Machine Learning

FIB, Master in Data Science

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Topic 1: Linear regression

Outline

1. Solving least squares linear regression problem by optimization
2. Probabilistic perspective:
   - maximum likelihood
   - bias/variance decomposition of MSE
   - maximum a posteriori, regularization

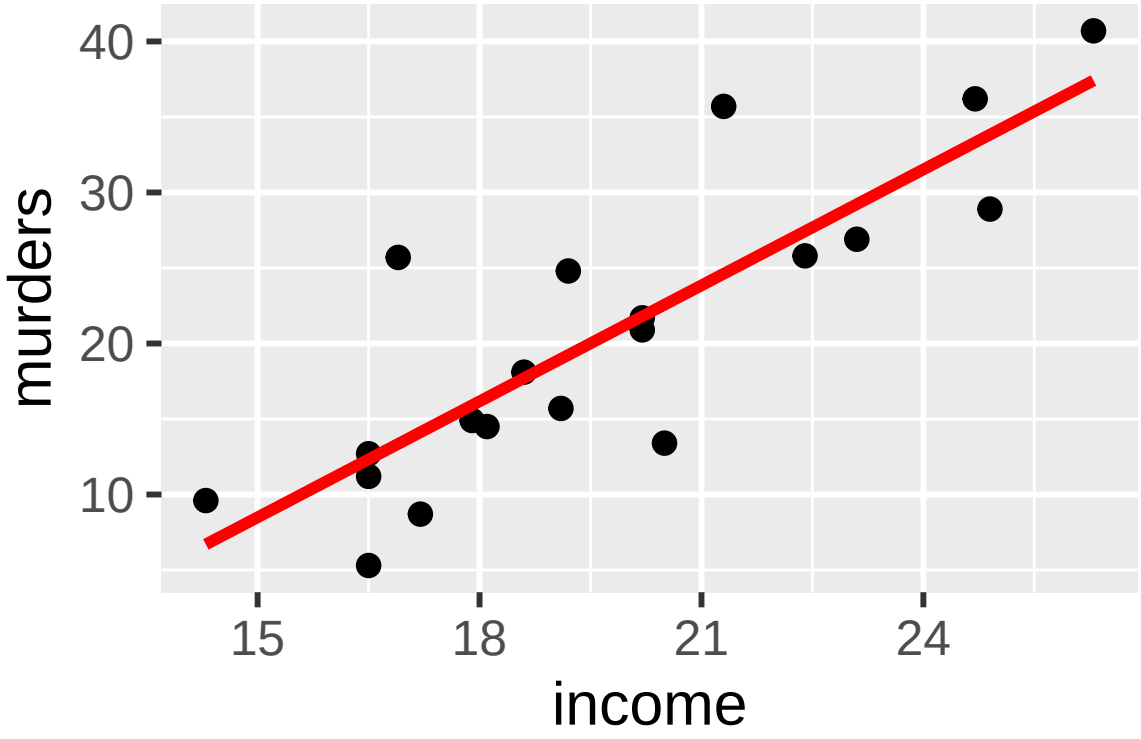
Regression

We have a dataset with data for 20 cities; for each city we have information on:

1. Nr. of inhabitants (in 10^3)
2. Percentage of families' incomes below 5000 USD
3. Percentage of unemployed
4. Number of murders per 10^6 inhabitants per annum

inhabitants	*income*	*unemployed*	*murders*
587	16.50	6.20	11.20
643	20.50	6.40	13.40
635	26.30	9.30	40.70
692	16.50	5.30	5.30
⋮	⋮	⋮	⋮
3353	16.90	6.70	25.70

Let us focus on a *single* variable (2D example)



Each point in the plot corresponds to a **row** of our data, and its coordinates are the (income, murders) values of that row.

The **red line** is "*the best*" linear model for this univariate regression model.

The optimization way

2D example, cont.

For $i = 1, .., 20$, we have plotted (x_i, y_i), where x_i is the income and y_i is the murders rate for city i.

Want a line that approximates murders as a function of income. The slope θ_1 and intercept θ_0 define the shape of the line:

$$\hat{y}(x_i) = \hat{y}_i = \theta_0 + x_i\theta_1$$

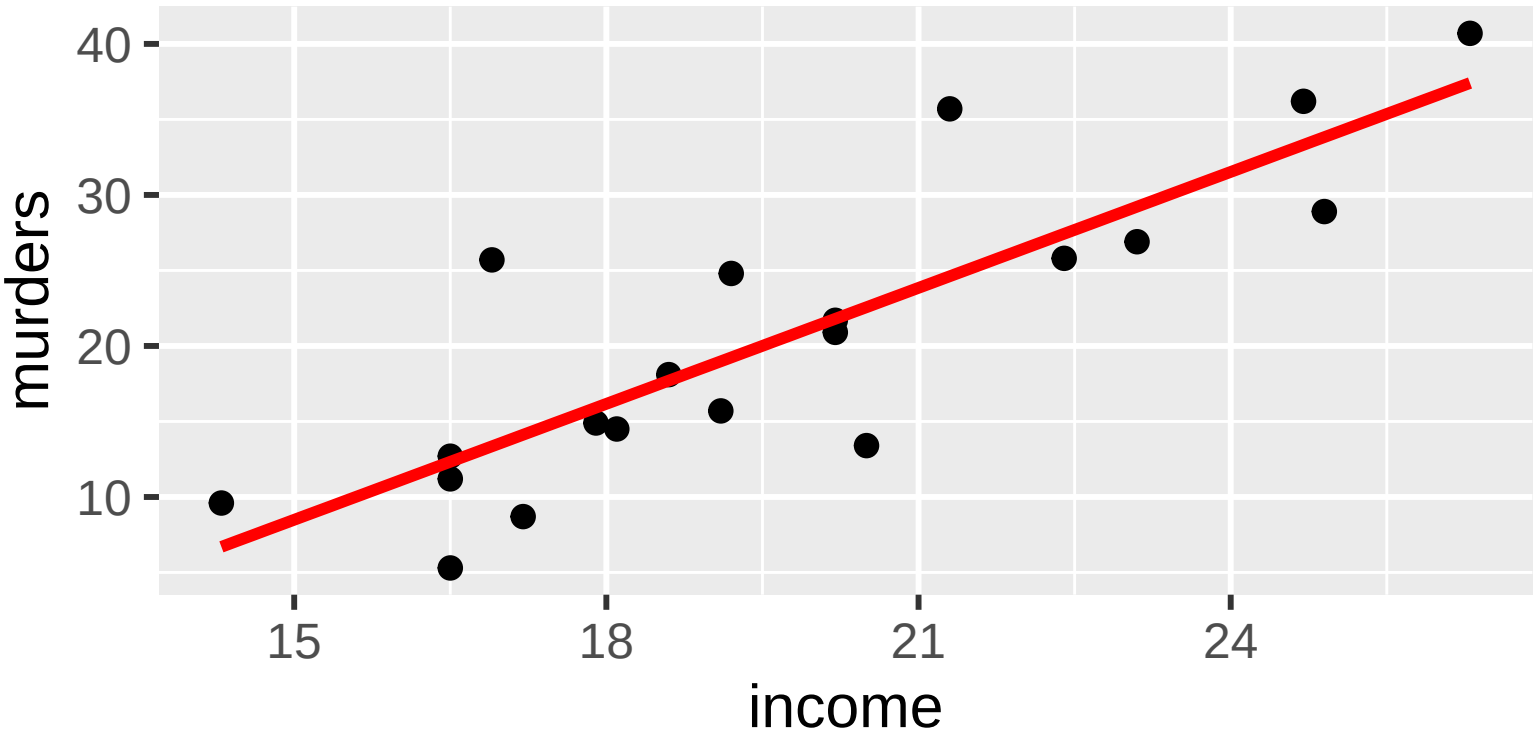
The **least squares** linear regression method tells us to choose the line that minimizes the following **error function** (a.k.a. objective function, loss function, cost function, ..):

$$J(\theta_0, \theta_1) = \sum_{i=1}^{20} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{20} (y_i - \theta_0 - x_i\theta_1)^2$$

This function depends on the **parameters** θ_0, θ_1, since data is assumed fixed (whatever was observed)

2D example, cont.

$$J(\theta_0, \theta_1) = \sum_{i=1}^{20} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{20} (y_i - \theta_0 - x_i\theta_1)^2$$



2D example, cont.

