# Machine Learning

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# Section 4

# Regression

# Regression basics

- In regression we assume that a response variable $y \in \mathbb{R}$ is a noisy function of the input variable $\boldsymbol{x} \in \mathbb{R}^d$.

$$y = f(\boldsymbol{x}) + \eta.$$

- We often assume that $f$ is linear, $f(\boldsymbol{x}) = \boldsymbol{w}^t \boldsymbol{x}$, and that $\eta$ has a zero-mean Gaussian distribution with constant variance, $\eta \sim N(0, \sigma^2)$.
- This is can equivalently be written as

$$p(y|\boldsymbol{x}) = N(\mu(\boldsymbol{x}), \sigma^2), \text{ with } \mu(\boldsymbol{x}) = \boldsymbol{w}^t \boldsymbol{x}.$$

- In one dimension: $\mu(\boldsymbol{x}) = w_0 + w_1 x$ and $\boldsymbol{x} = (1, x)$.
  $w_0$ is the **intercept** or bias term and $w_1$ is the **slope.**
- If $w_1 > 0$, we expect the output to increase as the input increases.

# Least Squares and Maximum Likelihood

- Fit $n$ data points $(\boldsymbol{x}_i, y_i)$ to a model that has $d+1$ parameters $w_j,\ j = 0, \ldots, d$.
- Notation: $\boldsymbol{x} \leftarrow (1, \boldsymbol{x}) \rightsquigarrow w_0$ is the intercept.
- Frequentist view: $\boldsymbol{w}$ is an unknown parameter vector, not a RV.
- We assume that the $n$ observations are **iid**.
- **Linear model:** $y_i = \boldsymbol{w}^t \boldsymbol{x}_i + \eta_i, \quad \eta_i \sim N(0, \sigma^2)$.
  Observed $y_i$ generated from a normal distribution centered at $\boldsymbol{w}^t \boldsymbol{x}_i$.
- Model predicts linear relationship between **conditional expectation** of **observations** $y_i$ and **inputs** $\boldsymbol{x}_i$:

$$E[y_i|\boldsymbol{x}_i] = w_0 + w_1 x_{i1} + \cdots + w_d x_{id} = \boldsymbol{w}^t \boldsymbol{x}_i = f(\boldsymbol{x}_i; \boldsymbol{w}).$$

  Note: the expectation operator is linear and $E[\eta_i] = 0$.
  **Regression function = conditional expectation.**

# LS and Maximum Likelihood

- **Likelihood function:** conditional probability of all observed $y_i$ given their explanation, treated as a function of the model parameters $\boldsymbol{w}$:

$$L(\boldsymbol{w}) \propto \prod_i \exp\left[-\frac{1}{2\sigma^2}(y_i - \boldsymbol{w}^t \boldsymbol{x}_i)^2\right]$$

- **Maximizing $L$ = finding model that best explains observations:**

$$\begin{aligned} \hat{\boldsymbol{w}} &= \arg\max_{\boldsymbol{w}} L(\boldsymbol{w}) = \arg\min_{\boldsymbol{w}}[-L(\boldsymbol{w})] = \arg\min_{\boldsymbol{w}}[-\log(L(\boldsymbol{w}))] \\ &= \arg\min_{\boldsymbol{w}} \sum_i (y_i - \boldsymbol{w}^t \boldsymbol{x}_i)^2 \end{aligned}$$

**Least-squares fit = ML solution under Gaussian error model.**

- $\hat{\boldsymbol{w}}_{MLE}$ minimizes the **residual sum of squares**

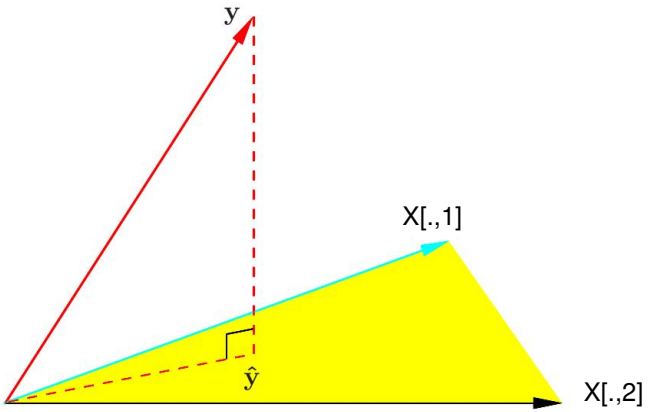
$$RSS(\boldsymbol{w}) = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} [y_i - f(\boldsymbol{x}_i; \boldsymbol{w})]^2 = \|\boldsymbol{y} - X\boldsymbol{w}\|^2.$$

