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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 $\boldsymbol{\theta}$.



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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

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



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

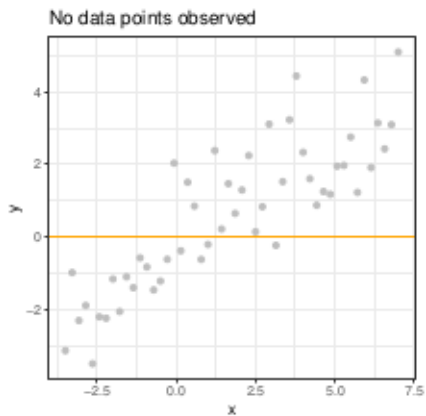
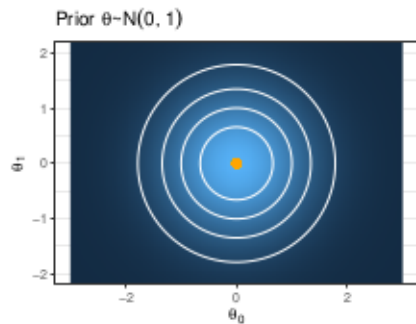
$$\theta \mid \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\sigma^{-2} \mathbf{A}^{-1} \mathbf{X}^{\top} \mathbf{y}, \mathbf{A}^{-1})$$

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

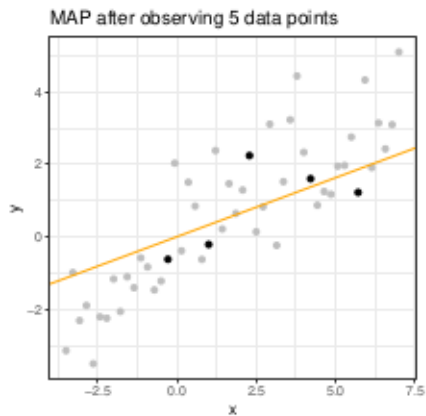
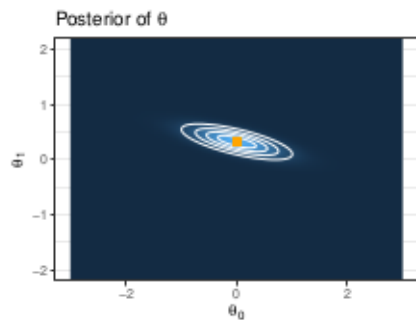
Note: If the posterior distribution $p(\theta \mid \mathbf{X}, \mathbf{y})$ are in the same probability distribution family as the prior $q(\theta)$ w.r.t. a specific likelihood function $p(\mathbf{y} \mid \mathbf{X}, \theta)$, they are called **conjugate distributions**. The prior is then called a **conjugate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



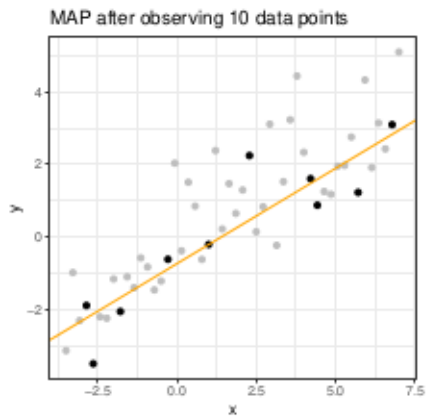
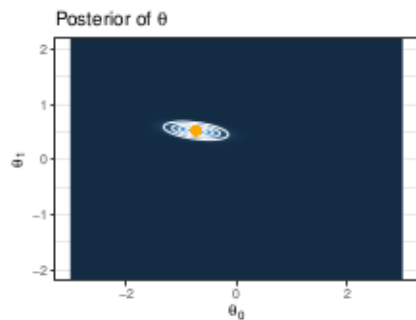
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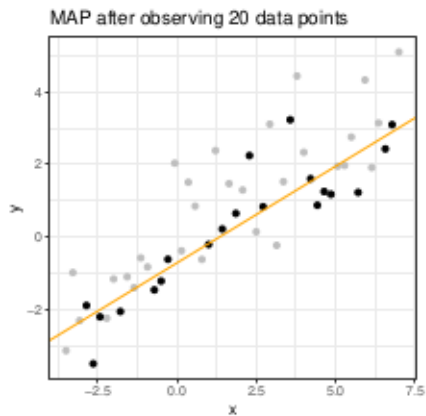
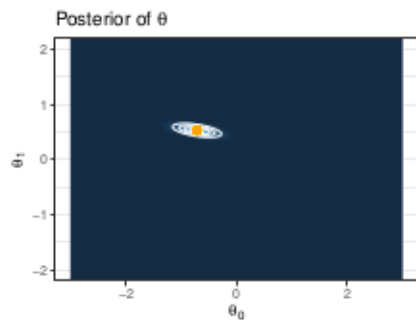
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Proof:

We want to show that

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

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

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

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



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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:

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

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.



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Based on the posterior distribution

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

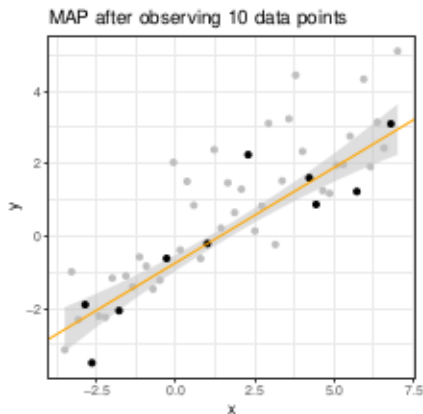
we can derive the predictive distribution for a new observations \mathbf{x}_* . The predictive distribution for the Bayesian linear model, i.e. the distribution of $\theta^{\top} \mathbf{x}_*$, is

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

(applying the rules for linear transformations of Gaussians).

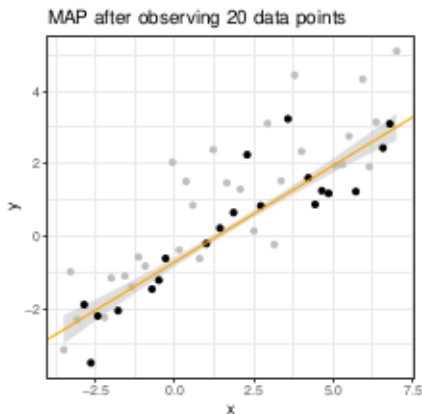


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For every test input \mathbf{x}_* , we get a distribution over the prediction y_* . In particular, we get a posterior mean (orange) and a posterior variance (grey region equals \pm two times standard deviation).

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