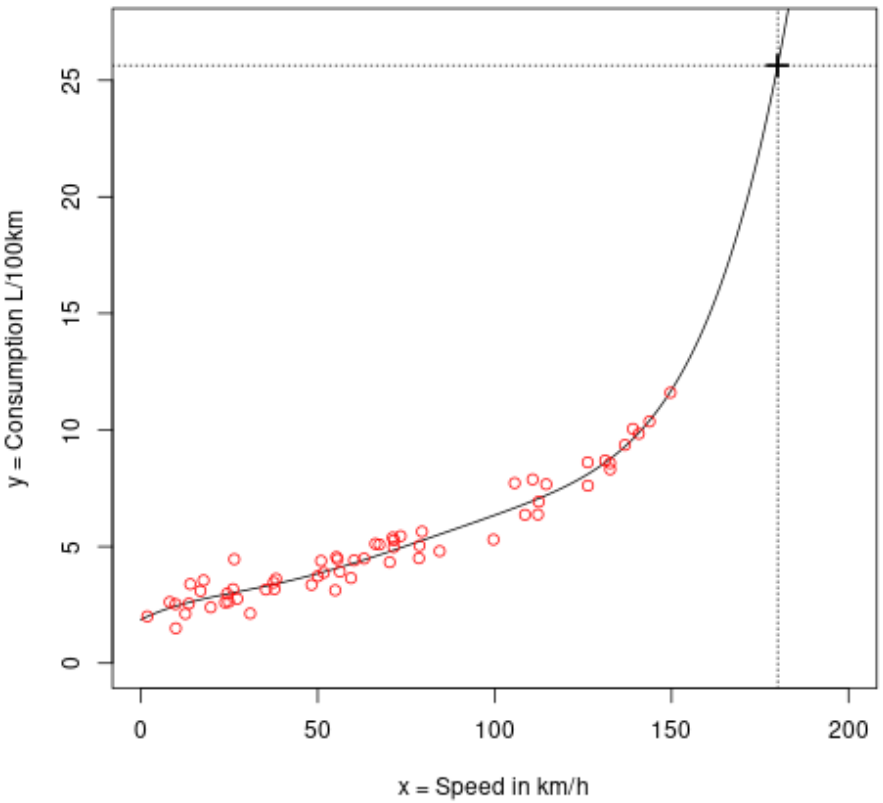

Worked-out example: toward more complex models

Informal definition

We will say that the polynomial model of degree 5 is more **expressive** than the linear regression.

Parameters: the more the better?

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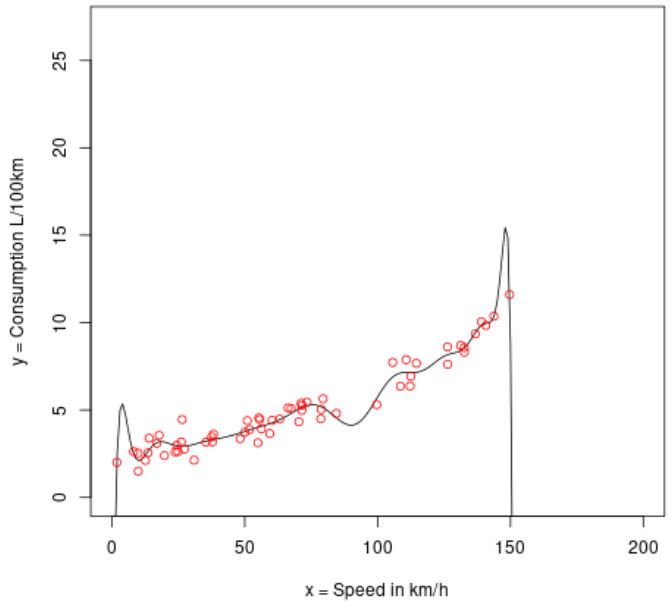