# Least squares regression: Geometry

$$\begin{aligned}
\frac{\partial RSS(\boldsymbol{w})}{\partial \boldsymbol{w}} &= \frac{\partial}{\partial \boldsymbol{w}} \left[\boldsymbol{y}^t \boldsymbol{y} - 2\boldsymbol{y}^t X \boldsymbol{w} + \boldsymbol{w}^t X^t X \boldsymbol{w}\right] \\
&= -2X^t \boldsymbol{y} + 2X^t X \boldsymbol{w} \stackrel{!}{=} \boldsymbol{0} \\
\Rightarrow \quad & \hat{\boldsymbol{w}} = (X^t X)^{-1} X^t \boldsymbol{y} \\
\Rightarrow \quad & X^t(\boldsymbol{y} - X\hat{\boldsymbol{w}}) = X^t \hat{\boldsymbol{r}} = \boldsymbol{0}.
\end{aligned}$$

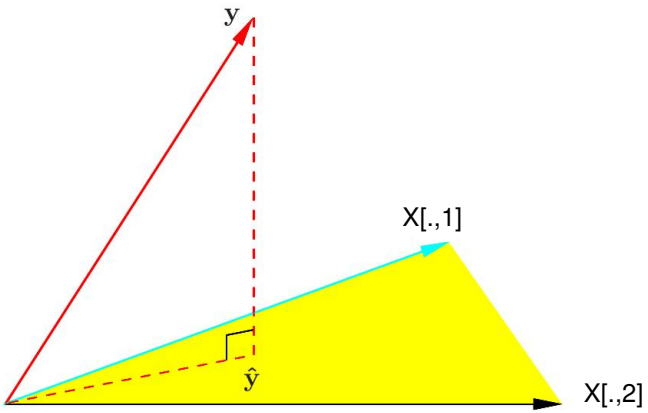
If follows that $\sum_{i=1}^{n} X_{ij} r_i = 0, \ \forall j = 0, 1, \ldots, d$.

**Residual is orthogonal to 1 $(j = 0)$ and to every input dimension $X_{\bullet j}$.**




Adapted from Fig. 3.2 in (Hastie, Tibshirani, Friedman)

# Least squares regression: Geometry




Adapted from Fig. 3.2 in (Hastie, Tibshirani, Friedman)

- The fitted values at the training inputs are
$$(\hat{f}(\boldsymbol{x}_1), \ldots, \hat{f}(\boldsymbol{x}_n))^t = \hat{\boldsymbol{y}} = X\hat{\boldsymbol{w}} = X(X^tX)^{-1}X^t\boldsymbol{y}.$$
- $H = X(X^tX)^{-1}X^t$ is called "hat" matrix (puts hat on $\boldsymbol{y}$)
- Column vectors of $X$ span the **column space** of $X \subset \mathbb{R}^n$.
- Minimizing $RSS(\boldsymbol{w}) \rightsquigarrow$ choose $\hat{\boldsymbol{w}}$ such that $\boldsymbol{r}$ is orthogonal.
- Fitted values $\hat{\boldsymbol{y}}$ are **orthogonal projection** of $\boldsymbol{y}$ on column space.

# Least squares regression: Algebra

- $H$ is **orthogonal projection** on **column space** of $X$:
$$HX = X(X^tX)^{-1}X^tX = X.$$
- **Fundamental theorem of linear algebra:** the **nullspace** of $X^t$ is the orthogonal complement of the column space of $X$.
- $M = I_n - H$ is **orthogonal projection** on **nullspace** of $X^t$:
$$MX = (I_n - H)X = X - X = 0.$$
- $H$ and $M$ are symmetric ($H^t = H$) and idempotent ($MM = M$)

## The Algebra of Least Squares

- $H$ creates fitted values: $\hat{\boldsymbol{y}} = H\boldsymbol{y} \rightsquigarrow \hat{\boldsymbol{y}} \in \mathrm{Col}(X)$
- $M$ creates residuals: $\boldsymbol{r} = M\boldsymbol{y} \rightsquigarrow \hat{\boldsymbol{r}} \in \mathrm{Null}(X^t) \Leftrightarrow X^t\boldsymbol{r} = \boldsymbol{0}$

