


Linear Regression

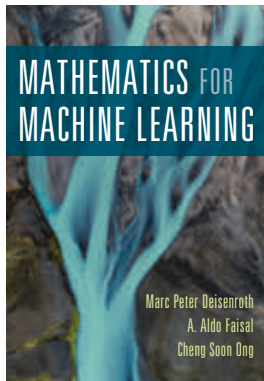
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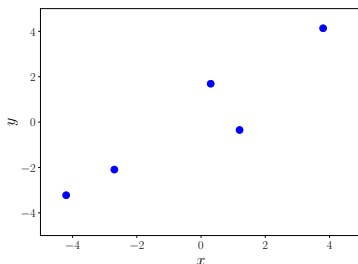


<https://mml-book.com>

Chapter 9

Regression (curve fitting)

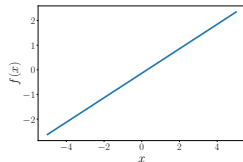
Given inputs $x \in \mathbb{R}^D$ and corresponding observations $y \in \mathbb{R}$ find a function f that models the relationship between x and y .



- Typically parametrize the function f with parameters θ
- Linear regression: Consider functions f that are **linear in the parameters**

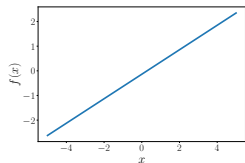
■ Straight lines

$$y = f(x, \boldsymbol{\theta}) = \theta_0 + \theta_1 x = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix}$$



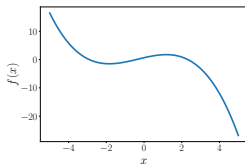
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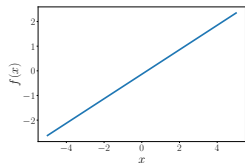
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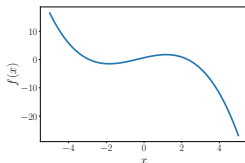
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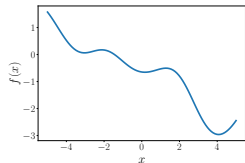
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■ Radial basis function networks

$$y = f(x, \boldsymbol{\theta}) = \sum_{m=1}^M \theta_m \exp\left(-\frac{1}{2}(x - \mu_m)^2\right)$$



$$y = \mathbf{x}^\top \boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- Given a training set $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$ we seek optimal parameters $\boldsymbol{\theta}^*$

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- Given a training set $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$ we seek optimal parameters $\boldsymbol{\theta}^*$
 - ▶▶ **Maximum Likelihood Estimation**
 - ▶▶ **Maximum a Posteriori Estimation**

- Define $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N]^\top \in \mathbb{R}^{N \times D}$ and $\mathbf{y} = [y_1, \dots, y_N]^\top \in \mathbb{R}^N$
- Find parameters θ^* that maximize the [likelihood](#)

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$$p(y_1, \dots, y_N | \mathbf{x}_1, \dots, \mathbf{x}_N, \boldsymbol{\theta}) = p(\mathbf{y} | \mathbf{X}, \boldsymbol{\theta}) = \prod_{n=1}^N \mathcal{N}(y_n | \mathbf{x}_n^\top \boldsymbol{\theta}, \sigma^2)$$

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- Log-transformation **▶ Maximize the log likelihood**

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- Log-transformation ► **Maximize the log likelihood**

$$\log p(\mathbf{y} | \mathbf{X}, \boldsymbol{\theta}) = \sum_{n=1}^N \log \mathcal{N}(y_n | \mathbf{x}_n^\top \boldsymbol{\theta}, \sigma^2),$$
$$\log \mathcal{N}(y_n | \mathbf{x}_n^\top \boldsymbol{\theta}, \sigma^2) = -\frac{1}{2\sigma^2} (y_n - \mathbf{x}_n^\top \boldsymbol{\theta})^2 + \text{const}$$

With

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- Computing the gradient with respect to $\boldsymbol{\theta}$ and setting it to $\mathbf{0}$ gives the **maximum likelihood estimator** (least-squares estimator)

