Machine Learning

FIB, Master in Innovation and Research in Informatics

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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, regression
3. Bayesian linear regression

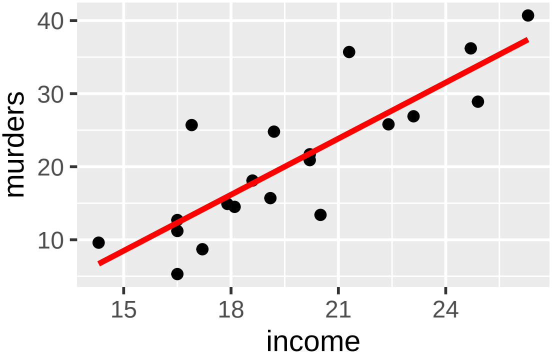
Regression

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:

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

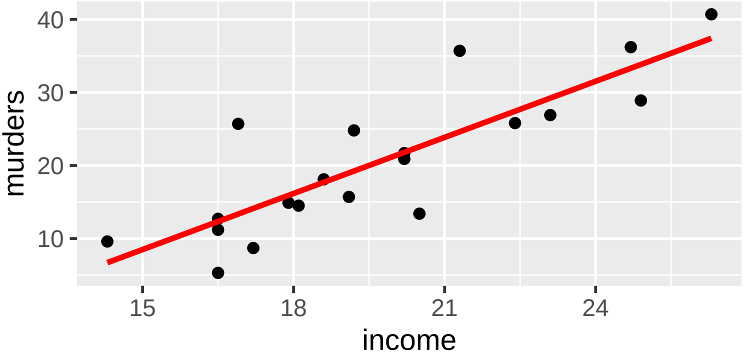
The **least squares** linear regression method tells us to choose the line that minimizes the following **error function** (a.k.a. objective function, loss function, cost function, ..):

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

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 $\theta = \begin{bmatrix} \theta_0 \; \theta_1 \; \ldots \theta_d \end{bmatrix}^T$:

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

Spelling it out this is:

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

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 $x' = \left[x'_1 \; x'_2 \ldots x'_d\right]^T$ all we need to do is compute

$$y' = \left[1 \; x'_1 \; x'_2 \ldots x'_d\right] \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} = \theta_0 + \sum_{j=1}^{d} x'_j \theta_j$$

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 $\mathbf{X}$

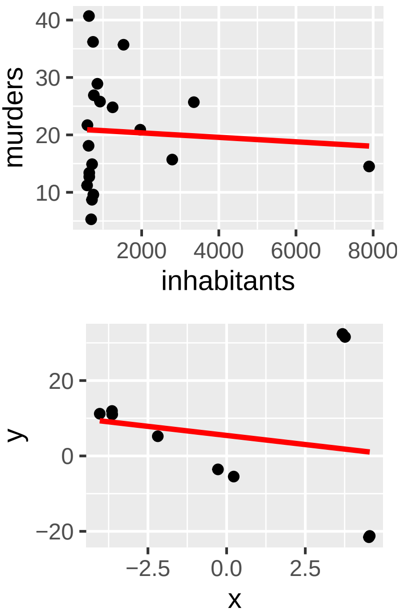
Then:

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

```python
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

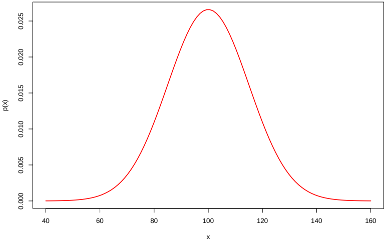
using probabilities to quantify uncertainty

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*:

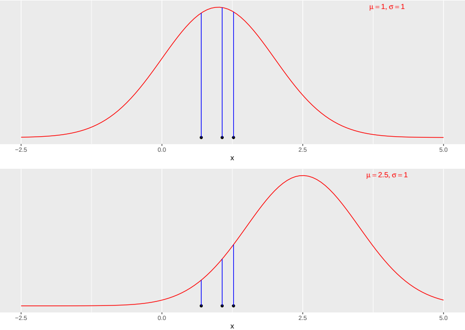
$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2} \quad \text{when } x \sim \mathcal{N}(\mu, \sigma^2)$$



Maximum likelihood principle

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

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

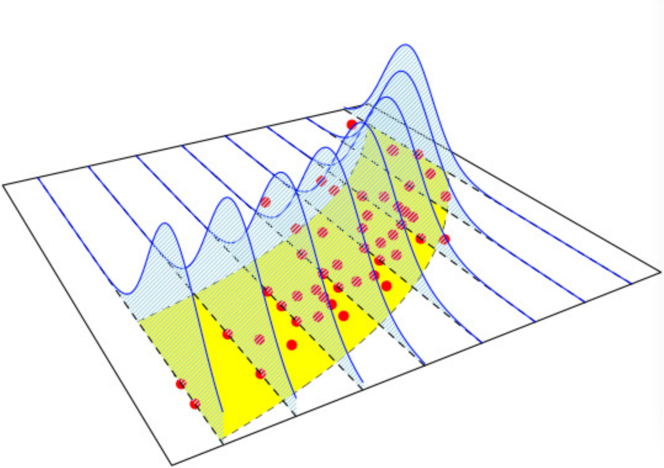


Note that the likelihood is a **function of the parameters**, assuming the data is fixed. Additionally, we assume that all x_i are *independent and identically distributed* according to $\mathcal{N}(\mu, \sigma^2)$.

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

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

leads to:

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

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

Tension between two concepts

Bias-Variance decomposition

Assume the following:

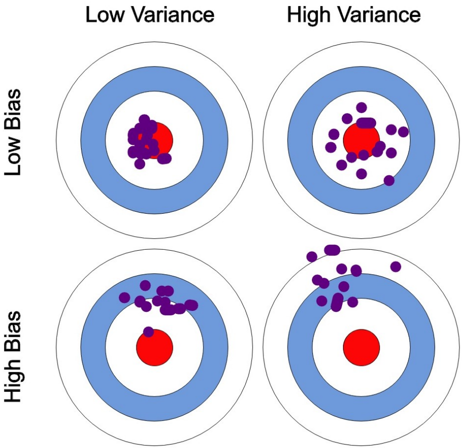
- let $f : \mathbb{R}^d \to \mathbb{R}$ be the **true function** that we are trying to approximate
- let D be a finite dataset for training $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)\}$, where $y_i = f(\mathbf{x}_i) + \epsilon_i$, and all ϵ_i are iid according to $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$
- 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 decomposition, dartboard intuition



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 $f(\mathbf{x})$

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

Bias-Variance decomposition, conclusion

For one test example we had that:

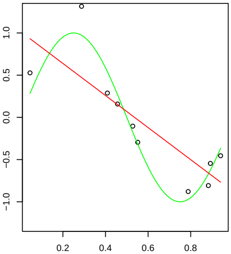
$$\mathbb{E}[(f(\mathbf{x})-\hat{f}(\mathbf{x};D))^2] = Bias_D[\hat{f}(\mathbf{x};D)]^2 + Var_D[\hat{f}(\mathbf{x};D)] + \sigma^2$$

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

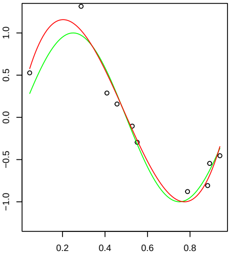
$$\begin{aligned} MSE_{true} &= \int_{\mathbf{x}} \left[Bias_D[\hat{f}(\mathbf{x};D)]^2 + Var_D[\hat{f}(\mathbf{x};D)] + \sigma^2\right] p(\mathbf{x}) d\mathbf{x} \\ &= \mathbb{E}_x \left[Bias_D[\hat{f}(\mathbf{x};D)]^2 + Var_D[\hat{f}(\mathbf{x};D)]\right] + \sigma^2 \end{aligned}$$

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

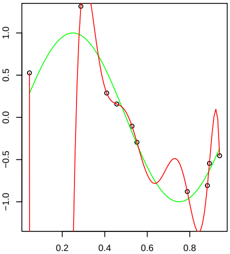
Bias-Variance decomposition, relation to over/underfitting



Poly fit of degree 1



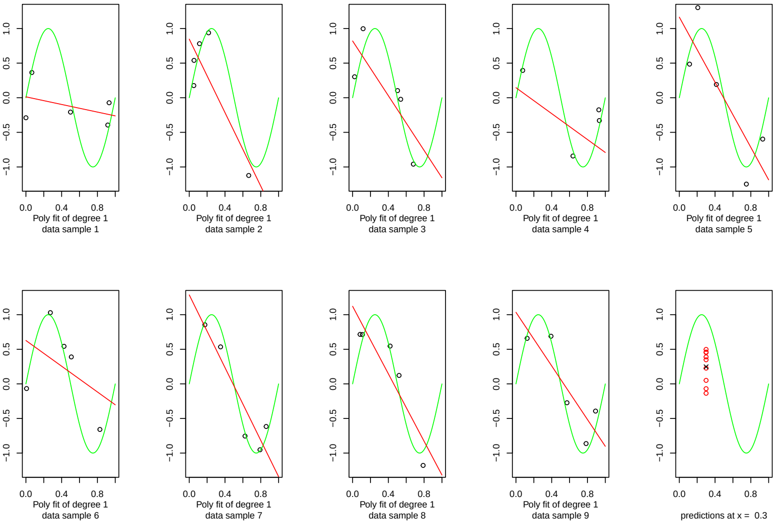
Poly fit of degree 3



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)



Poly fit of degree 1
data sample 1

Poly fit of degree 1
data sample 2

Poly fit of degree 1
data sample 3

Poly fit of degree 1
data sample 4

