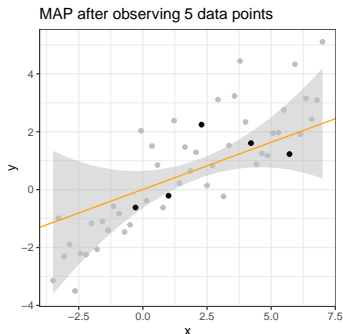
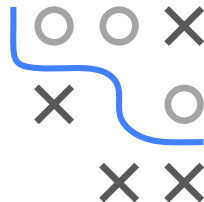


Introduction to Machine Learning

Gaussian Processes

Bayesian Linear Model

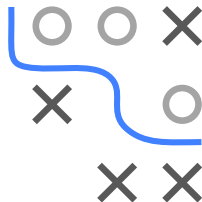
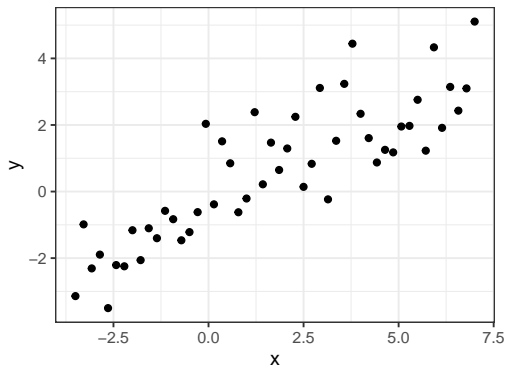


Learning goals

- Know the Bayesian linear model
- The Bayesian LM returns a (posterior) distribution instead of a point estimate
- Know how to derive the posterior distribution for a Bayesian LM

REVIEW: THE BAYESIAN LINEAR MODEL

Let $\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)})\}$ be a training set of i.i.d. observations from some unknown distribution.



Let $\mathbf{y} = (y^{(1)}, \dots, y^{(n)})^\top$ and $\mathbf{X} \in \mathbb{R}^{n \times p}$ be the design matrix where the i -th row contains vector $\mathbf{x}^{(i)}$.

REVIEW: THE BAYESIAN LINEAR MODEL / 2

The linear regression model is defined as

$$y = f(\mathbf{x}) + \epsilon = \boldsymbol{\theta}^T \mathbf{x} + \epsilon$$

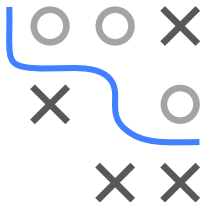
or on the data:

$$y^{(i)} = f(\mathbf{x}^{(i)}) + \epsilon^{(i)} = \boldsymbol{\theta}^T \mathbf{x}^{(i)} + \epsilon^{(i)}, \quad \text{for } i \in \{1, \dots, n\}$$

We now assume (from a Bayesian perspective) that also our parameter vector $\boldsymbol{\theta}$ is stochastic and follows a distribution. The observed values $y^{(i)}$ differ from the function values $f(\mathbf{x}^{(i)})$ by some additive noise, which is assumed to be i.i.d. Gaussian

$$\epsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$$

and independent of \mathbf{x} and $\boldsymbol{\theta}$.

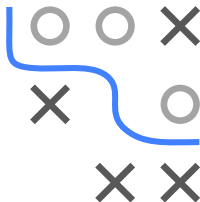


REVIEW: THE BAYESIAN LINEAR MODEL / 3

Let us assume we have **prior beliefs** about the parameter θ that are represented in a prior distribution $\theta \sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}_p)$.

Whenever data points are observed, we update the parameters' prior distribution according to Bayes' rule

$$\underbrace{p(\theta|\mathbf{X}, \mathbf{y})}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y}|\mathbf{X}, \theta)}^{\text{likelihood}} \overbrace{q(\theta)}^{\text{prior}}}{\underbrace{p(\mathbf{y}|\mathbf{X})}_{\text{marginal}}}.$$



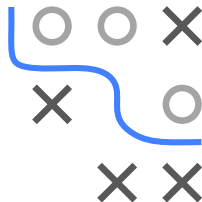
REVIEW: THE BAYESIAN LINEAR MODEL / 4

The posterior distribution of the parameter θ is again normal distributed (the Gaussian family is self-conjugate):