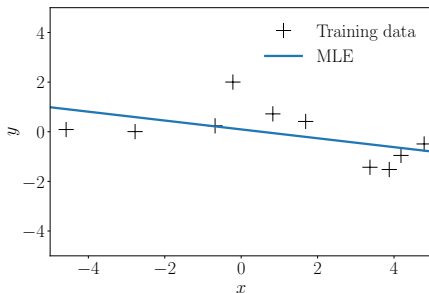
$$\boldsymbol{\theta}^{\text{ML}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

$$y = \mathbf{x}^\top \boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

Given an arbitrary input \mathbf{x}_* , we can predict the corresponding observation y_* using the maximum likelihood parameter:

$$p(y_* | \mathbf{x}_*, \boldsymbol{\theta}^{\text{ML}}) = \mathcal{N}(y_* | \mathbf{x}_*^\top \boldsymbol{\theta}^{\text{ML}}, \sigma^2)$$

- Measurement noise variance σ^2 assumed known
- In the absence of noise ($\sigma^2 = 0$), the prediction will be deterministic



$$y = \theta_0 + \theta_1 x + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- At any query point x_* we obtain the mean prediction as

$$\mathbb{E}[y_* | \theta^{\text{ML}}, x_*] = \theta_0^{\text{ML}} + \theta_1^{\text{ML}} x_*$$

$$y = \phi(\mathbf{x})^\top \boldsymbol{\theta} + \epsilon = \sum_{m=0}^M \theta_m x^m + \epsilon$$

- Polynomial regression with features

$$\phi(x) = [1, x, x^2, \dots, x^M]^\top$$

- Maximum likelihood estimator:

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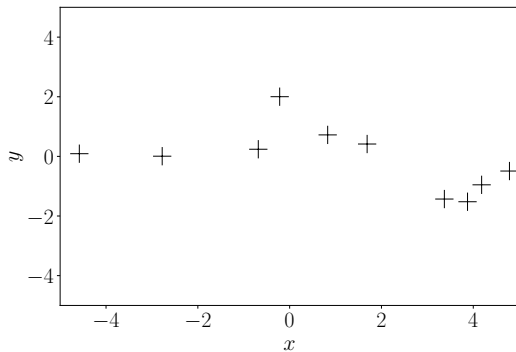