# Frequentist confidence limits

- **Recall:** $y_i = f(\boldsymbol{x}_i; \boldsymbol{w}) + \eta_i$, with independent Gaussian noise.
- In matrix-vector form: $\boldsymbol{y} = X\boldsymbol{w} + \boldsymbol{\eta}$, with $\boldsymbol{\eta} \sim N(\boldsymbol{0}, \sigma^2 I_n)$.

$$\begin{aligned} \hat{\boldsymbol{w}} &= (X^t X)^{-1} X^t \boldsymbol{y} \\ &= (X^t X)^{-1} X^t X \boldsymbol{w} + (X^t X)^{-1} X^t \boldsymbol{\eta} \\ &= \boldsymbol{w} + (X^t X)^{-1} X^t \boldsymbol{\eta} \end{aligned}$$

$$\Rightarrow \quad \hat{\boldsymbol{w}} - \boldsymbol{w} = (X^t X)^{-1} X^t \boldsymbol{\eta} =: A\boldsymbol{\eta}$$

- **Linear** functions of normals are normal:

$$\boldsymbol{\eta} \sim N(\boldsymbol{0}, \sigma^2 I_n) \;\Rightarrow\; A\boldsymbol{\eta} \sim N(\boldsymbol{0}, \sigma^2 AA^t).$$

Here: $A = (X^t X)^{-1} X^t \;\Rightarrow\; AA^t = (X^t X)^{-1}$

- Conditioned on $X$ and $\sigma^2$:

$$\hat{\boldsymbol{w}} - \boldsymbol{w} | X, \sigma^2 \sim N\left(\boldsymbol{0}, \sigma^2 (X^t X)^{-1}\right).$$

# Frequentist confidence limits

- Distribution completely specified $\rightsquigarrow$ **confidence limits:**

  $$\hat{w}_k - w_k \sim N(0, \sigma^2 S^{kk}),$$

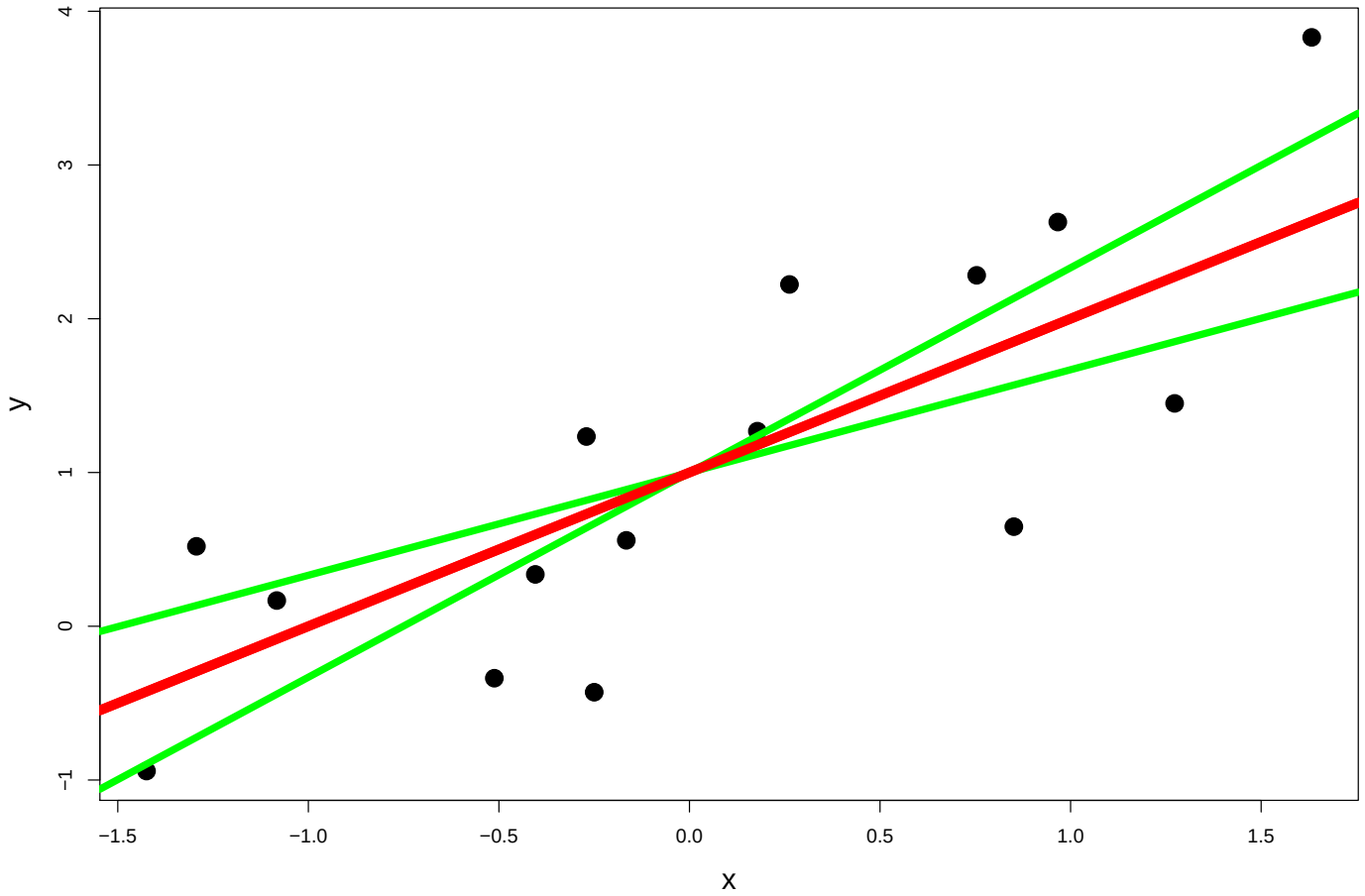
  where $S^{kk}$ denotes the $k$th diagonal element of $(X^t X)^{-1}$.
- Thus, both $z'_k$ and $z_k = -z'_k$ are standard normal:

  $$z_k := (w_k - \hat{w}_k)/\sqrt{\sigma^2 S^{kk}} \sim N(0,1)$$
- CDF:

  $$P(z_k < k_c) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{k_c} e^{-t^2/2}\, dt =: \Phi(k_c) = 1 - c$$
- Upper limit for $w_k$:

$$\begin{aligned} P(z_k < k_c) &= P(\sqrt{\sigma^2 S^{kk}} z_k < \sqrt{\sigma^2 S^{kk}} k_c) \\ &= P(w_k - (w_k - \hat{w}_k) > w_k - \sqrt{\sigma^2 S^{kk}} k_c) \\ &= P(\hat{w}_k > w_k - \sqrt{\sigma^2 S^{kk}} k_c) \\ &= P(w_k < \hat{w}_k + \sqrt{\sigma^2 S^{kk}} k_c) = 1 - c. \end{aligned}$$

# Frequentist confidence limits




Least-squares fit (red) and two lines with slopes according to upper (lower) 95% confidence limit (green).

# Standard parametric rate

- Assume we have estimated the parameters based on $n$ samples:

$$\begin{aligned}(\hat{\boldsymbol{w}}_n - \boldsymbol{w}) &\sim N(\mathbf{0}, \sigma^2 \left(X^t X\right)^{-1}) \\ &= N(\mathbf{0}, \sigma^2 \left(X^t X/n\right)^{-1} \cdot 1/n) \\ \sqrt{n}(\hat{\boldsymbol{w}}_n - \boldsymbol{w}) &\sim N(\mathbf{0}, \sigma^2 \underbrace{\left(X^t X/n\right)}_{\to \Sigma}{}^{-1})\end{aligned}$$

- Since for $n \to \infty$, $X^t X/n \to \Sigma = const$, this means that **$\hat{\boldsymbol{w}}_n$ converges to $\boldsymbol{w}$ at a rate of $1/\sqrt{n}$.**
- This is a very general result that holds in an asymptotic sense even without assuming normality $\rightsquigarrow$ **central limit theorem.**
- Due to its universality, it is called the **standard parametric rate.**