With 30 parameters: $\theta_0, ...\theta_{29}$

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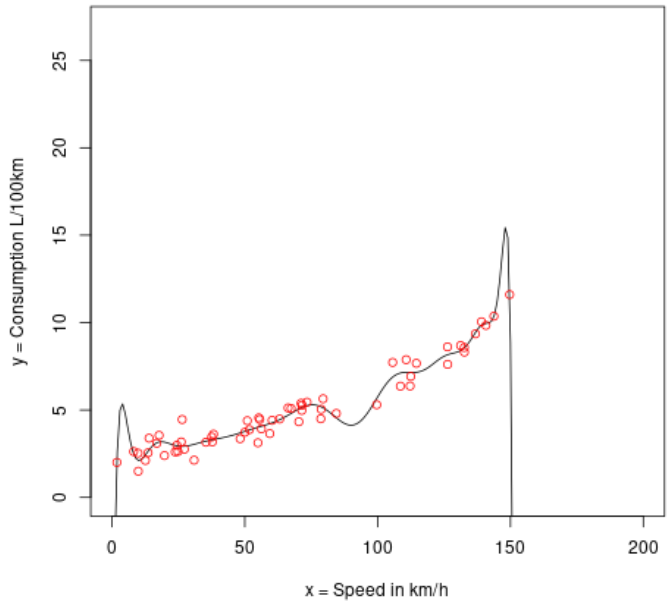

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Definition

The phenomenon is called **overfit**.

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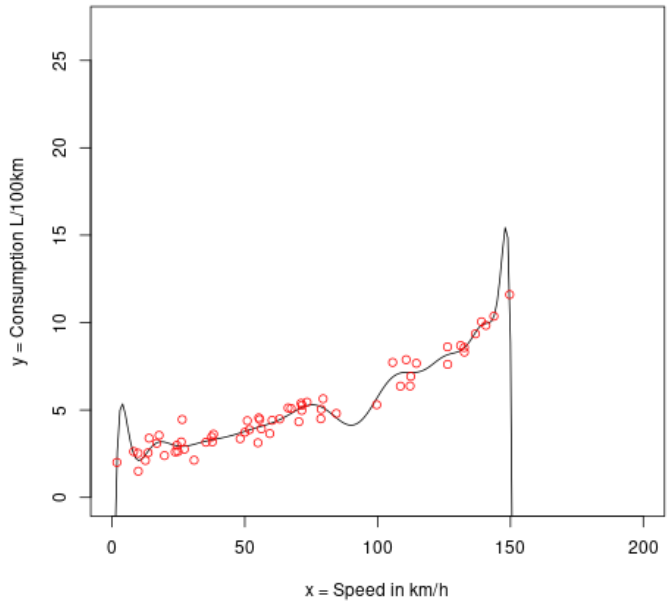

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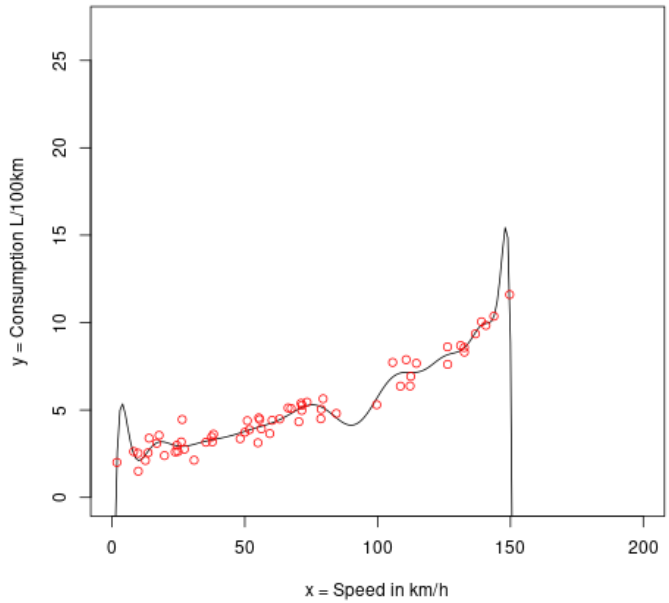

