Bayesian Linear Regression

Mark van der Wilk

Department of Computing Imperial College London **y**@markvanderwilk m.vdwilk@imperial.ac.uk

November 16, 2021

Reference

Mathematics for Machine Learning:

https://mml-book.com

Chapter 9

Probabilistic model: Model of the data is a probability distribution.

Probabilistic model: Model of the data is a probability distribution.

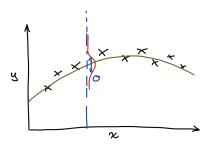
$$y_n = f(\mathbf{x}_n; \boldsymbol{\theta}) + \epsilon_n$$

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

Probabilistic model: Model of the data is a probability distribution.

$$y_n = f(\mathbf{x}_n; \boldsymbol{\theta}) + \epsilon_n$$
 $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$

We can now also estimate the **unpredictability** of our problem:



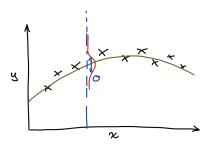
$$(\boldsymbol{\theta}^*, \sigma^{2^*}) = \operatorname{argmax}_{\boldsymbol{\theta}, \sigma^2} \log p(\mathbf{y}|\boldsymbol{\theta}, \sigma^2, X)$$
 (1)

Unpredictability remains even if we **know** underlying function. Goes by many names... e.g. **aleatoric uncertainty**.

Probabilistic model: Model of the data is a probability distribution.

$$y_n = f(\mathbf{x}_n; \boldsymbol{\theta}) + \epsilon_n$$
 $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$

We can now also estimate the **unpredictability** of our problem:

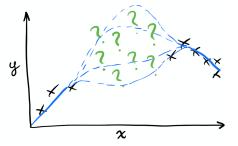


$$(\boldsymbol{\theta}^*, \sigma^{2^*}) = \operatorname{argmax}_{\boldsymbol{\theta}, \sigma^2} \log p(\mathbf{y}|\boldsymbol{\theta}, \sigma^2, X)$$
 (1)

Unpredictability remains even if we **know** underlying function. Goes by many names... e.g. **aleatoric uncertainty**.

Uncertainty in Parameters/Function

Aren't we also uncertain when we have a lack of data?



This is uncertainty in the parameters that define the function! Also goes by many names... e.g. **epistemic uncertainty**.

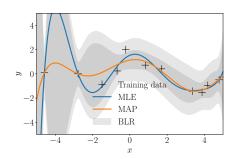
Quantifying Uncertainty with Bayesian Inference

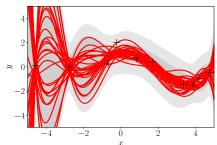
If we knew that for a series of problems, our parameters θ were sampled from $p(\theta)$, then Bayes' rule would give us the probability distribution after observing our data y:

$$\underbrace{p(\boldsymbol{\theta}|\mathbf{y})}_{\text{posterior}} = \underbrace{\frac{p(\mathbf{y}|\boldsymbol{\theta})}{p(\boldsymbol{\theta})} \underbrace{p(\boldsymbol{\theta})}_{\text{evidence}}}_{\text{likelihood prior}} p(\mathbf{y})$$
(2)

- Allows us to quantify uncertainty in parameters θ .
- Bayesian inference makes a leap of faith: Choose a prior and assume this is the correct one.
- ► Choosing priors is important ⇒ Probabilistic Inference (Spring).

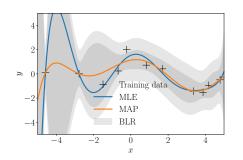
Example

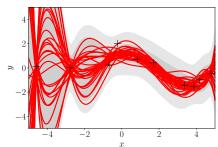




- Light-gray: uncertainty due to noise (aleatoric uncertainty / unpredictability)
- Dark-gray: uncertainty due to parameter uncertainty (epistemic uncertainty)

Example



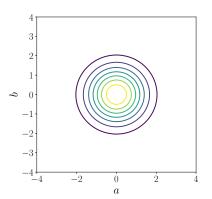


- Light-gray: uncertainty due to noise (aleatoric uncertainty / unpredictability)
- Dark-gray: uncertainty due to parameter uncertainty (epistemic uncertainty)
- Right: Plausible functions under the parameter distribution (every single parameter setting describes one function)

Distribution over Functions

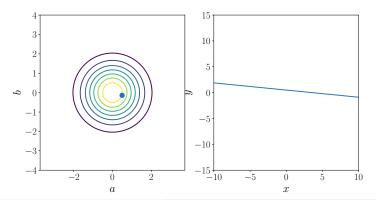
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$