Figure: Training data

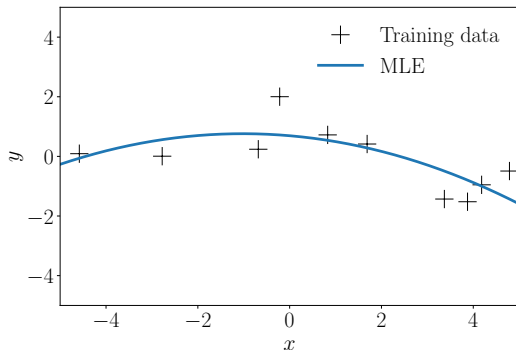


Figure: 2nd-order polynomial

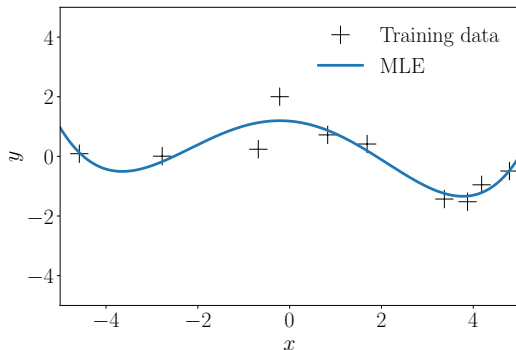


Figure: 4th-order polynomial

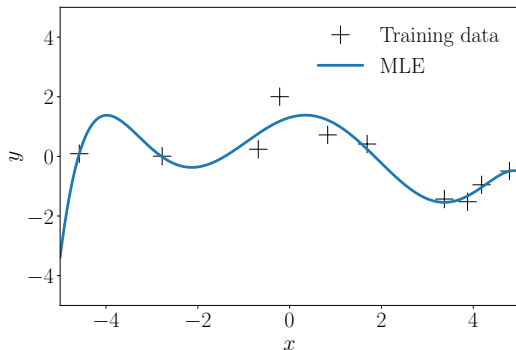


Figure: 6th-order polynomial

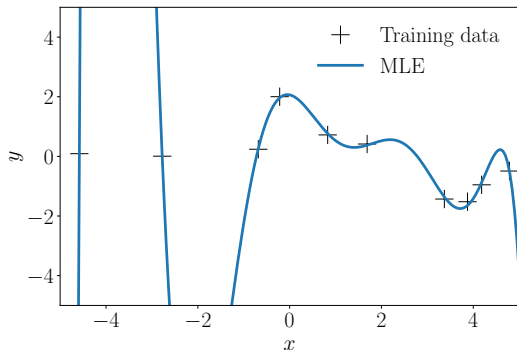


Figure: 8th-order polynomial

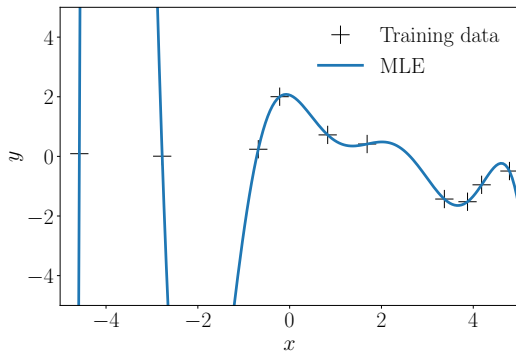
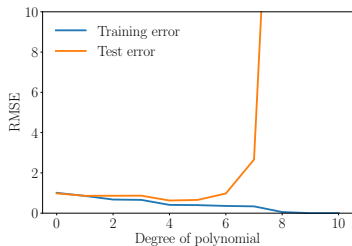
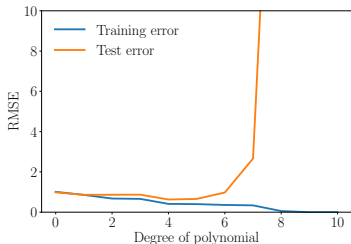


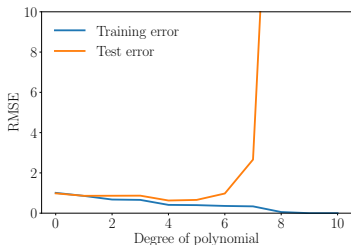
Figure: 10th-order polynomial



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- We are not so much interested in the training error, but in the **generalization error**: How well does the model perform when we predict at previously unseen input locations?
- Maximum likelihood often runs into **overfitting** problems, i.e., we exploit the flexibility of the model to fit to the noise in the data

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- Choose $\boldsymbol{\theta}^*$ as the parameter that **maximizes the (log) parameter posterior**

$$\log p(\boldsymbol{\theta} | \mathbf{X}, \mathbf{y}) = \underbrace{\log p(\mathbf{y} | \mathbf{X}, \boldsymbol{\theta})}_{\text{log-likelihood}} + \underbrace{\log p(\boldsymbol{\theta})}_{\text{log-prior}} + \text{const}$$

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- Log-prior induces a direct penalty on the parameters
- **Maximum a posteriori estimate** (regularized least squares)

- Gaussian parameter prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$
- Log-posterior distribution:

$$\begin{aligned}\log p(\boldsymbol{\theta} | \mathbf{X}, \mathbf{y}) &= -\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) - \frac{1}{2\alpha^2} \boldsymbol{\theta}^\top \boldsymbol{\theta} + \text{const} \\ &= -\frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|^2 - \frac{1}{2\alpha^2} \|\boldsymbol{\theta}\|^2 + \text{const}\end{aligned}$$

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- Compute gradient with respect to $\boldsymbol{\theta}$, set it to 0
 - ▶ **Maximum a posteriori estimate:**

$$\boldsymbol{\theta}^{\text{MAP}} = (\mathbf{X}^\top \mathbf{X} + \frac{\sigma^2}{\alpha^2} \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

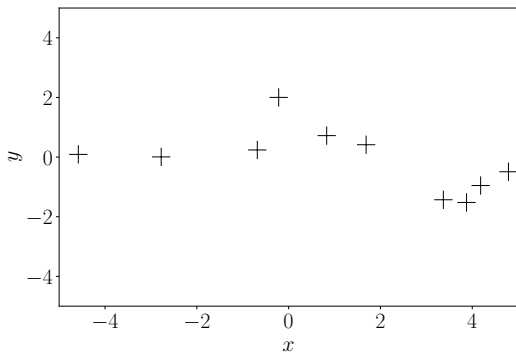
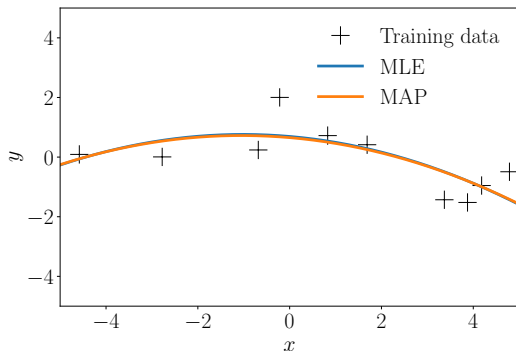