To find θ_0, θ_1 s.t. $J(\theta_0, \theta_1)$ is minimized we will compute partial derivatives, set them to 0 and solve for θ_0, θ_1.

Least squares regression: multi-variate case

But let us solve the general case, using all three features available. Now we have that the least squares solution is no longer a line, but a **hyperplane in 4D** given by the equation:

$$\hat{y}(\mathbf{x}_i) = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \theta_3 x_{i3} = \theta_0 + \sum_{j=1}^{3} x_{ij}\theta_j = \sum_{j=0}^{3} x_{ij}\theta_j$$

where we introduce $x_{i0} = 1$ for all i

Least squares regression: multi-variate case

For ease of notation, we will use vector and matrix operations for the multi-variate case

	inhabitants	*income*	*unemployed*	*murders*
1	587	16.50	6.20	11.20
2	643	20.50	6.40	13.40
3	635	26.30	9.30	40.70
4	692	16.50	5.30	5.30
⋮	⋮	⋮	⋮	⋮
20	3353	16.90	6.70	25.70

is represented as

$$\mathbf{X} = \begin{bmatrix} 1 & 587 & 16.50 & 6.20 \\ 1 & 643 & 20.50 & 6.40 \\ 1 & 635 & 26.30 & 9.30 \\ 1 & 692 & 16.50 & 5.30 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 3353 & 16.90 & 6.70 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 11.20 \\ 13.40 \\ 40.70 \\ 5.30 \\ \vdots \\ 25.70 \end{bmatrix}$$

Least squares regression: multi-variate case, cont.

$$\mathbf{X} = \begin{bmatrix} 1 & 587 & 16.50 & 6.20 \\ 1 & 643 & 20.50 & 6.40 \\ 1 & 635 & 26.30 & 9.30 \\ 1 & 692 & 16.50 & 5.30 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 3353 & 16.90 & 6.70 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 11.20 \\ 13.40 \\ 40.70 \\ 5.30 \\ \vdots \\ 25.70 \end{bmatrix}$$

placing all coefficients θ_j into a column vector $\theta = \begin{bmatrix} \theta_0 & \theta_1 & \dots \theta_d \end{bmatrix}^T$:

$$\hat{\mathbf{y}} = \mathbf{X}\theta$$

Spelling it out this is:

$$\begin{bmatrix} \hat{y_1} \\ \hat{y_2} \\ \vdots \\ \hat{y_n} \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1d} \\ 1 & x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

Least squares regression: multi-variate case, cont.

$$J(\theta) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = (\mathbf{y} - \hat{\mathbf{y}})^T (\mathbf{y} - \hat{\mathbf{y}}) = (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta)$$

And so the least squares linear regression problem is solved by setting $\frac{\partial J(\theta)}{\partial \theta} = 0$ and solving for θ. Here, we will use the following facts: $\frac{\partial \mathbf{A}\theta}{\partial \theta} = \mathbf{A}^T$ and $\frac{\partial \theta^T \mathbf{B}\theta}{\partial \theta} = 2\mathbf{B}\theta$ if $\mathbf{B}$ symmetric:

$$\begin{aligned}
\frac{\partial J(\theta)}{\partial \theta} &= \frac{\partial (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta)}{\partial \theta} \\
&= \frac{\partial}{\partial \theta} \left[\mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\theta - \theta^T \mathbf{X}^T \mathbf{y} + \theta^T \mathbf{X}^T \mathbf{X}\theta \right] \\
&= \frac{\partial}{\partial \theta} \left[\mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\theta + \theta^T \mathbf{X}^T \mathbf{X}\theta \right] \\
&= 0 - 2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X}\theta
\end{aligned}$$

So $2\mathbf{X}^T \mathbf{X}\theta = 2\mathbf{X}^T \mathbf{y}$ implies

$$\theta_{lse} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Least squares regression: multi-variate case, cont.

The "best" linear model (defined by the one that minimizes least squares error) is given by

$$\theta_{lse} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Now, in order to make predictions on unseen test data $x' = \begin{bmatrix} x'_1 & x'_2 \dots x'_d \end{bmatrix}^T$ all we need to do is compute

$$y' = \begin{bmatrix} 1 & x'_1 & x'_2 \dots x'_d \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} = \theta_0 + \sum_{j=1}^{d} x'_j\theta_j$$

*This is the **optimization** view of learning; (1) set up error function as a fn. of parameters, (2) optimize it to find suitable values for the parameters, (3) use values to make predictions.*

Computation of least squares solution via the SVD

Let us look closely at the solution for coefficients θ via minimization of the squared error:

$$\theta_{lse} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- $\mathbf{X} \in \mathbb{R}^{n\times(d+1)}$
- $\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{(d+1)\times(d+1)}$
- If $\mathbf{X}$ has independent columns, then $\mathbf{X}^T\mathbf{X}$ is invertible
- Inverting this matrix can have numerical problems and so the SVD is used instead

Singular Value Decomposition of a rectangular matrix $A \in \mathbb{R}^{m \times n}$

Any matrix $A \in \mathbb{R}^{m \times n}$ with $m > n$ can be expressed as

$$A = U \Sigma V^T$$

where:

- $U \in \mathbb{R}^{m \times n}$ has orthonormal columns (so $U^T U = I$)
- $\Sigma \in \mathbb{R}^{n \times n}$ is diagonal and contains the singular values in its diagonal
- $V \in \mathbb{R}^{n \times n}$ has orthonormal rows and columns (so $V^T V = I$, $V V^T = I$ and $V^{-1} = V^T$)

Visually:

$$A = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \cdots \\ \mathbf{v}_n^T \end{bmatrix}$$

$$= \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^T + \ldots + \sigma_n \mathbf{u}_n \mathbf{v}_n^T$$

Computing least squares solution via the SVD

Let $\mathbf{X} = U\Sigma V^T$ be the SVD decomposition of data matrix $\mathbf{X}$

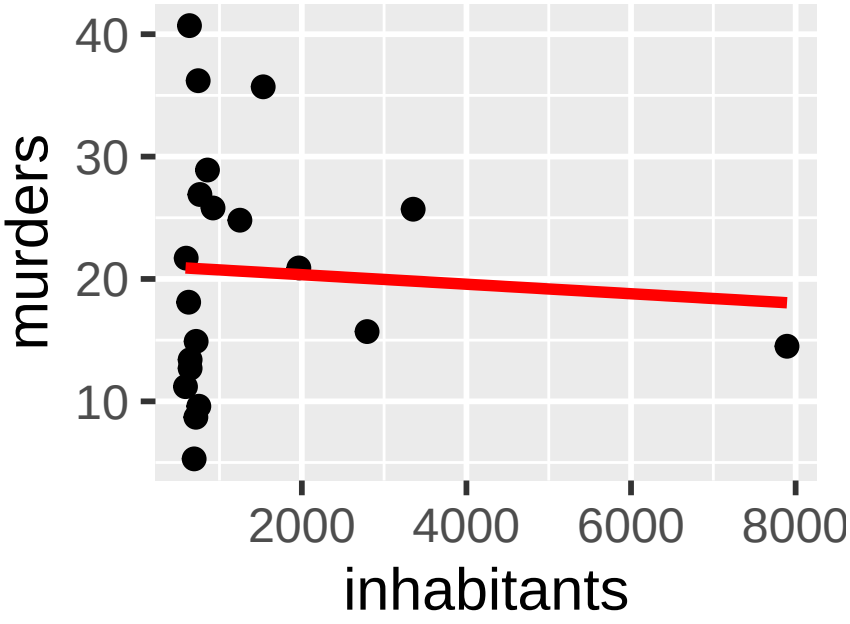
Then:

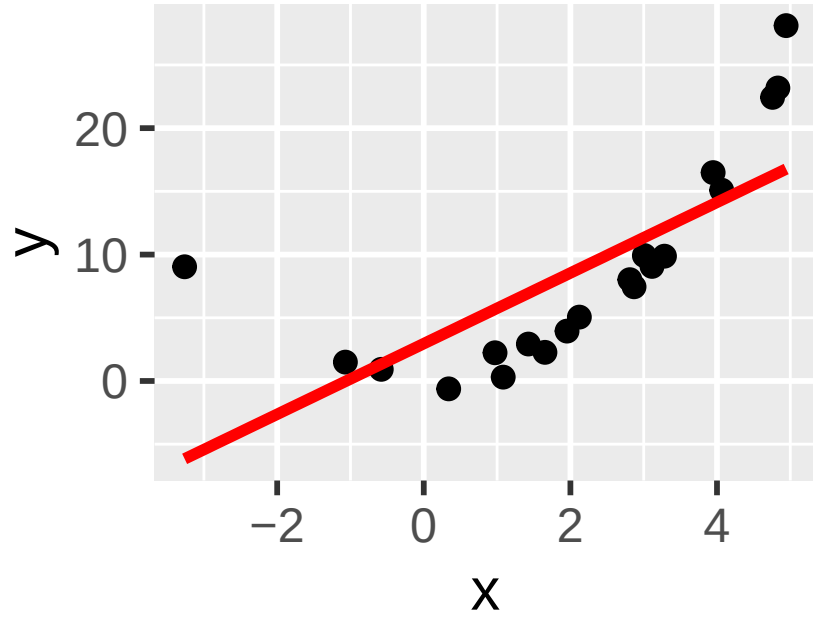
$$\begin{aligned}
\theta_{lse} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\
&= ((U\Sigma V^T)^T U\Sigma V^T)^{-1}(U\Sigma V^T)^T\mathbf{y} \\
&= (V\Sigma U^T U\Sigma V^T)^{-1}V\Sigma U^T\mathbf{y} \\
&= (V\Sigma^2 V^T)^{-1}V\Sigma U^T\mathbf{y} \\
&= (V^T)^{-1}\Sigma^{-2}V^{-1}V\Sigma U^T\mathbf{y} \\
&= V\Sigma^{-1}U^T\mathbf{y}
\end{aligned}$$

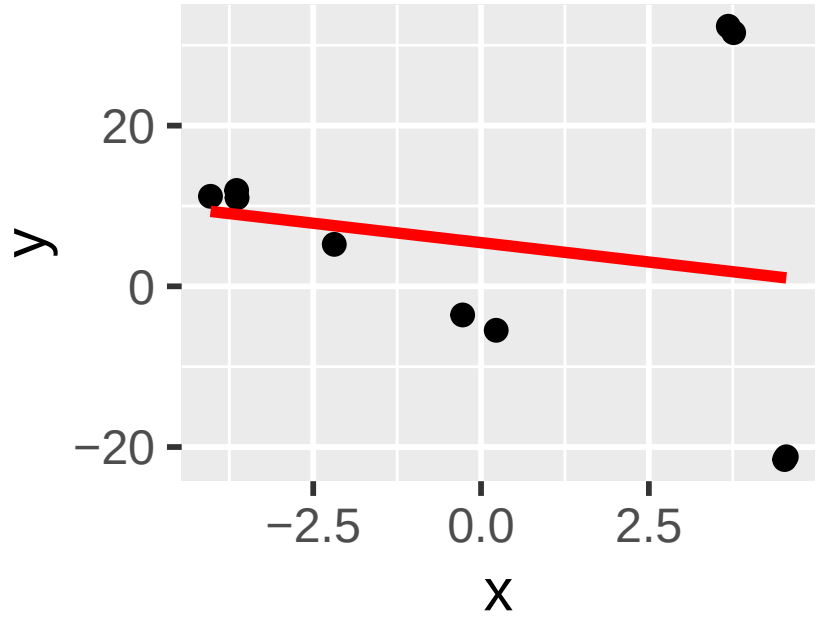
```
import numpy as np

U, d, Vt = np.linalg.svd(X, full_matrices=False)
D = np.diag(1/d)
theta = Vt.T @ D @ U.T @ y
```

Things that could go wrong







Fixing the second problem.. use basis functions!

Linear regression with non-linear input features

What if we could do linear regression on and *expanded input*? In particular, if the new inputs are non-linear, we increment the expressive power of our prediction function. The predictive function is still **linear** because linearlity is defined with respect to the *parameters* of the functions.

In general, the feature mapping is a non-linear transformation of the inputs $\phi : \mathbb{R}^d \to \mathbb{R}^k$. The resulting predictive function is $y = \phi(x)\theta$.

For example, we could use a **polynomial expansion of degree** k so that:

- $\phi(x) = (1 \; x \; x^2 \; \ldots \; x^k)$
- $y = \phi(x)\theta = \theta_0 + x\theta_1 + x^2\theta_2 + \cdots + x^k\theta_k$

Note that functions start to have more complexity (if k is very high for example), so **complexity control** is going to be crucial to **avoid overfitting**.

Fixing the second problem.. use basis functions!

Linear regression with non-linear input features

The *new input data matrix becomes*

$$\Phi = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_n) \end{bmatrix} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \dots & \phi_k(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \dots & \phi_k(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_n) & \phi_2(x_n) & \dots & \phi_k(x_n) \end{bmatrix}$$

And the *optimal* solution is:

$$\begin{aligned} \theta_{min} &= \arg\min_{\theta} (\mathbf{y} - \Phi\theta)^T (\mathbf{y} - \Phi\theta) \\ &= (\Phi^T \Phi)^{-1} \Phi^T \mathbf{y} \end{aligned}$$

The probabilistic perspective

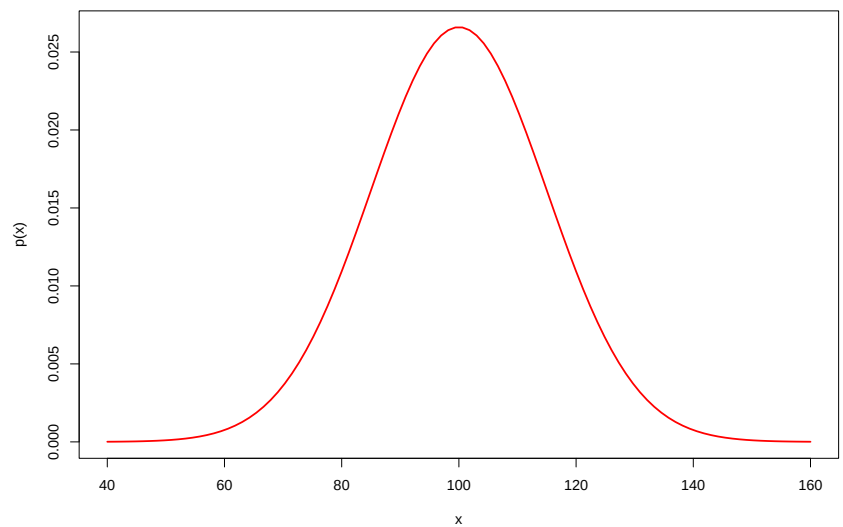
using probabilities to quantify uncertainty

Least squares regression, from a probabilistic perspective

Now we cast the problem in a probabilistic setting, and use the principle of **maximum likelihood** to derive the same linear regression estimates.

A key player is the **univariate Gaussian distribution** – the **normal** distribution – with *probability density function*:

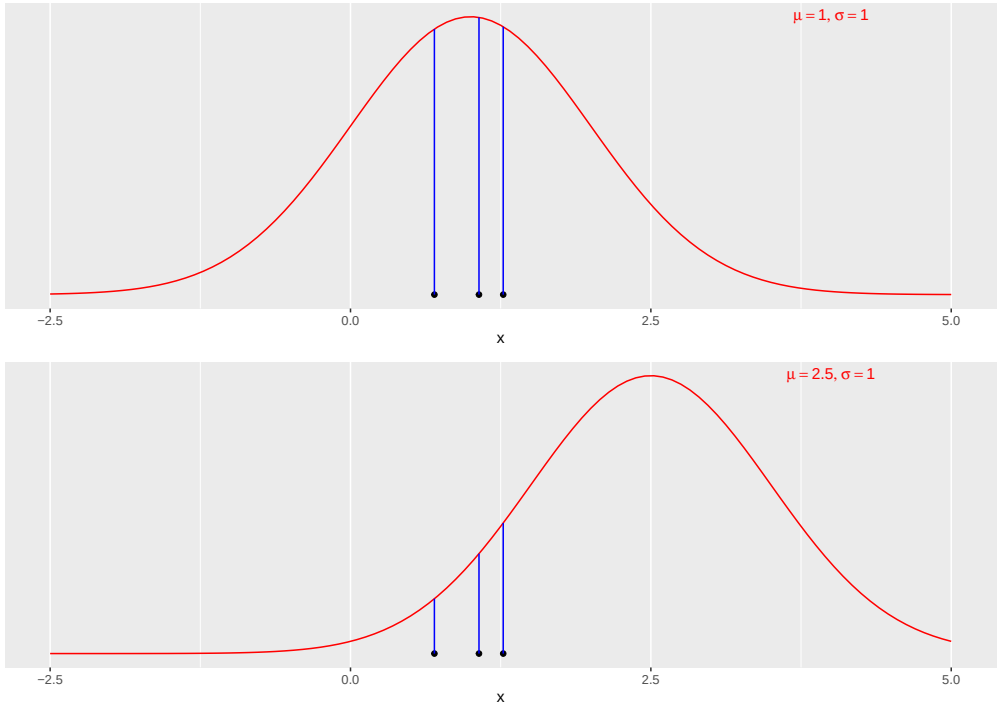
$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2} \quad \text{when } x \sim \mathcal{N}(\mu, \sigma^2)$$