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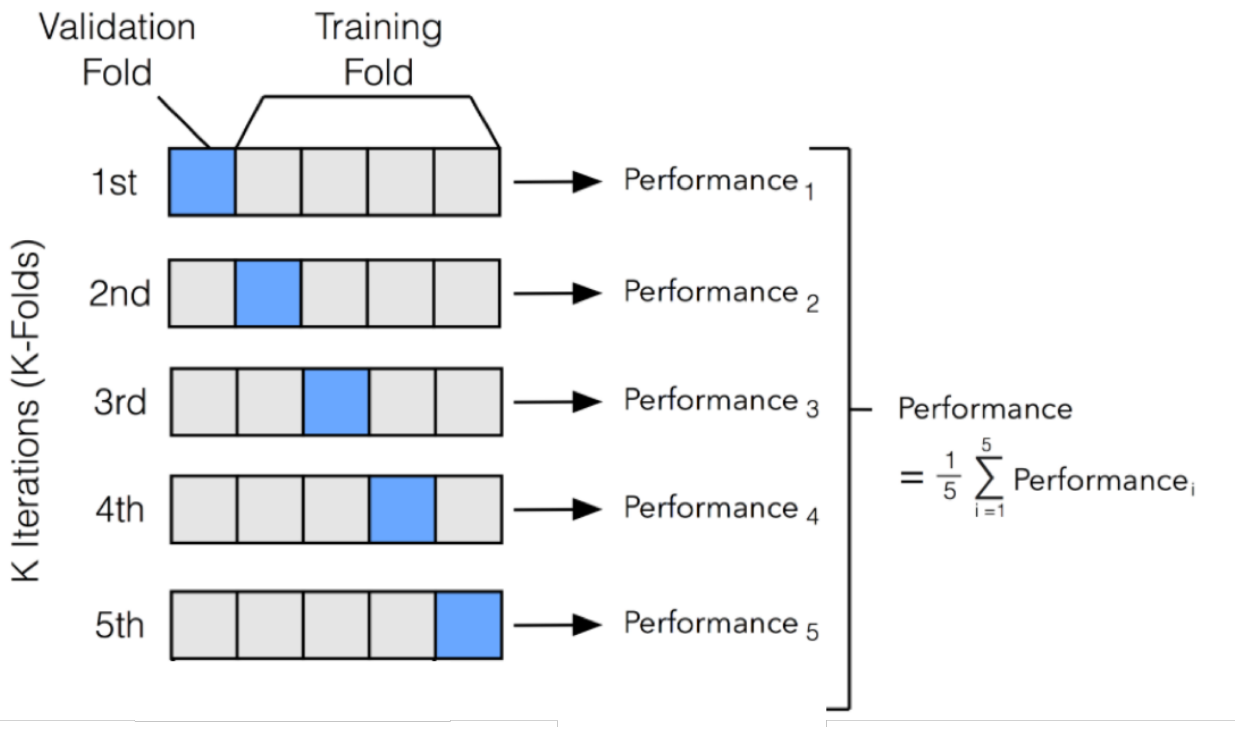
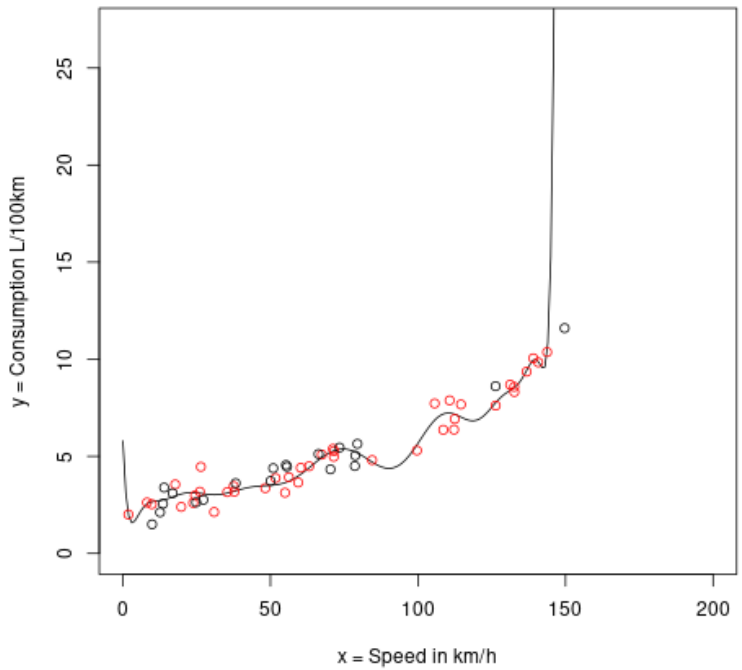
How to control overfit?