Figure: Training data

Mean prediction:

$$\mathbb{E}[y_* | \mathbf{x}_*, \boldsymbol{\theta}^{\text{MAP}}] = \boldsymbol{\phi}^\top(\mathbf{x}_*) \boldsymbol{\theta}^{\text{MAP}}$$



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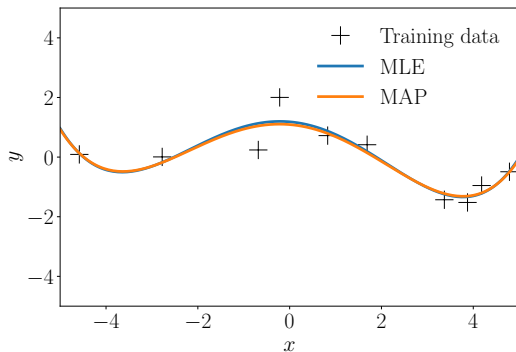


Figure: 4th-order polynomial

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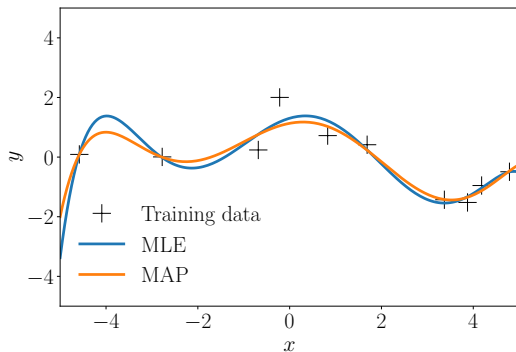


Figure: 6th-order polynomial

Mean prediction:

$$\mathbb{E}[y_* | \mathbf{x}_*, \boldsymbol{\theta}^{\text{MAP}}] = \boldsymbol{\phi}^\top(\mathbf{x}_*) \boldsymbol{\theta}^{\text{MAP}}$$

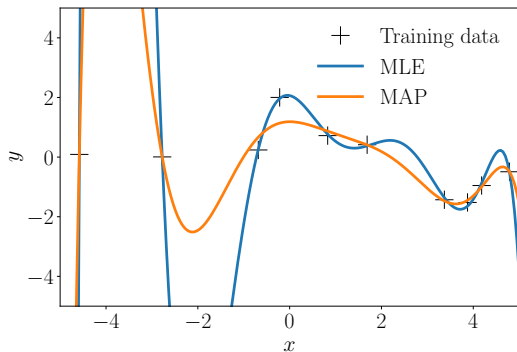


Figure: 8th-order polynomial

Mean prediction:

$$\mathbb{E}[y_* | \mathbf{x}_*, \boldsymbol{\theta}^{\text{MAP}}] = \boldsymbol{\phi}^\top(\mathbf{x}_*) \boldsymbol{\theta}^{\text{MAP}}$$

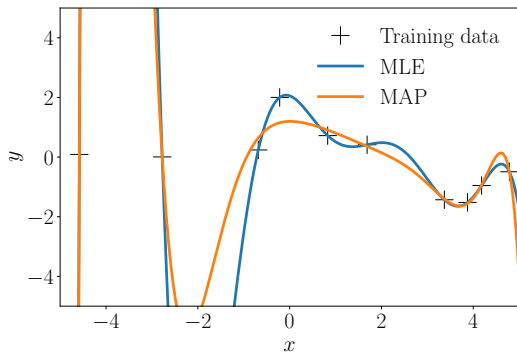
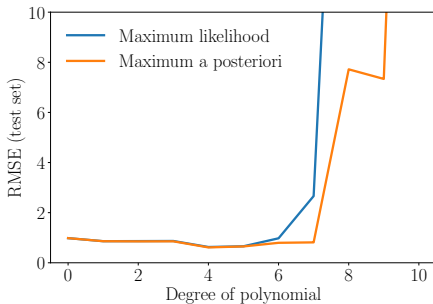