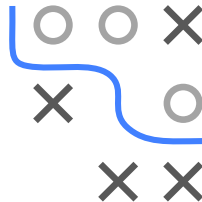
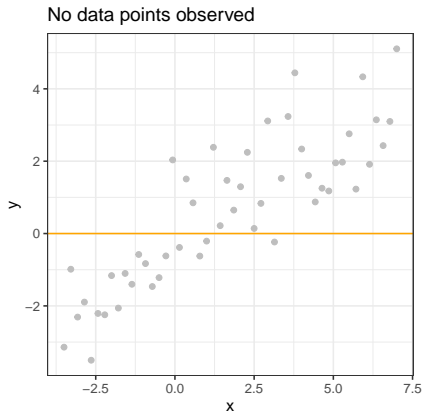
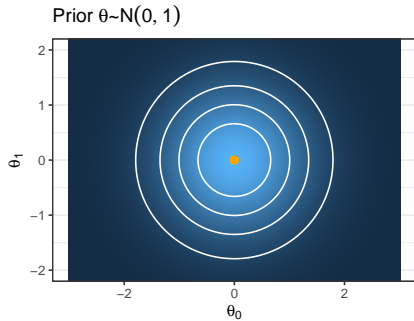
$$\theta \mid \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^{\top} \mathbf{y}, \mathbf{A}^{-1})$$

with $\mathbf{A} := \sigma^{-2} \mathbf{X}^{\top} \mathbf{X} + \frac{1}{\tau^2} \mathbf{I}_p$.

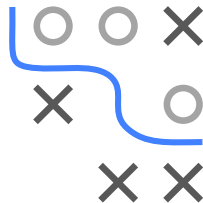
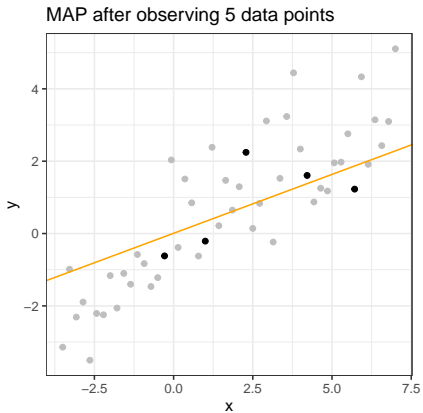
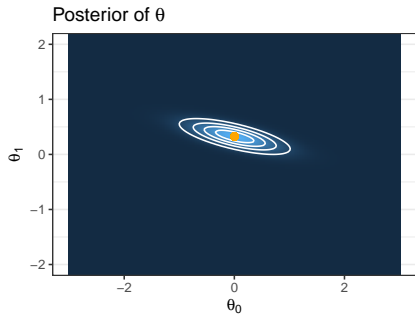
Note: If the posterior distribution $p(\theta \mid \mathbf{X}, \mathbf{y})$ are in the same probability distribution family as the prior $q(\theta)$ w.r.t. a specific likelihood function $p(\mathbf{y} \mid \mathbf{X}, \theta)$, they are called **conjugate distributions**. The prior is then called a **conjugate prior** for the likelihood. The Gaussian family is self-conjugate: Choosing a Gaussian prior for a Gaussian Likelihood ensures that the posterior is Gaussian.



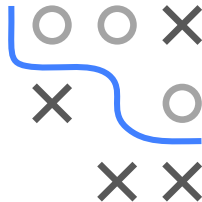
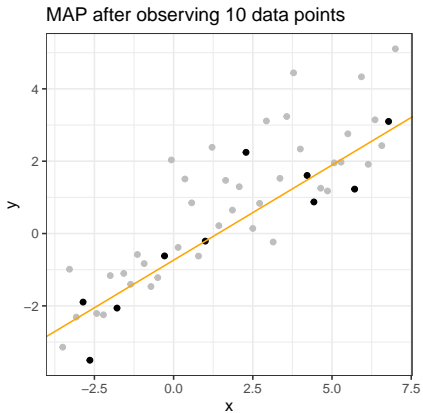
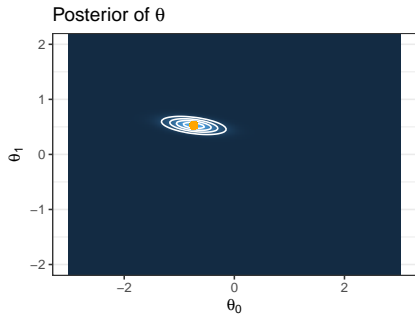
REVIEW: THE BAYESIAN LINEAR MODEL / 5