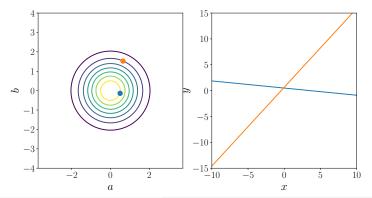
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



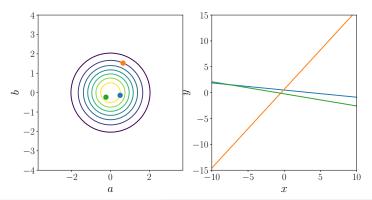
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



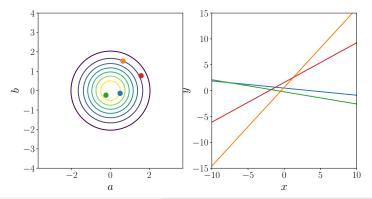
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



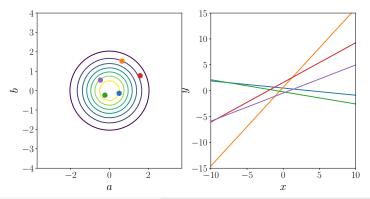
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



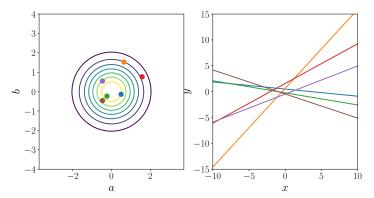
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



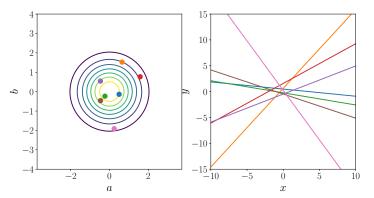
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



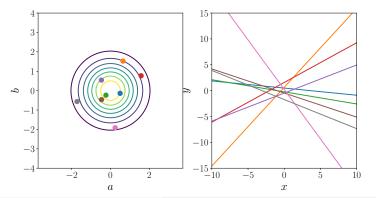
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



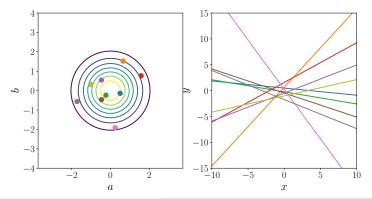
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$



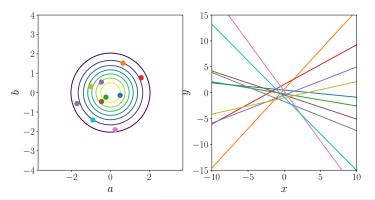
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$

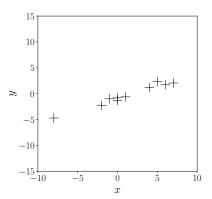


$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$

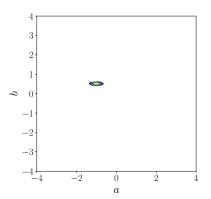


$$y = f(x) + \epsilon = a + bx + \epsilon$$
, $\epsilon \sim \mathcal{N}(0, \sigma_n^2)$
 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $\mathbf{X} = [x_1, \dots, x_N], \ \mathbf{y} = [y_1, \dots, y_N]$ Training inputs/targets



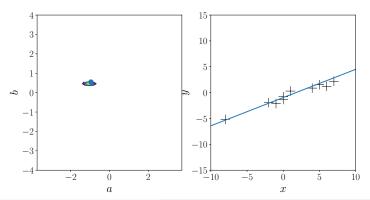
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a,b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $p(a,b|\mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$ Posterior



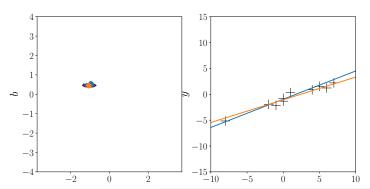
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | X, y)$
 $f_i = a_i + b_i x$



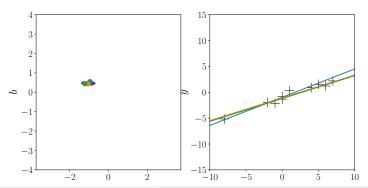
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



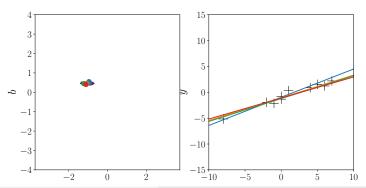
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