Poly fit of degree 1
data sample 5

Poly fit of degree 1
data sample 6

Poly fit of degree 1
data sample 7

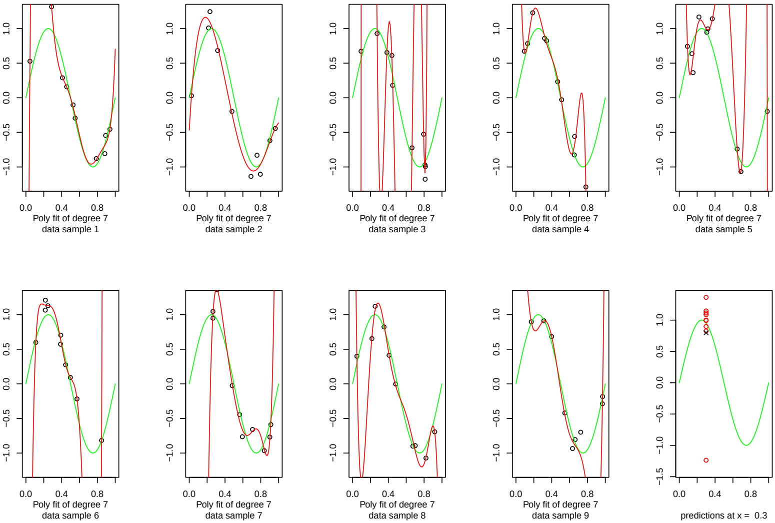
Poly fit of degree 1
data sample 8

Poly fit of degree 1
data sample 9

predictions at x = 0.3

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)



Poly fit of degree 7
data sample 1

Poly fit of degree 7
data sample 2

Poly fit of degree 7
data sample 3

Poly fit of degree 7
data sample 4

Poly fit of degree 7
data sample 5

Poly fit of degree 7
data sample 6

Poly fit of degree 7
data sample 7

Poly fit of degree 7
data sample 8

Poly fit of degree 7
data sample 9

predictions at x = 0.3

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*):

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

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

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

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:

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

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:

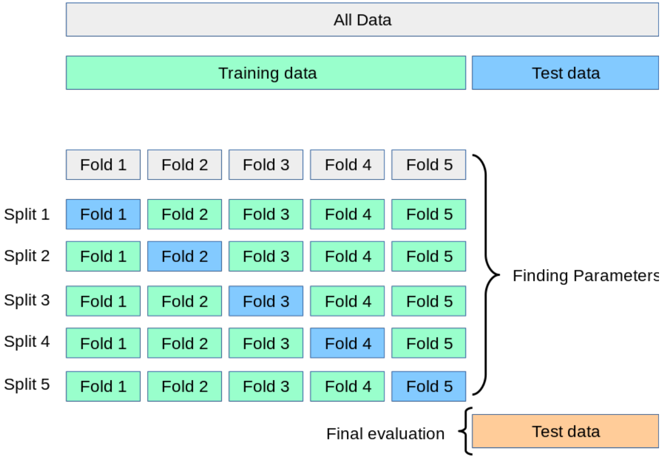
- λ controls the complexity of the solution θ (smaller “length” == smaller coefficients == simpler solution)
- $\mathbf{X}^T\mathbf{X}+\lambda I$ is guaranteed to be non-singular and behaves better numerically than $\mathbf{X}^T\mathbf{X}$, especially if the columns of $\mathbf{X}$ are highly correlated, 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



All Data

Training data | Test data

	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 4	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 5	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Finding Parameters

Final evaluation

Test data

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:

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

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.

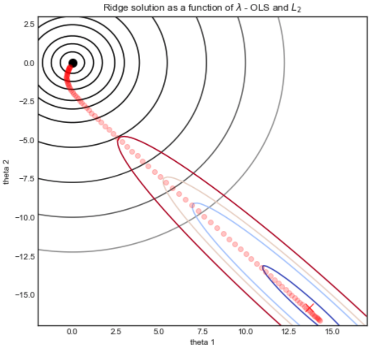
So **lasso** regression minimizes L1-norm of parameters and squared error:

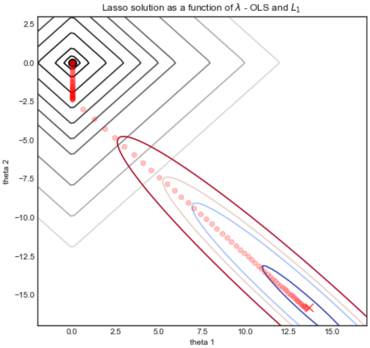
$$\theta_{lasso} = \arg\min_\theta \left[\|\mathbf{y} - \mathbf{X}\theta\|_2^2 + \lambda \|\theta\|_1 \right]$$

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**.

Some concepts to remember

- Linear regression as an example of learning
- Solving using loss minimization
- Solving using MLE
- Bias and variance tension
- Solving tension via regularization
- Cross validation to find best regularization parameter

The full-Bayesian perspective

Bayesian linear regression

Both ML and MAP produce point-estimates of the parameters; in contrast in Bayesian Learning we want the full **posterior** distribution of the parameters.

The key insight is that if we know the posterior distribution of the parameters (let's call it $p(\theta|D)$), then we can do a sort of "infinite weighted averaging" for doing predictions:

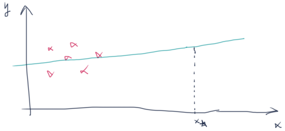
$$p(y_\star|x_\star, D) = \int_\Theta p(y_\star|x_\star, \theta, D)p(\theta|D)\ d\theta$$

So, instead of just using a single point-estimate $\hat{\theta}$ of the parameters, we use the full distribution and integrate the predictions. This, in turn, gives us a full distribution over the predictions as opposed to (again) to a single point-prediction that we get for ML or MAP.

Typically, computing this integral is going to be intractable and we have to resort to approximating it. Luckily in the context of linear regression all these expressions have closed-form formulas. For computational speed however we may use approximations as well.

Bayesian linear regression vs. ML and MAP

Technically, ML and MAP assume that $Y \sim \mathcal{N}(\mathbf{x}^T\theta, \sigma^2)$ so a prediction for a new test point $\mathbf{x}_\star$ is going to have distribution $\mathcal{N}(\mathbf{x}_\star^T\hat{\theta}, \hat{\sigma}^2)$. But note the lack of flexibility of this since the width of the normal distribution is going to be the same for any new test point, which may be a dangerous assumption e.g. in a situation as follows:



Linear regression problem, again

Just as a reminder, we describe the regression problem: we are given a sample $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$.

We assume

- $Y_1, \ldots, Y_n$ are independent given θ,
- $Y_i \sim \mathcal{N}(\mathbf{x}_i^T \theta, a^{-1})$, with $a > 0$ being the precision of the noise in the observations (so, $a = \frac{1}{\sigma^2}$)
- **parameter's prior** $p(\theta) \sim \mathcal{N}(0, b^{-1} I)$ with $b > 0$, i.e., spherical or isotropic Gaussian
- a, b known
- the only parameter variables are the coefficients $\theta = (\theta_0, \ldots, \theta_d)^T$

The likelihood function is

$$p(D|\theta) \propto \exp\left\{ -\frac{a}{2} (\mathbf{y} - X\theta)^T (\mathbf{y} - X\theta) \right\}$$

with $X = \begin{pmatrix} \text{------} & \mathbf{x}_1^T & \text{------} \\ & \vdots & \\ \text{------} & \mathbf{x}_n^T & \text{------} \end{pmatrix}$ and $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$.

The posterior distribution

Using Bayes as usual, we derive the posterior distribution

$$
\begin{aligned}
p(\theta|D) &\propto p(D|\theta)p(\theta) \\
&\propto \exp\left\{-\frac{a}{2}(\mathbf{y}-X\theta)^T(\mathbf{y}-X\theta)\right\}\exp\left\{-\frac{b}{2}\theta^T\theta\right\} \\
&\propto \exp\left\{-\frac{a}{2}(\mathbf{y}-X\theta)^T(\mathbf{y}-X\theta)-\frac{b}{2}\theta^T\theta\right\}
\end{aligned}
$$

It is important to notice that the exponent of the above expression is quadratic on θ, and so the above expression is going to be a multivariate Gaussian.