Cross-validation to control overfit



Cross-validation example: 30 parameters

Red: training set Black: validation set



30 parameters, fold 1

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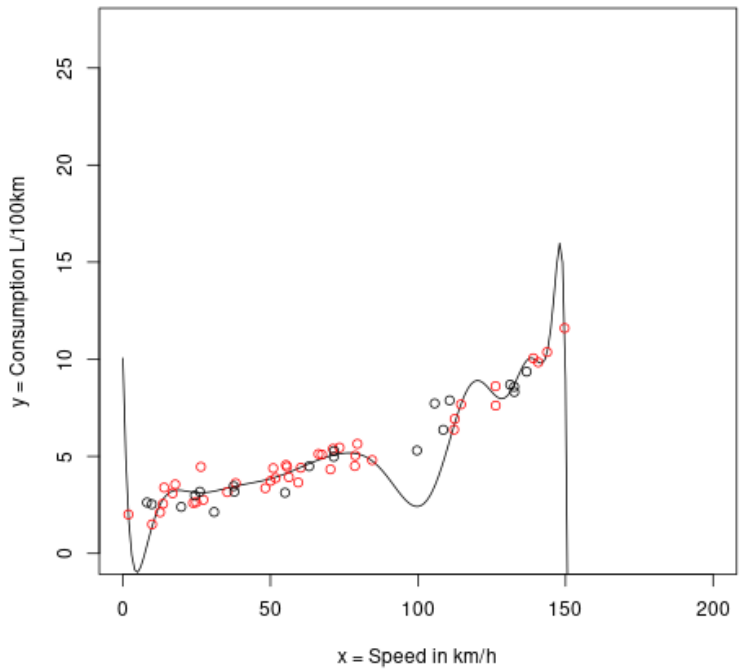

30 parameters, fold 2

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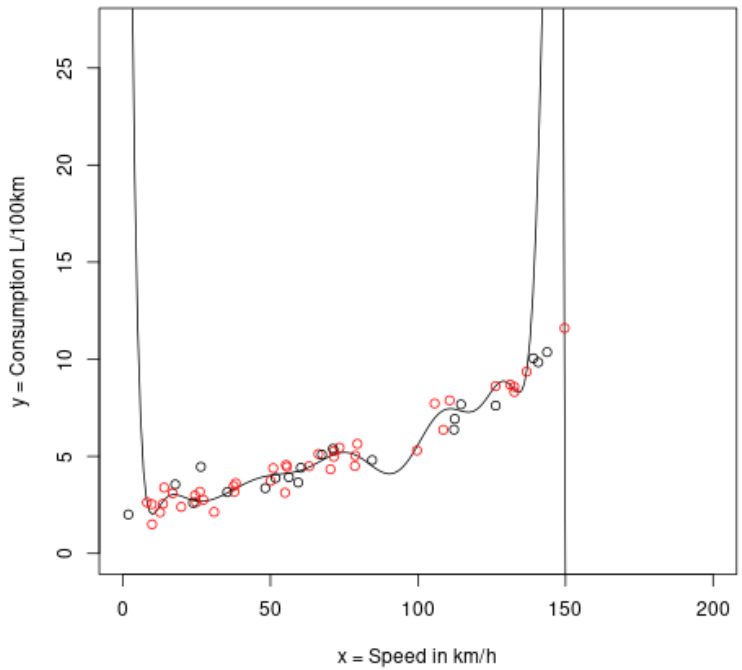

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Cross-validation example: 6 parameters

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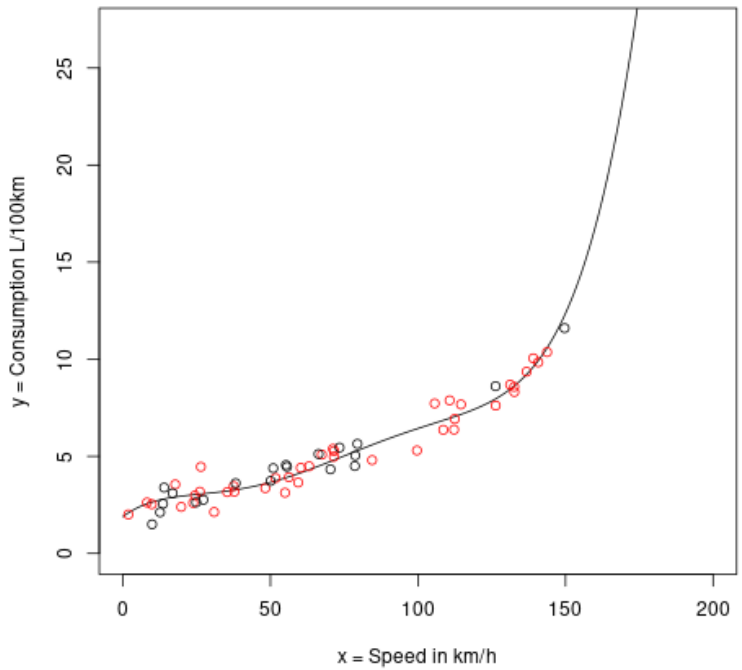