Maximum likelihood principle

Out of these two normal densities, we will prefer the one that **maximizes the likelihood**

$$\mathcal{L}(\mu, \sigma; \{x_1, x_2, x_3\}) := P(x_1, x_2, x_3; \mu, \sigma) = \prod_i p(x_i; \mu, \sigma)$$

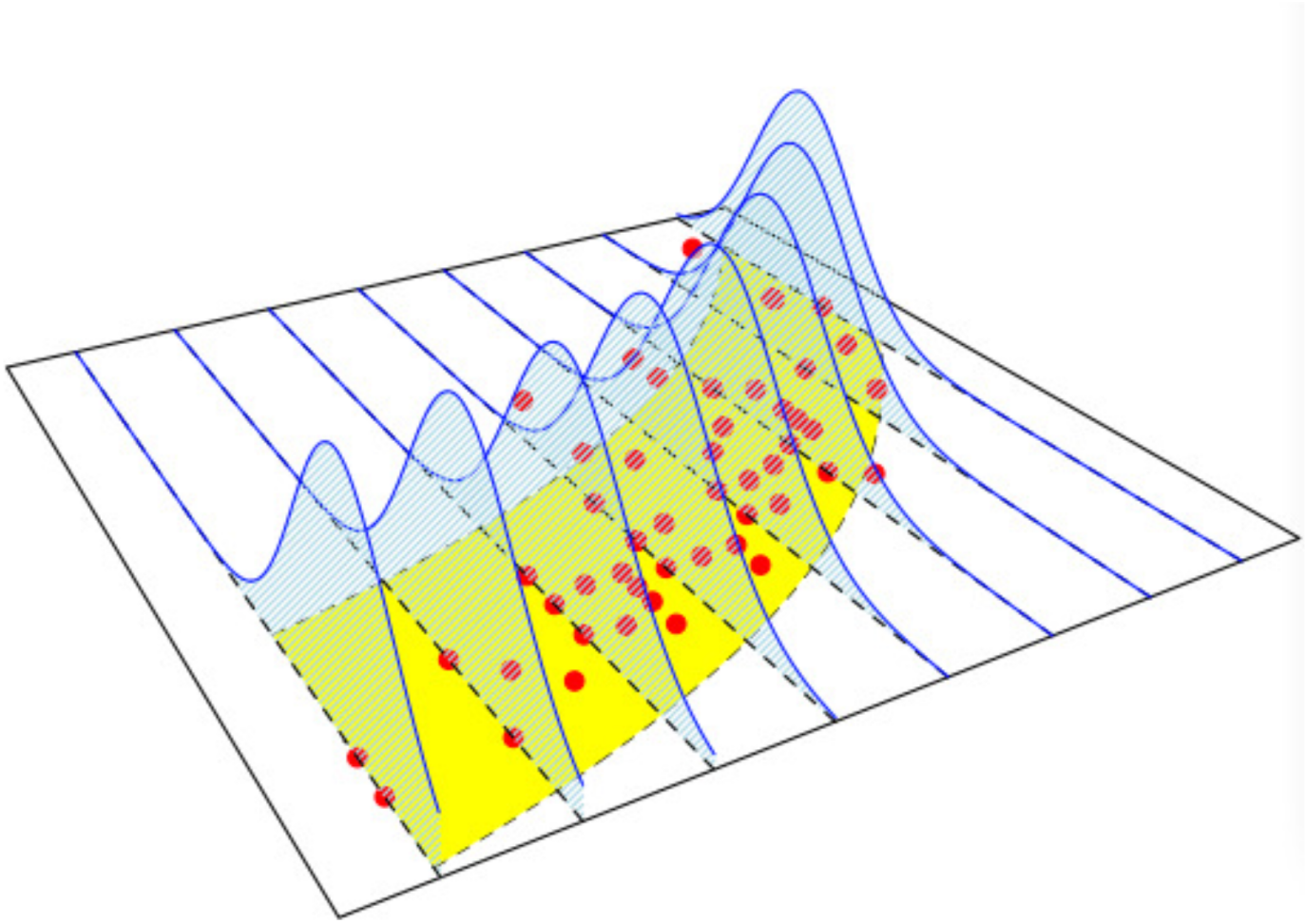


Note that the likelihood is a **function of the parameters**, assuming the data is fixed. Additionally, we assume that all x_i are *independent and identically distributed* according to $\mathcal{N}(\mu, \sigma^2)$.

Back to regression

In the probabilistic setting of linear regression, we assume that each label y_i we observe is normally distributed with mean $\mu = \mathbf{x}_i\theta$ and variance σ^2:

$$y_i = \mathbf{x}_i\theta + \epsilon_i, \text{ where } \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$



Maximum likelihood for linear regression

Our data is given by a set of n labelled examples $(\mathbf{x}_i, y_i)$ which are assumed to be iid according to $y_i \sim \mathcal{N}(\mathbf{x}_i\theta, \sigma^2)$ for unknown θ and σ.

As usual, it is convenient to place the data into a column vector $\mathbf{y}$ of labels and a data matrix $\mathbf{X}$:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1d} \\ 1 & x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix}$$

The likelihood of paramter vector θ is given by

$$\mathcal{L}(\theta, \sigma) := P(\mathbf{y}|\mathbf{X}; \theta, \sigma) = \prod_{i=1}^{n} p(y_i|\mathbf{x}_i; \theta, \sigma)$$

Maximum likelihood for linear regression, cont.

For numerical reasons we will maximize de *log-likelihood* instead:

$$
\begin{aligned}
l(\theta, \sigma) := \ln \mathcal{L}(\theta, \sigma) &= \ln \prod_i p(y_i | \mathbf{x}_i; \theta, \sigma) \\
&= \sum_i \ln p(y_i | \mathbf{x}_i; \theta, \sigma) \\
&= \sum_i \ln \left[\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i\theta)^2} \right] \\
&= \sum_{i=1}^{n} \left[\ln \frac{1}{\sqrt{2\pi\sigma^2}} + \ln \left(e^{-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i\theta)^2} \right) \right] \\
&= -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_i (y_i - \mathbf{x}_i\theta)^2 \\
&= -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta)
\end{aligned}
$$

Maximum likelihood for linear regression, cont.

$$l(\theta, \sigma) = -\frac{n}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\theta)^T(\mathbf{y} - \mathbf{X}\theta)$$

Differentiating w.r.t to paramters and setting equal to 0

$$\frac{\partial l(\theta, \sigma)}{\partial \theta} = -\frac{1}{2\sigma^2}(-2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\theta) = 0$$
$$\frac{\partial l(\theta, \sigma)}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4}(\mathbf{y} - \mathbf{X}\theta)^T(\mathbf{y} - \mathbf{X}\theta) = 0$$

leads to:

$$\theta_{ML} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$
$$\sigma^2_{ML} = \frac{1}{n}(\mathbf{y} - \mathbf{X}\theta)^T(\mathbf{y} - \mathbf{X}\theta) = \frac{1}{n}\sum_i (y_i - \mathbf{x}_i\theta_{ML})^2 = MSE$$

Maximum likelihood for linear regression, cont.

Notice that the maximum likelihood solution **coincides** with the one we found minimizing **squared error**. The squared loss is a consequence of assuming gaussian noise. Other types of distributions are of course possible, and they correspond to minimizing **other** error functions.