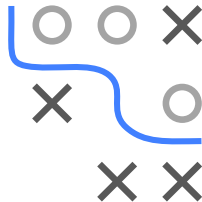
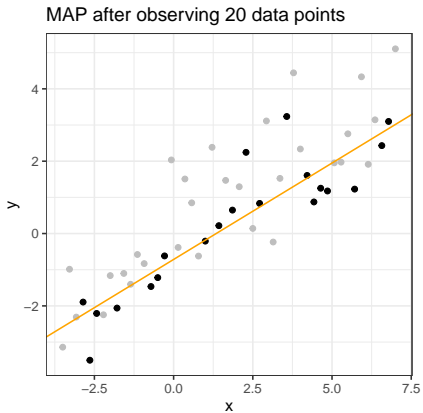
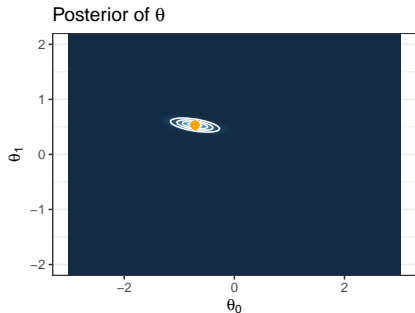
REVIEW: THE BAYESIAN LINEAR MODEL / 6



REVIEW: THE BAYESIAN LINEAR MODEL / 7



REVIEW: THE BAYESIAN LINEAR MODEL / 8



REVIEW: THE BAYESIAN LINEAR MODEL / 9

Proof:

We want to show that

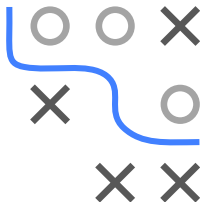
- for a Gaussian prior on $\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}_p)$
- for a Gaussian Likelihood $y \mid \mathbf{X}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}^\top \boldsymbol{\theta}, \sigma^2 \mathbf{I}_n)$

the resulting posterior is Gaussian $\mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^\top \mathbf{y}, \mathbf{A}^{-1})$ with $\mathbf{A} := \sigma^{-2} \mathbf{X}^\top \mathbf{X} + \frac{1}{\tau^2} \mathbf{I}_p$.

Plugging in Bayes' rule and multiplying out yields

$$\begin{aligned} p(\boldsymbol{\theta} \mid \mathbf{X}, \mathbf{y}) &\propto p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta}) q(\boldsymbol{\theta}) \propto \exp \left[-\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) - \frac{1}{2\tau^2} \boldsymbol{\theta}^\top \boldsymbol{\theta} \right] \\ &= \exp \left[-\frac{1}{2} \left(\underbrace{\sigma^{-2} \mathbf{y}^\top \mathbf{y}}_{\text{doesn't depend on } \boldsymbol{\theta}} - 2\sigma^{-2} \mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} + \sigma^{-2} \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} + \tau^{-2} \boldsymbol{\theta}^\top \boldsymbol{\theta} \right) \right] \\ &\propto \exp \left[-\frac{1}{2} \left(\sigma^{-2} \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\theta} + \tau^{-2} \boldsymbol{\theta}^\top \boldsymbol{\theta} - 2\sigma^{-2} \mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} \right) \right] \\ &= \exp \left[-\frac{1}{2} \boldsymbol{\theta}^\top \underbrace{\left(\sigma^{-2} \mathbf{X}^\top \mathbf{X} + \tau^{-2} \mathbf{I}_p \right)}_{:=\mathbf{A}} \boldsymbol{\theta} + \sigma^{-2} \mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} \right] \end{aligned}$$

This expression resembles a normal density - except for the term in red!



REVIEW: THE BAYESIAN LINEAR MODEL / 10

Note: We need not worry about the normalizing constant since its mere role is to convert probability functions to density functions with a total probability of one.

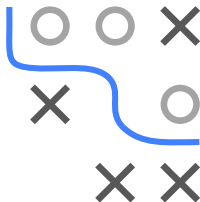
We subtract a (not yet defined) constant c while compensating for this change by adding the respective terms (“adding 0”), emphasized in green:

$$\begin{aligned} p(\theta|\mathbf{X}, \mathbf{y}) &\propto \exp \left[-\frac{1}{2}(\theta - \mathbf{c})^\top \mathbf{A}(\theta - \mathbf{c}) - \underbrace{\mathbf{c}^\top \mathbf{A} \theta}_{\text{doesn't depend on } \theta} + \sigma^{-2} \mathbf{y}^\top \mathbf{X} \theta \right] \\ &\propto \exp \left[-\frac{1}{2}(\theta - \mathbf{c})^\top \mathbf{A}(\theta - \mathbf{c}) - \mathbf{c}^\top \mathbf{A} \theta + \sigma^{-2} \mathbf{y}^\top \mathbf{X} \theta \right] \end{aligned}$$

If we choose \mathbf{c} such that $-\mathbf{c}^\top \mathbf{A} \theta + \sigma^{-2} \mathbf{y}^\top \mathbf{X} \theta = 0$, the posterior is normal with mean \mathbf{c} and covariance matrix \mathbf{A}^{-1} . Taking into account that \mathbf{A} is symmetric, this is if we choose

$$\begin{aligned} \sigma^{-2} \mathbf{y}^\top \mathbf{X} &= \mathbf{c}^\top \mathbf{A} \\ \Leftrightarrow \sigma^{-2} \mathbf{y}^\top \mathbf{X} \mathbf{A}^{-1} &= \mathbf{c}^\top \\ \Leftrightarrow \mathbf{c} &= \sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^\top \mathbf{y} \end{aligned}$$

as claimed.