Figure: 10th-order polynomial

Mean prediction:

$$\mathbb{E}[y_* | \mathbf{x}_*, \boldsymbol{\theta}^{\text{MAP}}] = \boldsymbol{\phi}^\top(\mathbf{x}_*) \boldsymbol{\theta}^{\text{MAP}}$$



- Maximum likelihood estimation “delays” the problem of overfitting
- It does not provide a general solution
- ▶▶ Need a more principled solution

$$y = \phi^\top(\mathbf{x})\boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

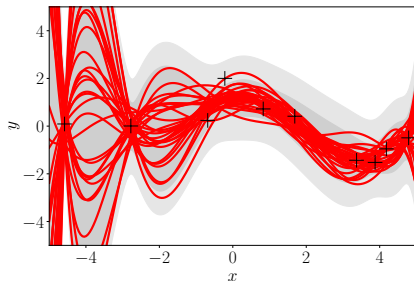
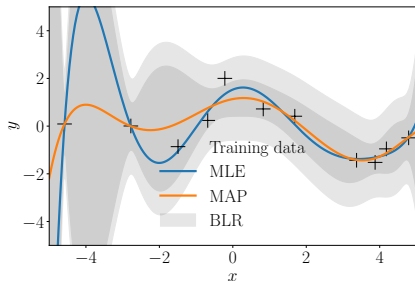
- Avoid overfitting by not fitting any parameters:
 - ▶▶ Integrate parameters out instead of optimizing them

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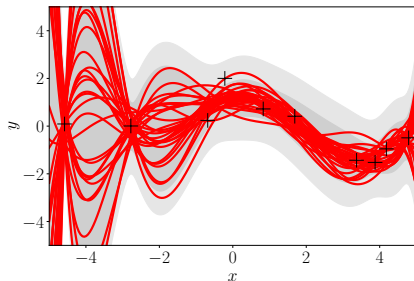
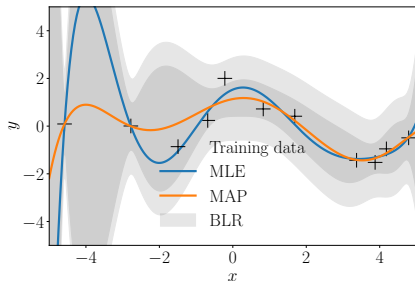
- Avoid overfitting by not fitting any parameters:
 - ▶ Integrate parameters out instead of optimizing them
- Use a full parameter distribution $p(\boldsymbol{\theta})$ (and not a single point estimate $\boldsymbol{\theta}^*$) when making predictions:

$$p(y_* | \mathbf{x}_*) = \int p(y_* | \mathbf{x}_*, \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

- ▶ Prediction no longer depends on $\boldsymbol{\theta}$
- Predictive distribution reflects the uncertainty about the “correct” parameter setting



- Light-gray: uncertainty due to noise (same as in MLE/MAP)
- Dark-gray: uncertainty due to parameter uncertainty



- Light-gray: uncertainty due to noise (same as in MLE/MAP)
- Dark-gray: uncertainty due to parameter uncertainty
- Right: Plausible functions under the parameter distribution (every single parameter setting describes one function)

Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0)$,

Likelihood $p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y | \boldsymbol{\phi}^\top(\mathbf{x})\boldsymbol{\theta}, \sigma^2)$

- Parameter $\boldsymbol{\theta}$ becomes a latent (random) variable
- Prior distribution induces a **distribution over plausible functions**
- Choose a conjugate Gaussian prior
 - Closed-form computations
 - Gaussian posterior

- Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{m}_0, \boldsymbol{S}_0)$ is Gaussian ► posterior is Gaussian:
►► **Derive this**

$$p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}(\boldsymbol{m}_N, \boldsymbol{S}_N)$$

$$\boldsymbol{S}_N = (\boldsymbol{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}$$

$$\boldsymbol{m}_N = \boldsymbol{S}_N(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{y})$$

- Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0)$ is Gaussian \blacktriangleright posterior is Gaussian:

$$p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{S}_N = (\mathbf{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}$$

$$\mathbf{m}_N = \mathbf{S}_N(\mathbf{S}_0^{-1}\mathbf{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y})$$