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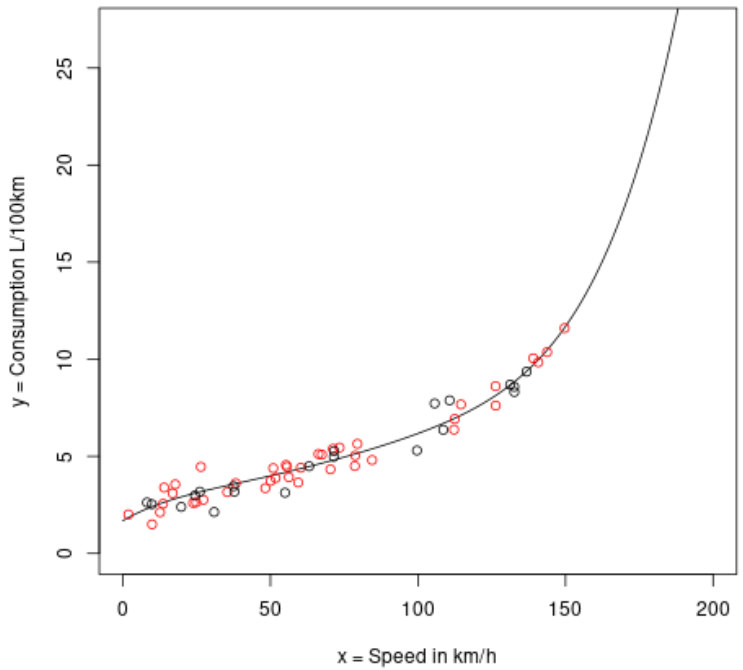

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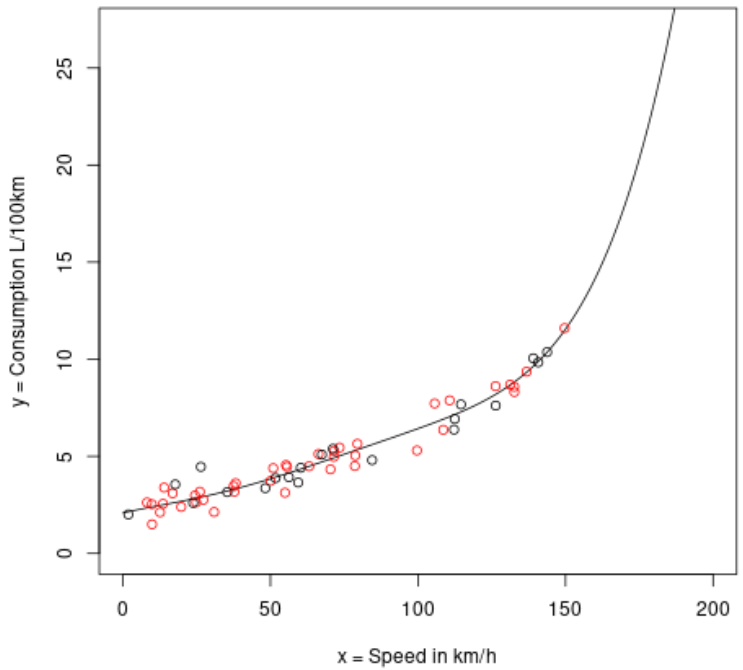

6 parameters, fold 3

What do you observe?

- Lower error on training with ___ parameters
- If the error on the validation is much higher than on the training set, it means that the model is ___.
- Naively, a model with ___ parameters will have ___ variance.

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What do you observe?

- Lower error on training with **more** parameters
- If the error on the validation is much higher than on the training set, it means that the model is **overfiting**.
- Naively, a model with **more (less)** parameters will have **more (less)** variance.