REVIEW: THE BAYESIAN LINEAR MODEL / 11

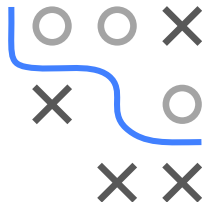
Based on the posterior distribution

$$\boldsymbol{\theta} \mid \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^{\top} \mathbf{y}, \mathbf{A}^{-1})$$

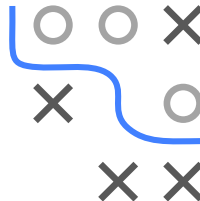
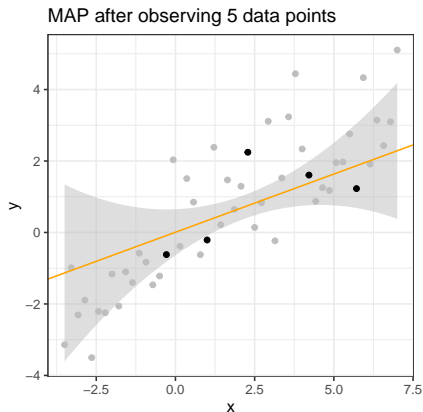
we can derive the predictive distribution for a new observations \mathbf{x}_* . The predictive distribution for the Bayesian linear model, i.e. the distribution of $\boldsymbol{\theta}^{\top} \mathbf{x}_*$, is

$$y_* \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_* \sim \mathcal{N}(\sigma^{-2} \mathbf{y}^{\top} \mathbf{X} \mathbf{A}^{-1} \mathbf{x}_*, \mathbf{x}_*^{\top} \mathbf{A}^{-1} \mathbf{x}_*)$$

(applying the rules for linear transformations of Gaussians).

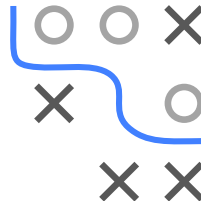
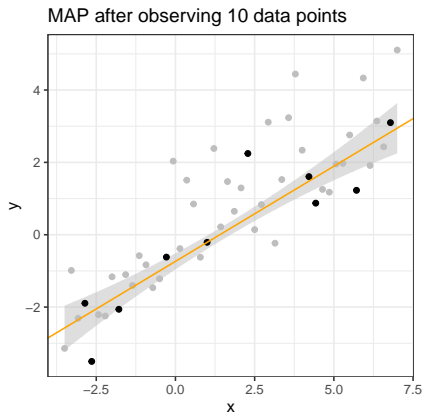


REVIEW: THE BAYESIAN LINEAR MODEL / 12



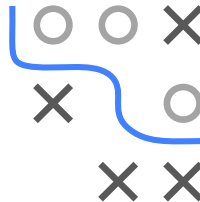
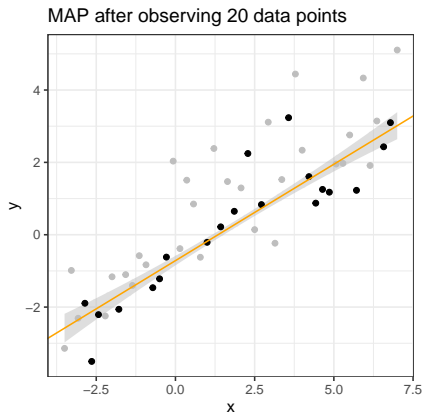
For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

REVIEW: THE BAYESIAN LINEAR MODEL / 13



For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

REVIEW: THE BAYESIAN LINEAR MODEL / 14



For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

SUMMARY: THE BAYESIAN LINEAR MODEL

- By switching to a Bayesian perspective, we do not only have point estimates for the parameter θ , but whole **distributions**
- From the posterior distribution of θ , we can derive a predictive distribution for $y_* = \theta^\top \mathbf{x}_*$.
- We can perform online updates: Whenever datapoints are observed, we can update the **posterior distribution** of θ

Next, we want to develop a theory for general shape functions, and not only for linear function.