So:

least squares linear regression == linear regression with Gaussian noise

and as a bonus, we get an estimate of how confident we can be on our predictions (given by the MSE)

Bias-Variance decomposition

Assume the following:

- let $f : \mathbb{R}^d \to \mathbb{R}$ be the **true function** that we are trying to approximate
- let D be a finite dataset for training $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)\}$, where $y_i = f(\mathbf{x}_i) + \epsilon_i$, and all ϵ_i are iid according to $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$
- let $\mathbf{x} \in \mathbb{R}^d$ be a test data point
- using D, we train a model $\hat{f}$; the prediction according to $\hat{f}$ is $\hat{y}_D = \hat{f}(\mathbf{x})$; here we add the subscript to emphasize that the prediction depends on the training dataset D

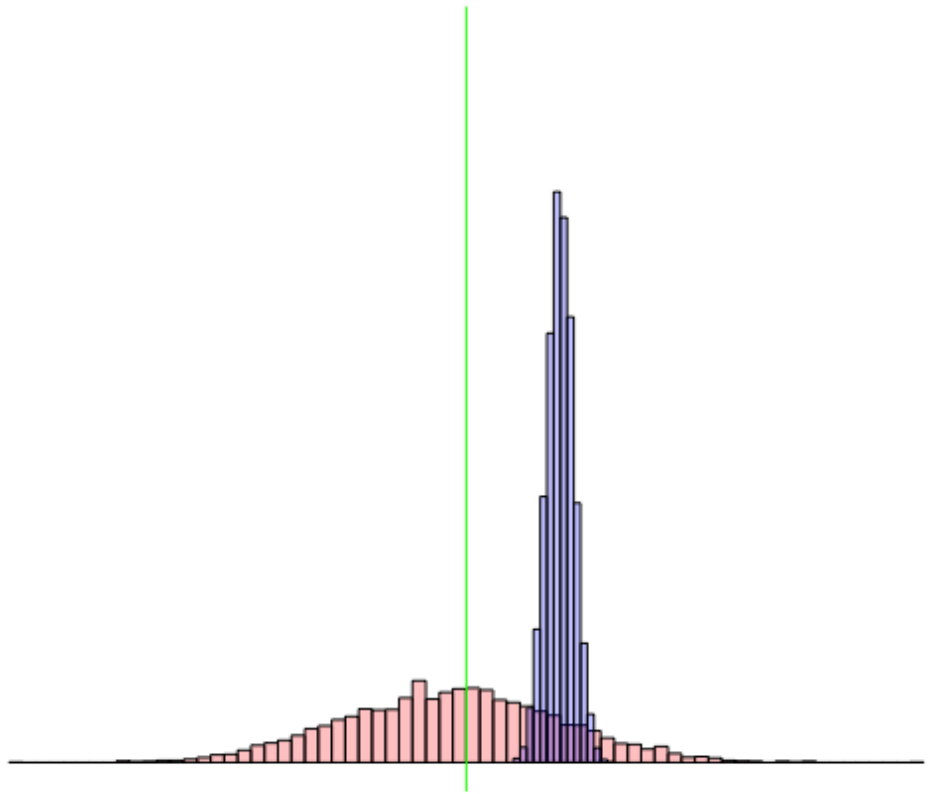
In this derivation we are going to see that its expected[1] squared error $(y - \hat{y}_D)^2$ can be decomposed as a sum of the following:

- the **irreducible error** given by σ^2
- the (squared) **bias** of the learning method; this is the systematic limitation that the modelling assumptions impose (e.g. using *linear functions* will never have low error on complex "non-linear" data)
- the **variance** of the learning method; this is how sensitive the modelling is to small variations of D

[1] this **expectation** is taken over the possible choices of D of size n

Bias-Variance trade-off, intuition

- true value given by *green* vertical line
- blue model has better variance, but worse bias
- red model has better bias, but worse variance
- which is best?



Bias-Variance decomposition, derivation

In the following derivation, we are using basic facts about expectations; for brevity, we use f for the true value of $f(\mathbf{x})$

$$
\begin{aligned}
\mathbb{E}[(y - \hat{y}_D)^2] &= \mathbb{E}[(f + \epsilon - \hat{y}_D)^2] \\
&= \mathbb{E}[(f + \epsilon - \hat{y}_D + \mathbb{E}[\hat{y}_D] - \mathbb{E}[\hat{y}_D])^2] \\
&= \mathbb{E}[(\underbrace{(f - \mathbb{E}[\hat{y}_D])}_{A} + \underbrace{\epsilon}_{B} + \underbrace{(\mathbb{E}[\hat{y}_D] - \hat{y}_D)}_{C})^2] \\
&= \mathbb{E}[\underbrace{(f - \mathbb{E}[\hat{y}_D])^2}_{A^2}] + \underbrace{\mathbb{E}[\epsilon^2]}_{B^2} + \underbrace{\mathbb{E}[(\mathbb{E}[\hat{y}_D] - \hat{y}_D)^2]}_{C^2} \\
&\quad + 2\underbrace{\mathbb{E}[(f - \mathbb{E}[\hat{y}_D])\epsilon]}_{AB} \\
&\quad + 2\underbrace{\mathbb{E}[(f - \mathbb{E}[\hat{y}_D])(\mathbb{E}[\hat{y}_D] - \hat{y}_D)]}_{AC} \\
&\quad + 2\underbrace{\mathbb{E}[\epsilon(\mathbb{E}[\hat{y}_D] - \hat{y}_D)]}_{BC} \\
&= \dots \\
&= \mathbb{E}[\underbrace{(f - \mathbb{E}[\hat{y}_D])^2}_{A^2}] + \underbrace{\mathbb{E}[\epsilon^2]}_{B^2} + \underbrace{\mathbb{E}[(\mathbb{E}[\hat{y}_D] - \hat{y}_D)^2]}_{C^2} \\
&= Bias[\hat{y}_D]^2 + \sigma^2 + Var[\hat{y}_D]
\end{aligned}
$$

Bias-Variance decomposition, conclusion

For one test example we had that:

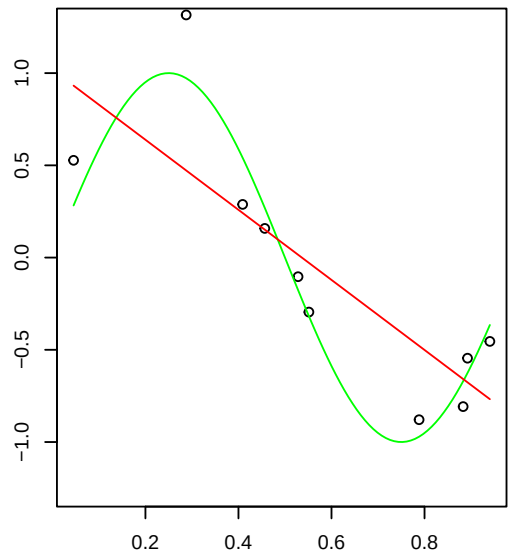
$$\mathbb{E}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}; D))^2] = Bias_D[\hat{f}(\mathbf{x}; D)]^2 + Var_D[\hat{f}(\mathbf{x}; D)] + \sigma^2$$

So, to take into account the whole space (true error) we integrate over all possible values of $\mathbf{x}$:

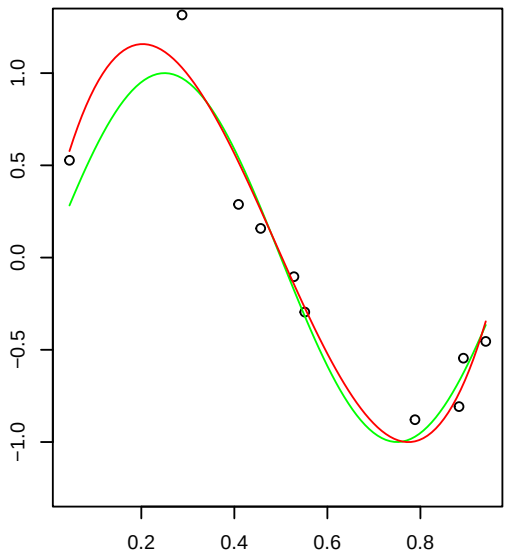
$$\begin{aligned} MSE_{true} &= \int_{\mathbf{x}} \left[Bias_D[\hat{f}(\mathbf{x}; D)]^2 + Var_D[\hat{f}(\mathbf{x}; D)] + \sigma^2 \right] p(\mathbf{x}) d\mathbf{x} \\ &= \mathbb{E}_x \left[Bias_D[\hat{f}(\mathbf{x}; D)]^2 + Var_D[\hat{f}(\mathbf{x}; D)] \right] + \sigma^2 \end{aligned}$$

which is the **expected true error** or **expected generalization error**

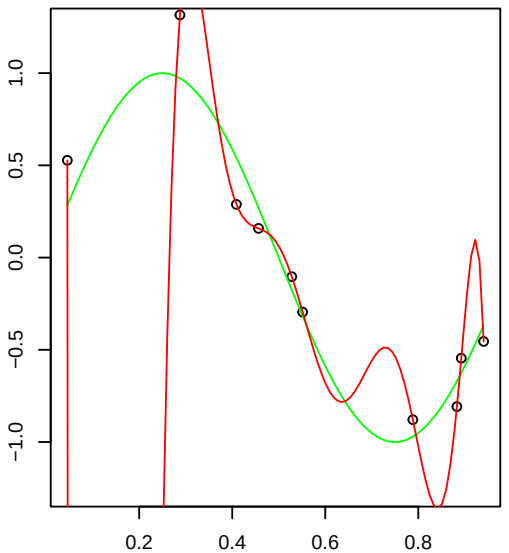
Bias-Variance decomposition, relation to over/underfitting