- Mean \mathbf{m}_N identical to MAP estimate

- Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0)$ is Gaussian \blacktriangleright posterior is Gaussian:

$$p(\boldsymbol{\theta} | \mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{S}_N = (\mathbf{S}_0^{-1} + \sigma^{-2} \boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1}$$

$$\mathbf{m}_N = \mathbf{S}_N (\mathbf{S}_0^{-1} \mathbf{m}_0 + \sigma^{-2} \boldsymbol{\Phi}^\top \mathbf{y})$$

- Mean \mathbf{m}_N identical to MAP estimate
- Assume a Gaussian distribution $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$. Then

$$p(y_* | \mathbf{x}_*) = \mathcal{N}(y | \boldsymbol{\phi}^\top(\mathbf{x}_*) \mathbf{m}_N, \boldsymbol{\phi}^\top(\mathbf{x}_*) \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x}_*) + \sigma^2)$$

- Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0)$ is Gaussian \blacktriangleright posterior is Gaussian:

$$p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{S}_N = (\mathbf{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi})^{-1}$$

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- $\boldsymbol{\phi}^\top(\mathbf{x}_*)\mathbf{S}_N\boldsymbol{\phi}(\mathbf{x}_*)$: Accounts for parameter uncertainty in predictive variance

More details \blacktriangleright <https://mml-book.com>, Chapter 9

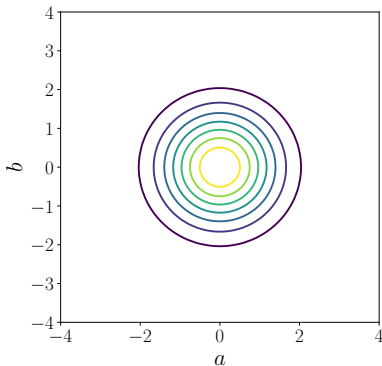
- Marginal likelihood can be computed analytically.
- With $p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta} = \mathcal{N}(\mathbf{y} | \boldsymbol{\Phi}\boldsymbol{\mu}, \boldsymbol{\Phi}\boldsymbol{\Sigma}\boldsymbol{\Phi}^\top + \sigma^2\mathbf{I})$$

- Derivation via completing the squares (see Section 9.3.5 of MML book)

Consider a linear regression setting

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



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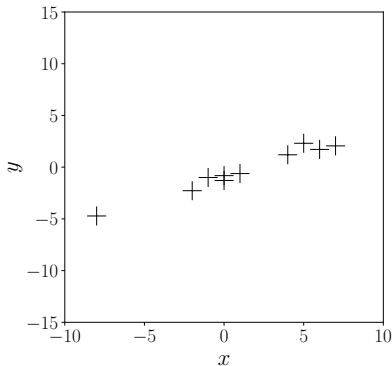
$$f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$$

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

$\mathbf{X} = [x_1, \dots, x_N]$, $\mathbf{y} = [y_1, \dots, y_N]$ Training inputs/targets

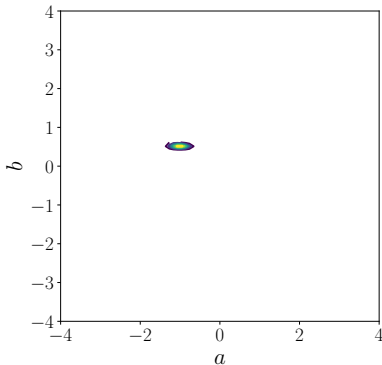


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$$p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$

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



Consider a linear regression setting

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

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

$$f_i = a_i + b_i x$$

- Fit nonlinear functions using (Bayesian) linear regression:
Linear combination of nonlinear features

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Linear combination of nonlinear features
- Example: Radial-basis-function (RBF) network

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Linear combination of nonlinear features
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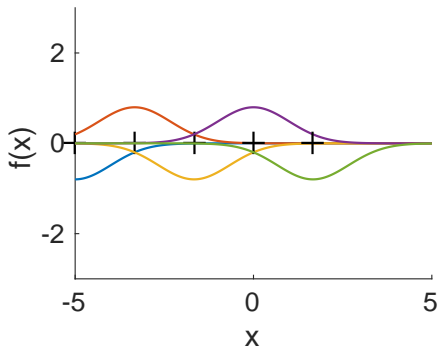
$$f(\mathbf{x}) = \sum_{i=1}^n \theta_i \phi_i(\mathbf{x}), \quad \theta_i \sim \mathcal{N}(0, \sigma_p^2)$$

where

$$\phi_i(\mathbf{x}) = \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^\top (\mathbf{x} - \boldsymbol{\mu}_i)\right)$$