More specifically, for N training sets $X_i \in X_{train}$ we compute N models f_i and their predictions $f_i(X_{test})$. The expectation of the squared error (mean sq error) of all models $\mathbb{E}[||y - \hat{y}||^2]$ can be decomposed as:

$$\begin{aligned}
\mathbb{E}[||y - \hat{y}||^2] &= \mathbb{E}[||y - \mathbb{E}[\hat{y}] + \mathbb{E}[\hat{y}] - \hat{y}||^2] \\
&= \mathbb{E}[||y - \mathbb{E}[\hat{y}]||^2] + 2 \times 0 + \mathbb{E}[||\mathbb{E}[\hat{y}] - \hat{y}||^2] \\
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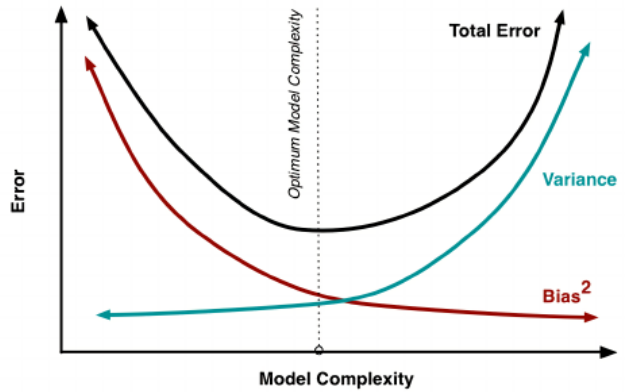
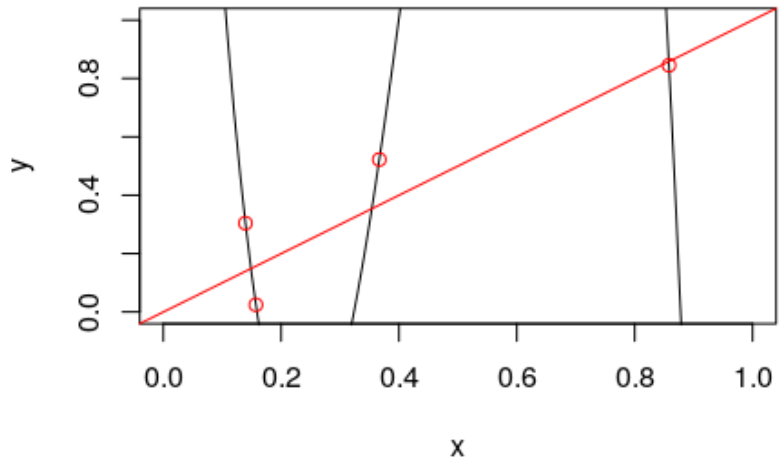
This is known as the **bias-variance trade-off**:



Regularization motivation

Let's come back to the model $y = \sum_{i=0}^{3} \theta_i x^i + \epsilon$.

The max likelihood with 4 points gives a θ fitting perfectly the points:



Maximum *likelihood* coefficients:

θ_0	θ_1	θ_2	θ_3
5.169	-54.388	155.755	-114.487

What makes you think that the model is wrong?

Regularization

The idea of regularization

Definition (well...)

Regularization is a set of methods for avoiding "unrealistic zones" in your parameter space.

Along the tutorials we will use:

- Ridge penalization (avoids high values of parameters)
- Lasso penalization (favors not using some parameters)

Other types of regularization (for Neural Networks in particular) include:

- Gaussian noise (augmenting data)
- Dropout (favors independence in the responsibilities of the parameters)

Prior distributions

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The model becomes:

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The θ_i are model **parameters** (inferred from the training data).
The μ_i and η_i are **hyperparameters** (not inferred from the training).

Worked out example

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1. Compute the posterior probability distribution

$$p(\theta|y, x) \propto p(y|\theta, x).p(\theta)$$

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$$\arg\min_{\theta} \sum_{i=0}^{N} (y_i - \theta.x_i)^2 + \lambda ||\theta||_2^2$$

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3. What it is the value of λ?

Toward Ridge regularization

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Toward Ridge regularization

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This is called **Ridge regularization**.

What is it enforcing?

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This is called **Ridge regularization**.

What is it enforcing?

It tells the model **to avoid high values** for the parameters.

General justification of Ridge regularization

Complexity

The complexity of a model is the dimensionality of the space it can describe, usually linked to the number of parameters.

A model with p binary parameters θ_i can describe ? outputs.

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where r is the radius where the parameters live and K_p a constant associated with the number of parameters.

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High dimension

In high dimension, there are "more" possible model outputs when parameters have high values.