Poly fit of degree 1



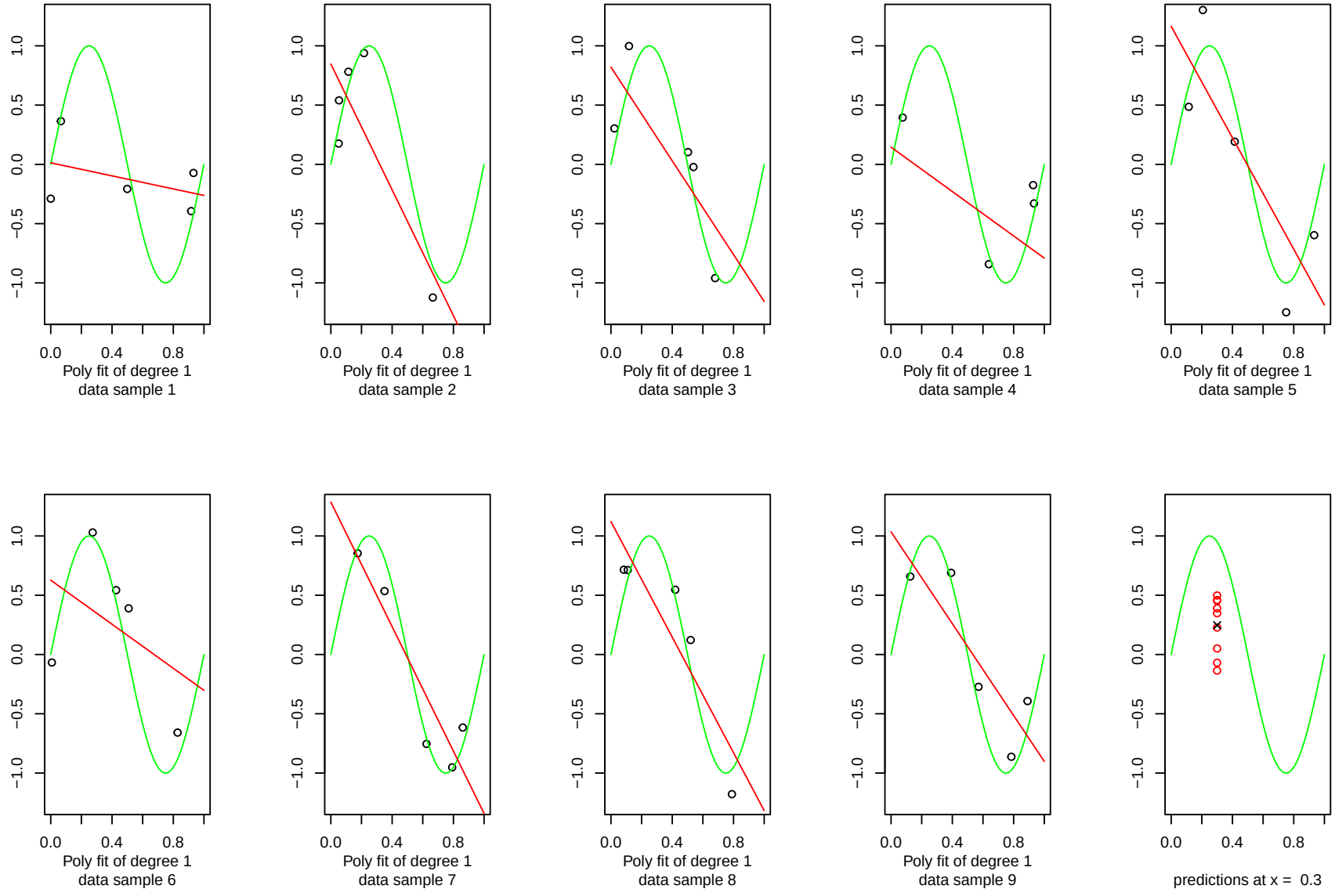
Poly fit of degree 3



Poly fit of degree 9

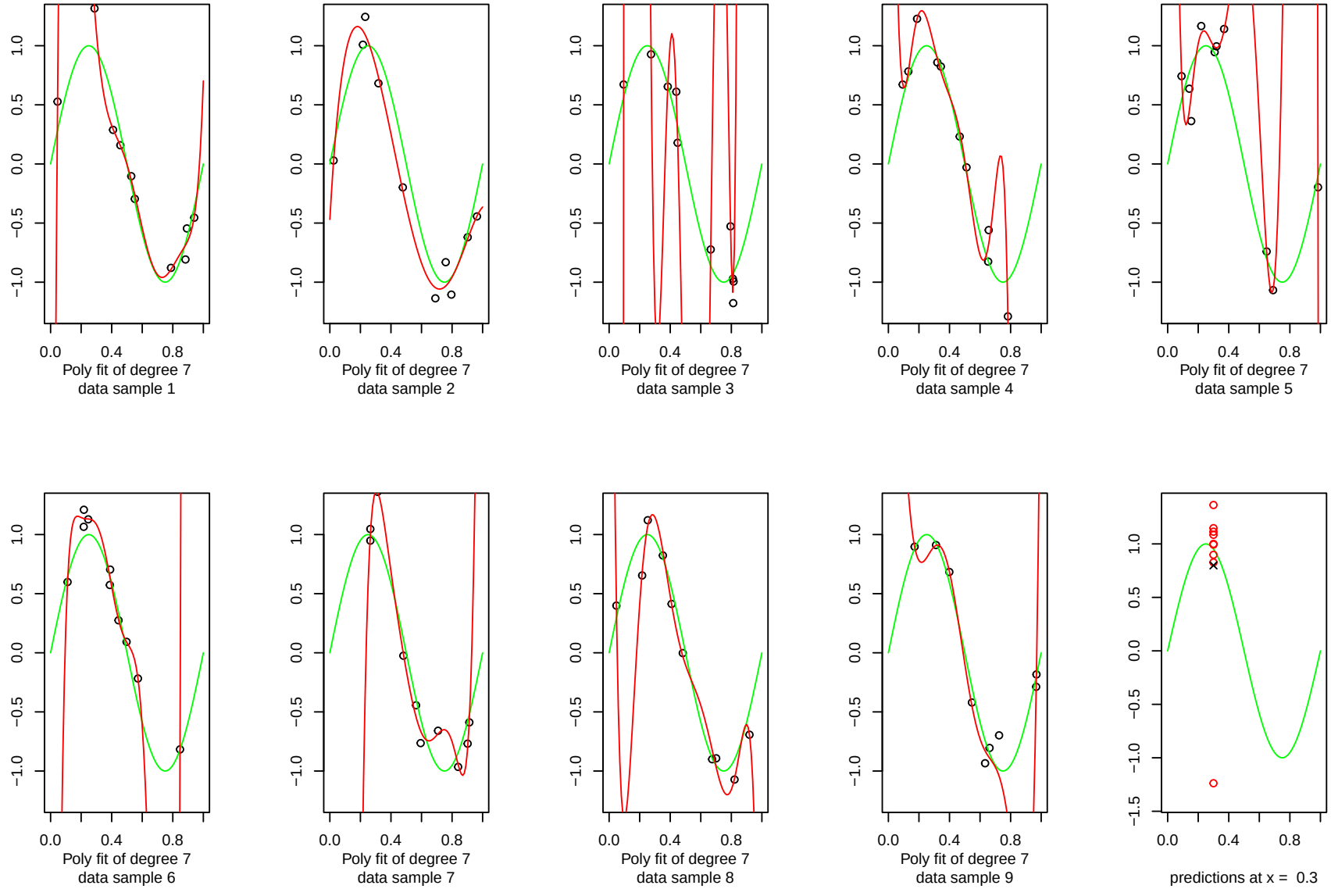
- high bias models will **underfit**
- high variance models will **overfit** especially if data is scarce (or: high variance model need tons of data to be fit properly)