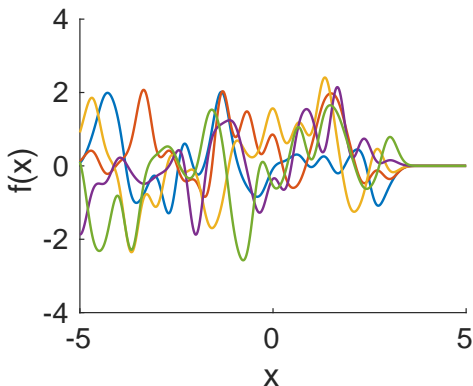
for given “centers” $\boldsymbol{\mu}_i$

$$\phi_i(\mathbf{x}) = \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^\top(\mathbf{x} - \boldsymbol{\mu}_i)\right)$$

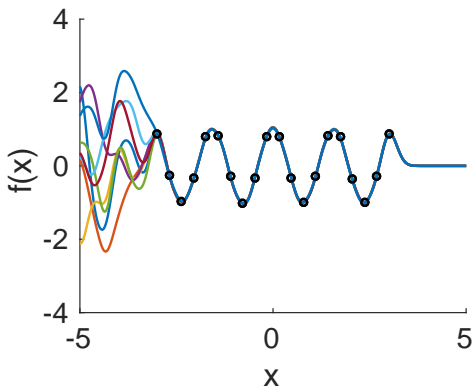


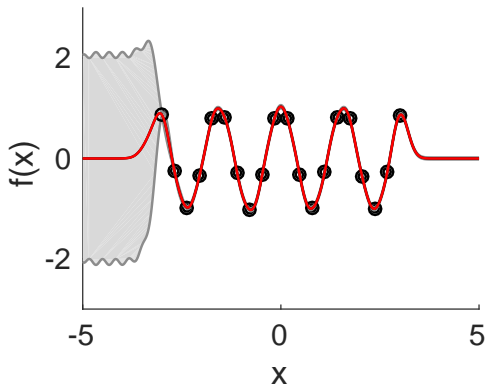
- Place Gaussian-shaped basis functions ϕ_i at 25 input locations μ_i , linearly spaced in the interval $[-5, 3]$

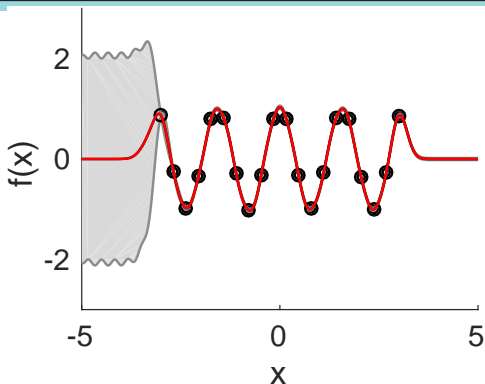
$$f(\mathbf{x}) = \sum_{i=1}^n \theta_i \phi_i(\mathbf{x}), \quad p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$



$$f(\mathbf{x}) = \sum_{i=1}^n \theta_i \phi_i(\mathbf{x}), \quad p(\boldsymbol{\theta} | \mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$$







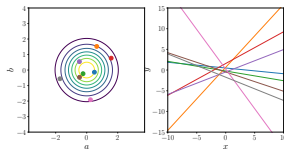
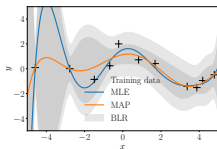
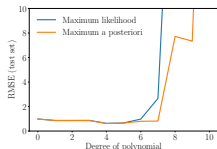
- Feature engineering (what basis functions to use?)
- Finite number of features:
 - Above: Without basis functions on the right, we cannot express any variability of the function
 - Ideally: Add more (infinitely many) basis functions

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 - ▶▶ Place a prior on functions
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- ▶▶ **Gaussian process**



- Regression = curve fitting
- Linear regression = linear in the parameters
- Parameter estimation via maximum likelihood and MAP estimation can lead to **overfitting**
- **Bayesian linear regression** addresses this issue, but may not be analytically tractable
- Predictive uncertainty in Bayesian linear regression explicitly accounts for parameter uncertainty
- Distribution over parameters **▶▶** Distribution over functions