Ridge regularization example

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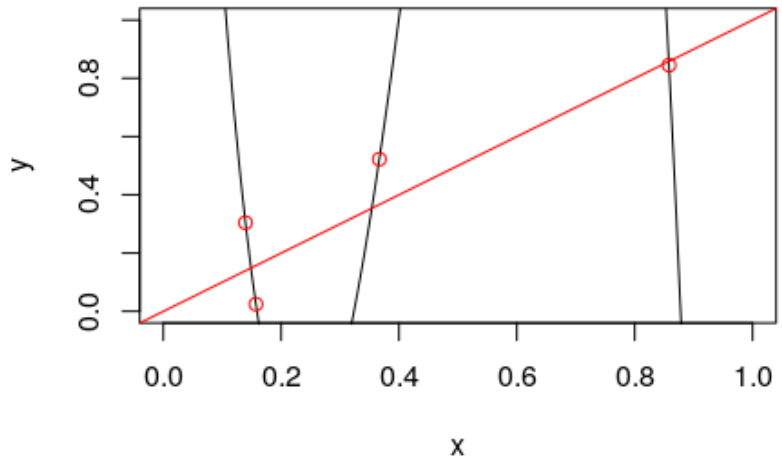
The maximum likelihood with 4 points will give a θ fitting perfectly the points:



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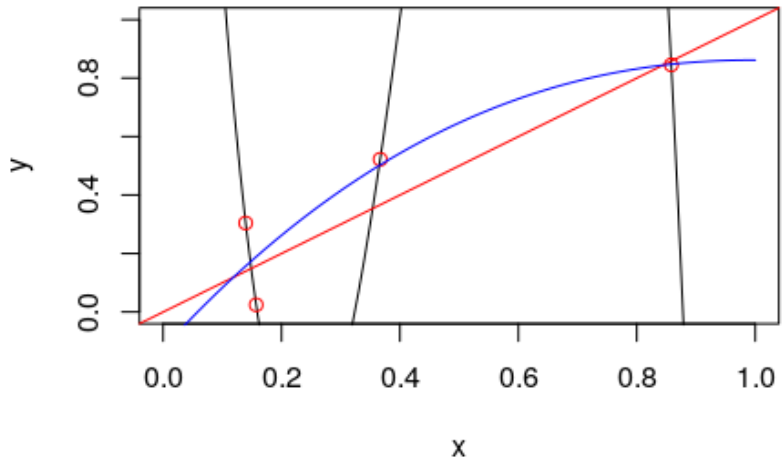
Ridge regularization example

Let's come back to the model $Y = \sum_{i=0}^{3} \theta_i x^i + \epsilon$.

With a prior $\mathcal{N}(0, \eta^2)$ the maximum a posteriori of the vector θ corresponds to (blue curve):



Maximum *a posteriori* coefficients

θ_0	θ_1	θ_2	θ_3
-0.1279	2.2561	-1.5779	0.3180

Sparse learning

Patient	Status	SNP1	SNP2	SNP3	SNP4	...
A	**0**	0	0	0	1	...
B	**1**	1	0	0	1	...
C	**1**	1	0	0	0	...
...						

From Ridge to Lasso

Suppose you model a variable Y depending on some explanatory variables x with a linear model:

$$Y = \theta_0 + \sum_{i=1}^{p} \theta_i . x_i + \epsilon$$

Imagine now that you know that actually **only few** variables actually explain your target variable.

Question

A Gaussian prior on θ_i centered on 0 avoids high values of θ_i.
Will this prior push the non-explanatory variables down to 0?