Bias, variance of low complexity models (degree 1)



1. the model is quite stable (therefore it has **low Variance**)
2. the model is quite bad on average (therefore it has **high Bias**)

Bias, variance of high complexity models (degree 7)



1. the model is quite unstable (therefore it has **high Variance**)
2. the model is quite good *on average* (therefore it has **low Bias**)

Common error functions used in regression

name	*abbrev.*	*formula*
mean squared error	MSE	$\frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbf{x}_i\theta)^2$
root mean squared error	$RMSE$	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \mathbf{x}_i\theta)^2}$
normalized root mean squared error	$NRMSE$	$\sqrt{\frac{MSE}{Var(y)}}$
coefficient of determination	R^2	$1 - \frac{MSE}{Var(y)} = 1 - NRMSE^2$
mean absolute error	MAE	$\frac{1}{n}\sum_{i=1}^{n}\lvert y_i - \mathbf{x}_i\theta\rvert$

Regularization by Maximum a Posteriori (MAP)

Looking at Bayes for learning

Before proceeding, let us refresh Bayes rule in the context of learning (here, θ are the *parameters* and D is the given *data*):

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)} = \frac{likelihood \ \times \ prior}{evidence} = posterior$$

And so, maximum likelihood ignores prior information on θ (or equivalently assumes all θ are equally likely before doing any modelling):

$$\theta_{ML} \stackrel{\text{def}}{=} \arg\max_{\theta} \log P(X|\theta)$$

If we do assume some prior distribution over the parameters θ that is we have a notion of what types of solution we prefer, then we can use **maximum a posteriori** estimate for θ:

$$\begin{aligned}\theta_{MAP} &\stackrel{\text{def}}{=} \arg\max_{\theta} \log \left[P(X|\theta)P(\theta)\right] \\ &= \arg\max_{\theta} \left[\log P(X|\theta) + \log P(\theta)\right]\end{aligned}$$

Ridge regression from Gaussian prior on θ

Let us turn to an example; assume Gaussian prior on d-dimensional θ. Here, we use the special case of an *isotropic Gaussian* (i.e. $\Sigma = \tau^2 I$) and so:

- $\Sigma^{-1} = \frac{1}{\tau^2} I$
- $\det \Sigma = \tau^{2d}$

$$\theta \sim \mathcal{N}(\mu = 0, \mathbf{\Sigma} = \tau^2 I)$$

And so:

$$\begin{aligned} P(\theta; \mu = 0, \mathbf{\Sigma} = \tau^2 I) &= \frac{1}{|\mathbf{\Sigma}|^{\frac{1}{2}} (2\pi)^{\frac{d}{2}}} \exp\left\{ -\frac{1}{2} (\theta - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-1} (\theta - \boldsymbol{\mu}) \right\} \\ &= \frac{1}{(2\pi\tau^2)^{\frac{d}{2}}} \exp\left\{ -\frac{1}{2\tau^2} \theta^T \ \theta \right\} \\ &= \frac{1}{(2\pi\tau^2)^{\frac{d}{2}}} \exp\left\{ -\frac{\|\theta\|^2}{2\tau^2} \right\} \end{aligned}$$

Ridge regression from Gaussian prior on θ, cont.

$$
\begin{aligned}
P(\theta|\mathbf{y},\mathbf{X}) &\propto P(\mathbf{y}|\mathbf{X},\theta)\ P(\theta) \\
&\propto \exp\left\{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)\right\}\exp\left\{-\frac{\|\theta\|^2}{2\tau^2}\right\} \\
&= \exp\left\{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)-\frac{\|\theta\|^2}{2\tau^2}\right\}
\end{aligned}
$$

And so the **maximum a posteriori** estimate becomes:

$$
\begin{aligned}
\theta_{MAP} &= \arg\max_{\theta} \log\left[P(\mathbf{y}|\mathbf{X},\theta)\ P(\theta)\right] \\
&= \arg\max_{\theta}\left[-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)-\frac{\|\theta\|^2}{2\tau^2}\right] \\
&= \arg\min_{\theta}\left[(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)+\frac{\sigma^2}{\tau^2}\|\theta\|^2\right] \\
&= \arg\min_{\theta}\left[(\mathbf{y}-\mathbf{X}\theta)^T(\mathbf{y}-\mathbf{X}\theta)+\lambda\|\theta\|^2\right]
\end{aligned}
$$

which is the **ridge regression** estimate when $\lambda = \frac{\sigma^2}{\tau^2}$

Ridge regression estimate

As we did with ordinary least squares regression, we differentiate and set to 0 in order to find the minimum:

$$\frac{\partial}{\partial \theta}\left\{\|\mathbf{y}-\mathbf{X}\theta\|^2+\lambda\|\theta\|^2\right\}=(-2\mathbf{X}^T\mathbf{y}+2\mathbf{X}^T\mathbf{X}\theta)+2\lambda\theta=0$$

leading to

$$\theta_{MAP}=\theta_{ridge}=(\mathbf{X}^T\mathbf{X}+\lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

Observations:

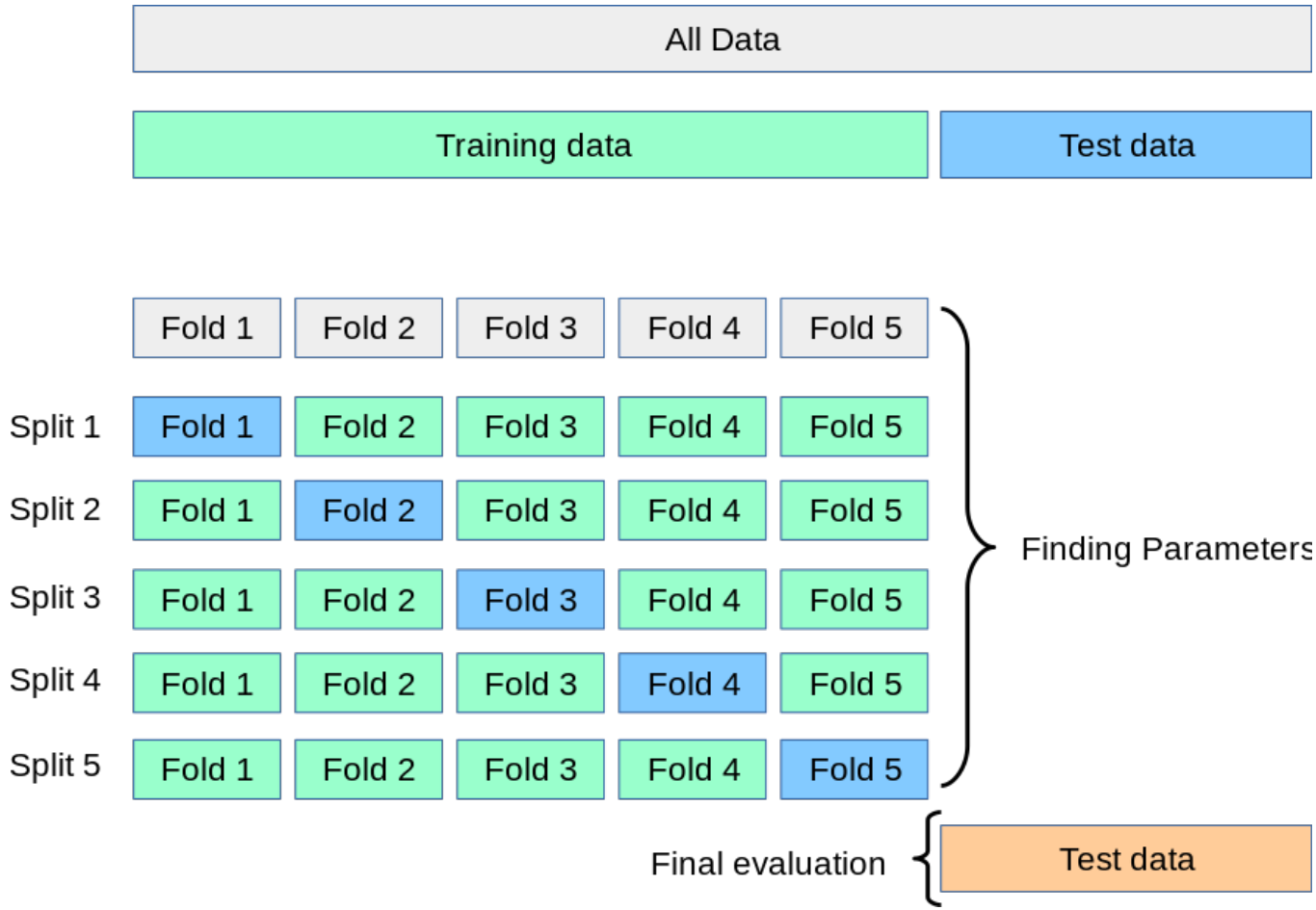
- λ controls the complexity of the solution θ (smaller "length" == smaller coefficients == simpler solution)
- $\mathbf{X}^T\mathbf{X}+\lambda I$ is guaranteed to be non-singular and behaves better numerically than $\mathbf{X}^T\mathbf{X}$, especially if the columns of $\mathbf{X}$ are highly correlated, or if there are few observations (rows of $\mathbf{X}$) relative to number of predictors (columns of $\mathbf{X}$).
- as a general recipe when we have a regularized objective function, is to use *potentially-more-complex-than-needed functions* and then adjust λ