We need to turn the above exponent into something resembling $(\theta-\mu)^T Q(\theta-\mu)$ (notice how we are using the *precision* instead of the *covariance* matrix) so that we can derive what the mean μ and the precision Q of the posterior density is.

The posterior distribution, cont.

We use the method of completing the square which you may remember from your school days.

In this method, we are going to "match" terms from our posterior exponent $a(\mathbf{y} - X\theta)^T(\mathbf{y} - X\theta) + b\theta^T\theta$ to the desired form $(\theta - \mu)^T Q(\theta - \mu)$. Note that we have divided both by $-\frac{1}{2}$ to simplify a little.

So we re-write these expressions so that we can match the terms, starting with the desired one:

$$\begin{aligned}(\theta - \mu)^T Q(\theta - \mu) &= \theta^T Q\theta - \theta^T Q\mu - \mu^T Q\theta + \mu^T\mu \\ &= \theta^T Q\theta - 2\theta^T Q\mu + const.\end{aligned}$$

We do not need to keep track of terms that do not contain θ, because we only care about proportionality. Now we multiply out the posterior density exponent:

$$\begin{aligned}& a(\mathbf{y} - X\theta)^T(\mathbf{y} - X\theta) + b\theta^T\theta \\ = \quad & a(\mathbf{y}^T\mathbf{y} - 2\theta^T X^T\mathbf{y} + \theta^T X^T X\theta) + b\theta^T\theta \\ = \quad & a\mathbf{y}^T\mathbf{y} - 2a\theta^T X^T\mathbf{y} + \theta^T(aX^TX + bI)\theta\end{aligned}$$

The posterior distribution, cont.

We need to match terms of

$$\theta^T Q\theta - 2\theta^T Q\mu$$

with terms of

$$a\mathbf{y}^T\mathbf{y} - 2a\theta^T X^T\mathbf{y} + \theta^T(aX^T X + bI)\theta$$

First, we match $\theta^T(aX^T X + bI)\theta$ with $\theta^T Q\theta$ and obtain $Q = aX^T X + bI$.

Next, we match $-2a\theta^T X^T\mathbf{y}$ with $-2\theta^T Q\mu$ and so[2]:

$$\begin{aligned} a\theta^T X^T\mathbf{y} = \theta^T Q\mu &\iff \\ aX^T\mathbf{y} = Q\mu &\iff \\ aQ^{-1}X^T\mathbf{y} = \mu & \end{aligned}$$

And so the density of the posterior $p(\theta|D) \sim \mathcal{N}(\mu, Q^{-1})$ where

- $Q = aX^T X + bI$
- $\mu = aQ^{-1}X^T\mathbf{y}$

[2] Notice that we can safely invert Q because it is a positive definite matrix (the $+bI$ part guarantees it even if $X^T X$ was PSD only).

The posterior distribution, cont.

MAP estimate

The posterior $p(\theta|D) \sim \mathcal{N}(\mu, Q^{-1})$, where

- $Q = aX^TX + bI$
- $\mu = aQ^{-1}X^T\mathbf{y}$

We can read the MAP estimate (which we have already derived in previous sections) directly from this since the maximum density is obtained at the mean in any Gaussian distribution.

$$\mu = aQ^{-1}X^T\mathbf{y} = a(aX^TX + bI)^{-1}X^T\mathbf{y} = (X^TX + \frac{b}{a}I)^{-1}X^T\mathbf{y}$$

Additionally, in ridge regression we let $\lambda := \frac{b}{a}$ and turn it into a parameter that we can tune to control complexity vs. training error.

Using the posterior distribution for predictions

Let us know turn to the issue of computing the **predictive distribution** for our model. Namely, we want to compute