Appendix

■ Joint Gaussian distribution

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N} \left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix} \right)$$

- Joint Gaussian distribution

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N} \left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix} \right)$$

- Marginal:

$$\begin{aligned} p(\mathbf{x}) &= \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \\ &= \mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx}) \end{aligned}$$

- Joint Gaussian distribution

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- Marginal:

$$\begin{aligned} p(\mathbf{x}) &= \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y} \\ &= \mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx}) \end{aligned}$$

- Conditional:

$$\begin{aligned} p(\mathbf{x}|\mathbf{y}) &= \mathcal{N}(\boldsymbol{\mu}_{x|y}, \boldsymbol{\Sigma}_{x|y}) \\ \boldsymbol{\mu}_{x|y} &= \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} (\mathbf{y} - \boldsymbol{\mu}_y) \\ \boldsymbol{\Sigma}_{x|y} &= \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy} \boldsymbol{\Sigma}_{yy}^{-1} \boldsymbol{\Sigma}_{yx} \end{aligned}$$

If $x \sim \mathcal{N}(x \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $z = \mathbf{A}x + \mathbf{b}$ then

$$p(z) = \mathcal{N}(z \mid \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top)$$

$\mathbf{x} \in \mathbb{R}^D$. Then:

$$\mathcal{N}(\mathbf{x} | \mathbf{a}, \mathbf{A})\mathcal{N}(\mathbf{x} | \mathbf{b}, \mathbf{B}) = Z\mathcal{N}(\mathbf{x} | \mathbf{c}, \mathbf{C})$$

$$\mathbf{C} = (\mathbf{A}^{-1} + \mathbf{B}^{-1})^{-1}$$

$$\mathbf{c} = \mathbf{C}(\mathbf{A}^{-1}\mathbf{a} + \mathbf{B}^{-1}\mathbf{b})$$

$$Z = (2\pi)^{-\frac{D}{2}} |\mathbf{A} + \mathbf{B}| \exp\left(-\frac{1}{2}(\mathbf{a} - \mathbf{b})^\top (\mathbf{A} + \mathbf{B})^{-1} (\mathbf{a} - \mathbf{b})\right)$$

$x \in \mathbb{R}^D$. Then:

$$\mathcal{N}(x | \mathbf{a}, \mathbf{A})\mathcal{N}(x | \mathbf{b}, \mathbf{B}) = Z\mathcal{N}(x | \mathbf{c}, \mathbf{C})$$

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- Product of two Gaussians is an unnormalized Gaussian

$\mathbf{x} \in \mathbb{R}^D$. Then:

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$$Z = (2\pi)^{-\frac{D}{2}} |\mathbf{A} + \mathbf{B}| \exp\left(-\frac{1}{2}(\mathbf{a} - \mathbf{b})^\top (\mathbf{A} + \mathbf{B})^{-1} (\mathbf{a} - \mathbf{b})\right)$$

- Product of two Gaussians is an unnormalized Gaussian
- The “un-normalizer” Z has a Gaussian functional form:

$$Z = \mathcal{N}(\mathbf{a} | \mathbf{b}, \mathbf{A} + \mathbf{B}) = \mathcal{N}(\mathbf{b} | \mathbf{a}, \mathbf{A} + \mathbf{B})$$

Note: This is not a distribution (no random variables)

$$p_1(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \mathbf{a}, \mathbf{A})$$

$$p_2(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \mathbf{b}, \mathbf{B})$$

Then

$$\int p_1(\mathbf{x})p_2(\mathbf{x})d\mathbf{x} = \quad \in \mathbb{R}$$

Note: In this context, \mathcal{N} is used to describe the functional relationship between \mathbf{a} , \mathbf{b} . Do not treat \mathbf{a} or \mathbf{b} as random variables—they are both deterministic quantities.

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Then

$$\int p_1(\mathbf{x})p_2(\mathbf{x})d\mathbf{x} = Z = \mathcal{N}(\mathbf{a} \mid \mathbf{b}, \mathbf{A} + \mathbf{B}) \in \mathbb{R}$$

Note: In this context, \mathcal{N} is used to describe the functional relationship between \mathbf{a} , \mathbf{b} . Do not treat \mathbf{a} or \mathbf{b} as random variables—they are both deterministic quantities.