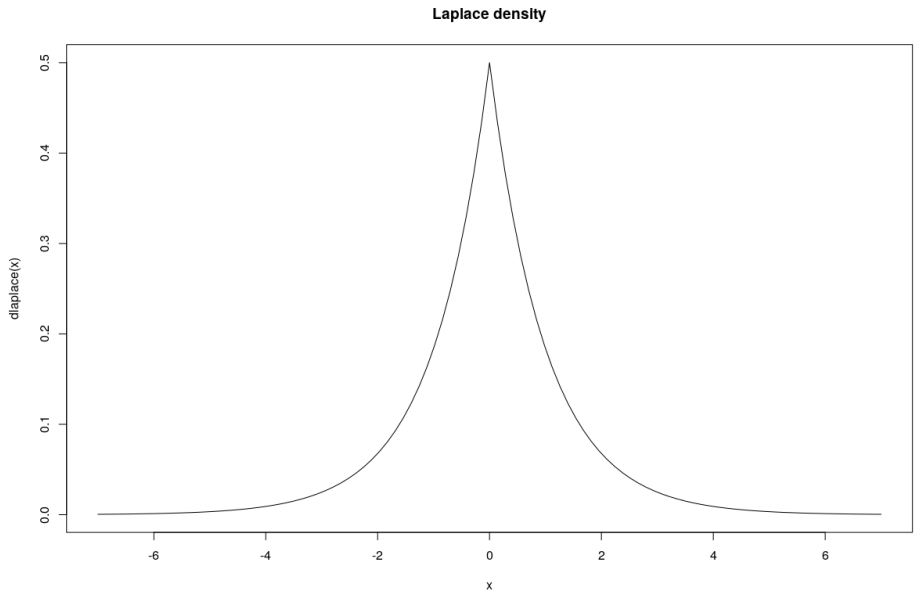
- Think individually - Draw - Rethink (5')
- Vote

Lasso penalization

What should be the shape around 0 of the prior distribution if we want to use less parameters?

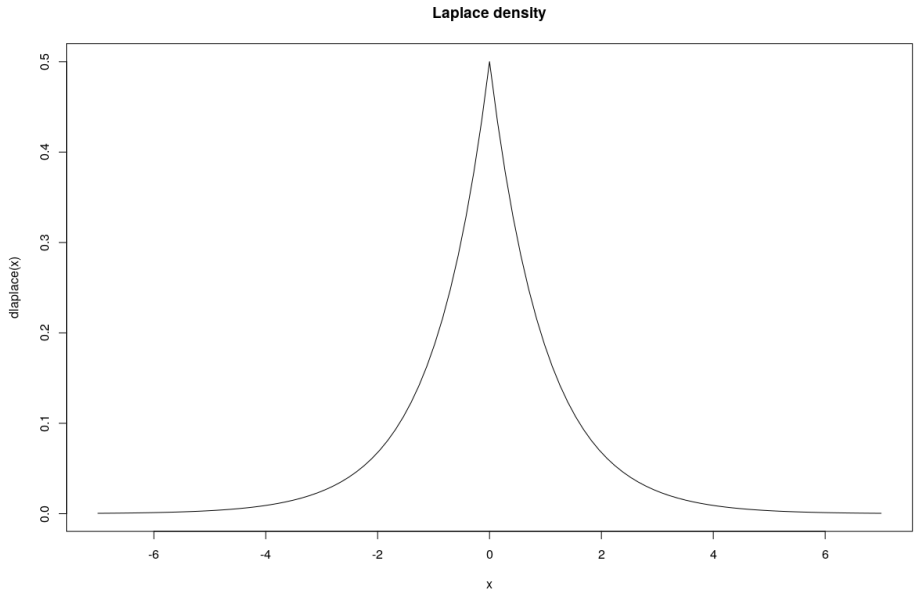
Lasso penalization

What should be the shape around 0 of the prior distribution if we want to use less parameters?
Something like the Laplace density:



$$f(x|\mu, b) = \frac{1}{2b} e^{-\frac{|x-\mu|}{b}}$$

Lasso penalization



$$f(x|\mu, b) = \frac{1}{2b} e^{-\frac{|x-\mu|}{b}}$$

Exercise

Compute the loss associated to a zero centered Laplace prior distribution.

Toward Lasso regularization

$$\min_{\theta} \sum_{i=0}^{N} (y_i - \theta.x_i)^2$$

Toward Lasso regularization

$$\min_{\theta} \sum_{i=0}^{N} (y_i - \theta.x_i)^2 \quad \rightarrow \quad \min_{\theta} \sum_{i=0}^{N} (y_i - \theta.x_i)^2 + \lambda ||\theta||_1$$

Toward Lasso regularization

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This is called **Lasso regularization**.

What is it enforcing?

Toward Lasso regularization

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This is called **Lasso regularization**.

What is it enforcing?

It tells the model **to use as few parameters** as possible.

The idea of regularization

Definition (well...)

Regularization is a set of methods for avoiding "unrealistic zones" in your parameter space.

We saw:

- Ridge penalization (avoids high values of parameters)
- Lasso penalization (favors not using some parameters)

Other types of regularization (for Neural Networks in particular) include:

- Gaussian noise (augmenting data)
- Dropout (favors independence in the responsibilities of the parameters)