$$p(y_\star | x_\star, D) = \int_\Theta p(y_\star | x_\star, \theta, D) p(\theta | D) \; d\theta$$

The predictive distribution

We substitute the densities $p(y_\star|x_\star, \theta, D)$ and $p(\theta|D)$ in the above expression, and start to work it out:

$$\begin{aligned} p(y_\star|x_\star, D) &= \int_\Theta \mathcal{N}(y_\star|\mathbf{x}_\star^T\theta, a^{-1})\mathcal{N}(\theta|\mu, Q^{-1})\ d\theta \\ &\propto \int_\Theta \exp\left\{-\frac{a}{2}(y_\star - \mathbf{x}_\star^T\theta)^2\right\}\exp\left\{-\frac{1}{2}(\theta-\mu)^T Q(\theta-\mu)\right\}\ d\theta \end{aligned}$$

The predictive distribution, cont.

We do not include the derivation here, but you can consult it in this video and its following 3 parts. The proof includes the following steps:

1. Factorizing the above expression into something like $\int \mathcal{N}(\theta|\dots)f(y_\star)\ d\theta$, where $f(y_\star)$ does not depend on θ using the complete the squares technique
2. Since $f(y_\star)$ does not depend on θ, we can take it out of the integral and get rid of it: $\int \mathcal{N}(\theta|\dots)f(y_\star)\ d\theta = f(y_\star)\int \mathcal{N}(\theta|\dots)\ d\theta = f(y_\star)$
3. Finally complete the squares (again!) on the remaining $f(y_\star)$ - as it turns out, $f(y_\star)$ is quadratic on $y_\star$ - to figure out the parameters for the predictive distribution.

The result after doing all this is that

$$p(y_\star|x_\star, D) \sim \mathcal{N}(m, s^{-1})$$

where

- $m = \mathbf{x}_\star^T \mu$
- $\frac{1}{s} = \frac{1}{a} + \mathbf{x}_\star^T Q \mathbf{x}_\star$, where
- $\mu = (X^T X + \frac{b}{a} I)^{-1} X^T \mathbf{y}$ is the mean of the posterior distribution $p(\theta|D)$
- Q is the precision matrix of the posterior distribution

The predictive distribution, cont.

As a final note, we see that the predictive distribution's mean prediction equals the point-prediction of the MAP. However, the variance of the prediction does depend on $\mathbf{x}_\star$ which is a good thing, since the uncertainty of our predictions depends on how far observed examples are, if near, then we should be more certain, but if far away, then we should be less certain.

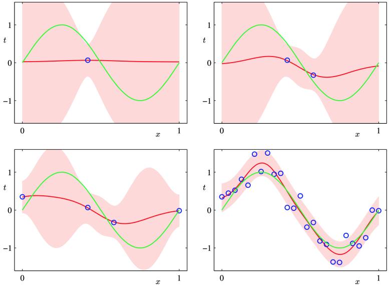


Figure 3.8 Examples of the predictive distribution (3.58) for a model consisting of 9 Gaussian basis functions of the form (3.4) using the synthetic sinusoidal data set of Section 1.1. See the text for a detailed discussion.

The predictive distribution, cont.

Bayesian learning is a very natural form of sequential learning

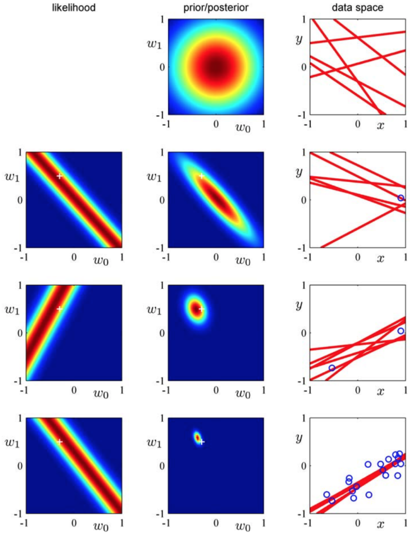


Figure 3.7 Illustration of sequential Bayesian learning for a simple linear model of the form $y(x, \mathbf{w}) = w_0 + w_1 x$. A detailed description of this figure is given in the text.