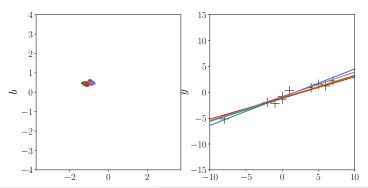
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



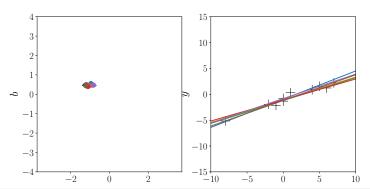
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



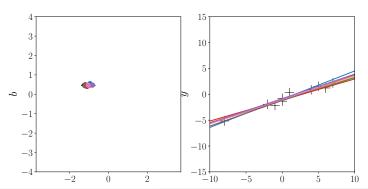
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



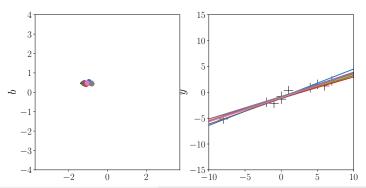
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



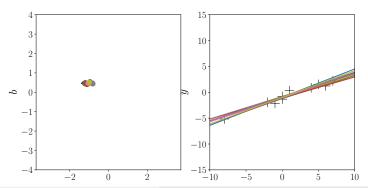
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



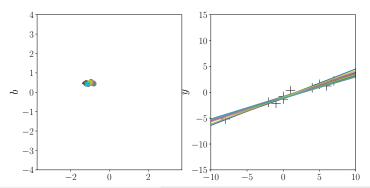
$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$
 $f_i = a_i + b_i x$



Model: Bayesian Linear Regression

We never put a distribution on any x_n , so we drop from conditioning.

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; 0, \mathbf{I}_M) \tag{3}$$

$$p(y_n|\boldsymbol{\theta}) = \mathcal{N}(y_n; \boldsymbol{\phi}(\mathbf{x}_n)^\mathsf{T}\boldsymbol{\theta}, \sigma^2)$$
 (4)

Model: Bayesian Linear Regression

We never put a distribution on any x_n , so we drop from conditioning.

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; 0, \mathbf{I}_M) \tag{3}$$

$$p(y_n|\boldsymbol{\theta}) = \mathcal{N}(y_n; \boldsymbol{\phi}(\mathbf{x}_n)^\mathsf{T}\boldsymbol{\theta}, \sigma^2)$$
 (4)

$$p(\mathbf{y}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{y}; \Phi(X)\boldsymbol{\theta}, \sigma^2 \mathbf{I}_N)$$
 (5)

Model: Bayesian Linear Regression

We never put a distribution on any x_n , so we drop from conditioning.

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; 0, I_M) \tag{3}$$

$$p(y_n|\boldsymbol{\theta}) = \mathcal{N}(y_n; \boldsymbol{\phi}(\mathbf{x}_n)^\mathsf{T}\boldsymbol{\theta}, \sigma^2)$$
 (4)

$$p(\mathbf{y}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{y}; \Phi(\mathbf{X})\boldsymbol{\theta}, \sigma^2 \mathbf{I}_N)$$
 (5)

Two goals:

- ▶ Find posterior over parameters $p(\theta|\mathbf{y})$
- Find predictive posterior $p(\mathbf{y}^*|\mathbf{y})$

Posterior over Parameters

Board:

- ► Equating coefficients (tests your matrix algebra skills!)
- ▶ Joint Gaussian
- Woodbury identity

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(X)\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(X)\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(6)

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta})^\mathsf{T} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^\mathsf{T}\boldsymbol{\theta}$$
(7)

This is a vector quadratic in θ ! board

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(X)\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(X)\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(6)

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(X)\boldsymbol{\theta})^\mathsf{T} (\mathbf{y} - \Phi(X)\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^\mathsf{T}\boldsymbol{\theta}$$
(7)

This is a vector quadratic in θ ! board \Longrightarrow Gaussian.

► Equate coefficients. Can rearrange...

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$
 (6)

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(7)

This is a vector quadratic in θ ! board \Longrightarrow Gaussian.