Tuning λ

We have a hyper-parameter λ. How do we set it?

1. training/validation split
2. cross-validation
3. leave-one-out-cross-validation (loocv)

Cross-validation



Cross-validation, cont.

1. Decide on a set of values for $\lambda \in \{\lambda_1, \ldots, \lambda_l\} = \Lambda$
2. Partition training data into $K > 1$ folds
3. Repeat for $k = 1, \ldots, K$:
   - use k-th fold for *validation*
   - use the remaining $K - 1$ for *training*; train with all λ values
   - estimate generalization on the one validation fold for all λ values
4. Average K generalization estimates, select λ that gives best cross-val estimation

Leave-one-out-cross-val is cross-validation for $K = n$ (one fold per example)

Notice that, in general, we have to train $K \times |\Lambda|$ times, so this may be costly ..

Loocv for ridge

As a particularity of linear and ridge regression, for a given λ value, only **one training** is necessary for *loocv*; so:

1. For each $\lambda \in \Lambda$:
   - compute optimal solution $\hat{\theta}_\lambda = (\mathbf{\Phi}^T\mathbf{\Phi} + \lambda I)^{-1}\mathbf{\Phi}^T\mathbf{y}$
   - compute "hat" matrix $H_\lambda = \mathbf{\Phi}(\mathbf{\Phi}^T\mathbf{\Phi} + \lambda I)^{-1}\mathbf{\Phi}^T$
   - compute loocv directly for each λ (no need to use folds etc.):

$$loocv(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \phi(\mathbf{x}_i)\theta_\lambda}{1 - h_{ii}}\right)^2$$

2. Return λ with minimum *loocv*

GCV for ridge

The *loocv* for each λ can be approximated by the (numerically more stable) GCV; here we have substituted each h_{ii} by the *average value of the elements in the diagonal*:

$$GCV(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \phi(\mathbf{x}_i)\theta_\lambda}{1 - \frac{Tr(H_\lambda)}{n}}\right)^2 = \frac{MSE_\lambda}{\left(1 - \frac{Tr(H_\lambda)}{n}\right)^2}$$

where $Tr(H_\lambda)$ is the trace of H_λ (sum of diagonal elements).

LASSO regression

The p-norm of vector θ is:

$$\|\theta\|_p \stackrel{\text{def}}{=} \left(\sum_d |\theta_d|^p \right)^{\frac{1}{p}}$$

As we have seen, assuming an isotropic Gaussian prior on the parameters leads to **ridge** regression, which joinly minimizes the (squared) of the L2-norm of θ (so, $p = 2$) and the squared error. Another very common choice is $p = 1$, which leads to **lasso** regression.

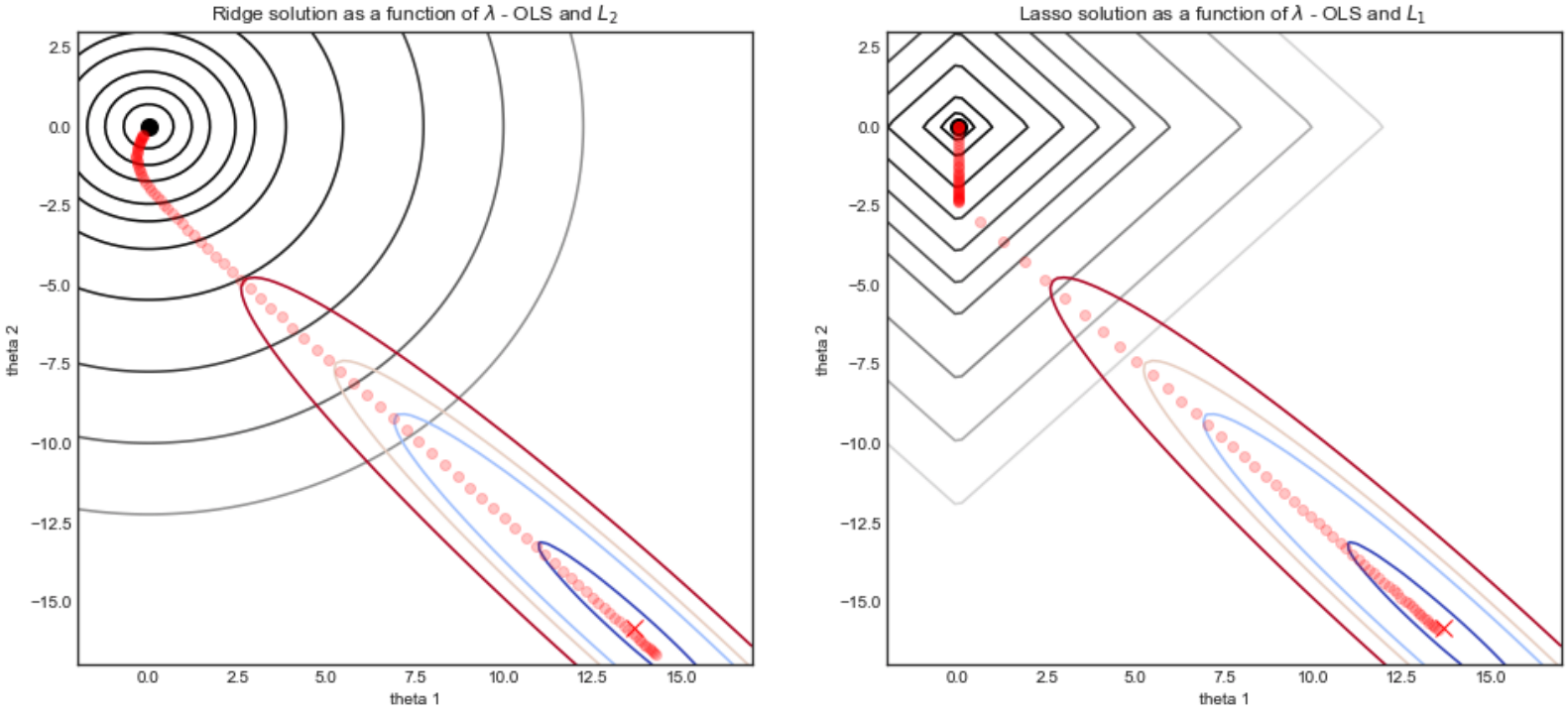
So **lasso** regression minimizes L1-norm of parameters and squared error:

$$\theta_{lasso} = \arg\min_{\theta} \left[\|\mathbf{y} - \mathbf{X}\theta\|_2^2 + \lambda \|\theta\|_1 \right]$$

Actually, **lasso** regression arises assuming a Laplace distribution prior over the parameters.

LASSO regression, cont.

Lasso regression gives **sparse** solutions in the sense that many of θ coefficients might be 0. So, it performs **feature selection**.



Lasso regularized cost function is no longer quadratic and has **no closed solution**, so an approximation procedure is used to optimize it called the **least angle regression**. This procedure exploits the special structure of the problem and provides an efficient way to compute the solutions for a list of possible values for $\lambda > 0$, giving the **regularization path**.