► Equate coefficients. Can rearrange... or find E+V by other means

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$
 (6)

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(7)

- ► Equate coefficients. Can rearrange... or find E+V by other means
- ▶ Find maximum to find mean board

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$
 (6)

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(7)

- ► Equate coefficients. Can rearrange... or find E+V by other means
- ► Find maximum to find mean board
- ► Find Hessian to find covariance board

$$\log p(\mathbf{y}|\boldsymbol{\theta}) = \log p(\mathbf{y}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$
 (6)

$$= c - \frac{1}{2\sigma^2} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta})^{\mathsf{T}} (\mathbf{y} - \Phi(\mathbf{X})\boldsymbol{\theta}) - \frac{1}{2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$
(7)

- ► Equate coefficients. Can rearrange... or find E+V by other means
- ► Find maximum to find mean board
- ► Find Hessian to find covariance board

$$p(\boldsymbol{\theta}|\mathbf{y}) = \mathcal{N}\left(\boldsymbol{\theta}; \left[\frac{1}{\sigma^2} \Phi(X)^\mathsf{T} \Phi(X) + \mathbf{I}_M\right]^{-1} \frac{1}{\sigma^2} \Phi(X)^\mathsf{T} \mathbf{y}\right)$$
(8)

$$\left[\frac{1}{\sigma^2}\Phi(X)^{\mathsf{T}}\Phi(X) + \mathbf{I}_M\right]^{-1} \tag{9}$$

Method 2: Joint Gaussian

Find

$$p(\boldsymbol{\theta}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\theta} \\ \mathbf{y} \end{bmatrix}; \begin{bmatrix} \mathbb{E}_{\boldsymbol{\theta}}[\boldsymbol{\theta}] \\ \mathbb{E}_{\mathbf{y}}[\mathbf{y}] \end{bmatrix}, \begin{bmatrix} \mathbb{V}[\boldsymbol{\theta}] & \mathbb{C}[\boldsymbol{\theta}, \mathbf{y}] \\ \mathbb{C}[\mathbf{y}, \boldsymbol{\theta}] & \mathbb{V}[\mathbf{y}] \end{bmatrix}\right)$$
(10)

board

$$p(\boldsymbol{\theta}|\mathbf{y}) = \mathcal{N}\left(\boldsymbol{\theta}; \boldsymbol{\Phi}(X)^{\mathsf{T}} \left[\boldsymbol{\Phi}(X)\boldsymbol{\Phi}(X)^{\mathsf{T}} + \sigma^{2} \boldsymbol{I}_{N}\right]^{-1} \mathbf{y},\right.$$
$$\left. \boldsymbol{I}_{M} - \boldsymbol{\Phi}(X)^{\mathsf{T}} \left[\boldsymbol{\Phi}(X)\boldsymbol{\Phi}(X)^{\mathsf{T}} + \sigma^{2} \boldsymbol{I}_{N}\right]^{-1} \boldsymbol{\Phi}(X)\right)$$
(11)

Computational Considerations

Woodbury identity

17

Predictive posterior

Board:

- Crunching densities
- ► Equating coefficients (tests your matrix algebra skills!)
- ► Joint Gaussian
- Woodbury identity

First, how to express our target in terms of densities we know.

First, how to express our target in terms of densities we know.

$$p(\mathbf{y}^*|\mathbf{y}) \stackrel{\text{AT}}{=} \int \frac{p(\mathbf{y}^*, \boldsymbol{\theta}, \mathbf{y})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (12)

(13)

First, how to express our target in terms of densities we know.

$$p(\mathbf{y}^*|\mathbf{y}) \stackrel{\text{AT}}{=} \int \frac{p(\mathbf{y}^*, \boldsymbol{\theta}, \mathbf{y})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (12)

$$\stackrel{\text{MA}}{=} \int p(\mathbf{y}^*|\boldsymbol{\theta}) \frac{p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (13)

19

First, how to express our target in terms of densities we know.

$$p(\mathbf{y}^*|\mathbf{y}) \stackrel{\text{AT}}{=} \int \frac{p(\mathbf{y}^*, \boldsymbol{\theta}, \mathbf{y})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (12)

$$\stackrel{\text{MA}}{=} \int p(\mathbf{y}^*|\boldsymbol{\theta}) \frac{p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (13)

Next do the integrals / equating coefficients.

First, how to express our target in terms of densities we know.

$$p(\mathbf{y}^*|\mathbf{y}) \stackrel{\text{AT}}{=} \int \frac{p(\mathbf{y}^*, \boldsymbol{\theta}, \mathbf{y})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (12)

$$\stackrel{\text{MA}}{=} \int p(\mathbf{y}^*|\boldsymbol{\theta}) \frac{p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{y})} d\boldsymbol{\theta}$$
 (13)

Next do the integrals / equating coefficients. \implies I recommend other method.

Conclusion