# Basis functions

- Can be generalized to model non-linear relationships by replacing $\boldsymbol{x}$ with some non-linear function of the inputs, $\phi(\boldsymbol{x})$:

$$p(y|\boldsymbol{x}) = N(\boldsymbol{w}^t \phi(\boldsymbol{x}), \sigma^2).$$

- Predictions can be based on a linear combination of a set of basis functions $\phi(\boldsymbol{x}) = \{g_0(\boldsymbol{x}), g_1(\boldsymbol{x}), \ldots, g_m(\boldsymbol{x})\}$, with $g_i(\boldsymbol{x}) : \mathbb{R}^d \mapsto \mathbb{R}$. Can model the intercept by setting $g_0(\boldsymbol{x}) = 1$:

$$f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 g_1(\boldsymbol{x}) + \cdots + w_m g_m(\boldsymbol{x}).$$

$\rightsquigarrow$ **additive models**

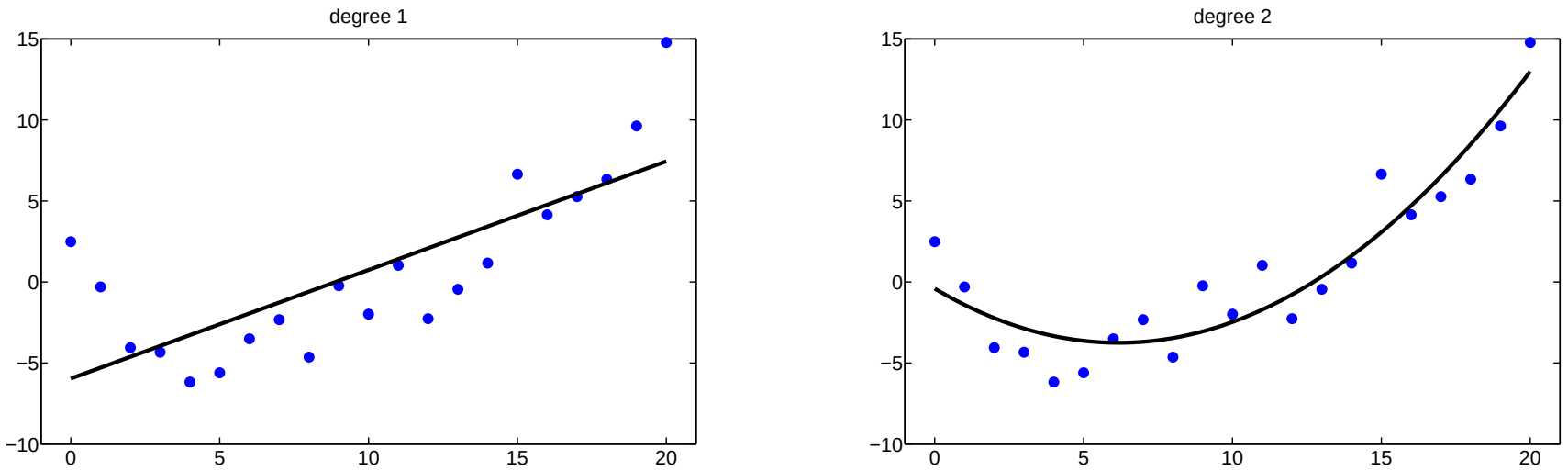



Fig 1.7 in K.Murphy

# Additive models

- Examples:
  If $x \in \mathbb{R}^d$ and $m = d+1$, $g_0(\boldsymbol{x}) = 1$ and $g_i(\boldsymbol{x}) = x_i$, $i = 1, \ldots, d$, then
  $$f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 x_1 + \cdots + w_d x_d.$$
  If $x \in \mathbb{R}$, $g_0(\boldsymbol{x}) = 1$ and $g_i(x) = x^i$, $i = 1, \ldots, m$, then
  $$f(x; \boldsymbol{w}) = w_0 + w_1 x^1 + \cdots + w_m x^m.$$
- Basis functions can **capture various properties of the inputs**.
  Example: **Document analysis**

$$\begin{aligned} \boldsymbol{x} &= \text{text document (collection of words)} \\ g_i(\boldsymbol{x}) &= \begin{cases} 1, & \text{if word i appears in the document} \\ 0, & \text{otherwise} \end{cases} \\ f(\boldsymbol{x}; \boldsymbol{w}) &= w_0 + \sum_{i \in \text{words}} w_i g_i(\boldsymbol{x}). \end{aligned}$$

# Additive models cont'd

- We can also make predictions by gauging the **similarity of examples to prototypes.**
- For example, our additive regression function could be

$$f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 g_1(\boldsymbol{x}) + \cdots + w_m g_m(\boldsymbol{x}),$$

where the basis functions are **radial basis functions**

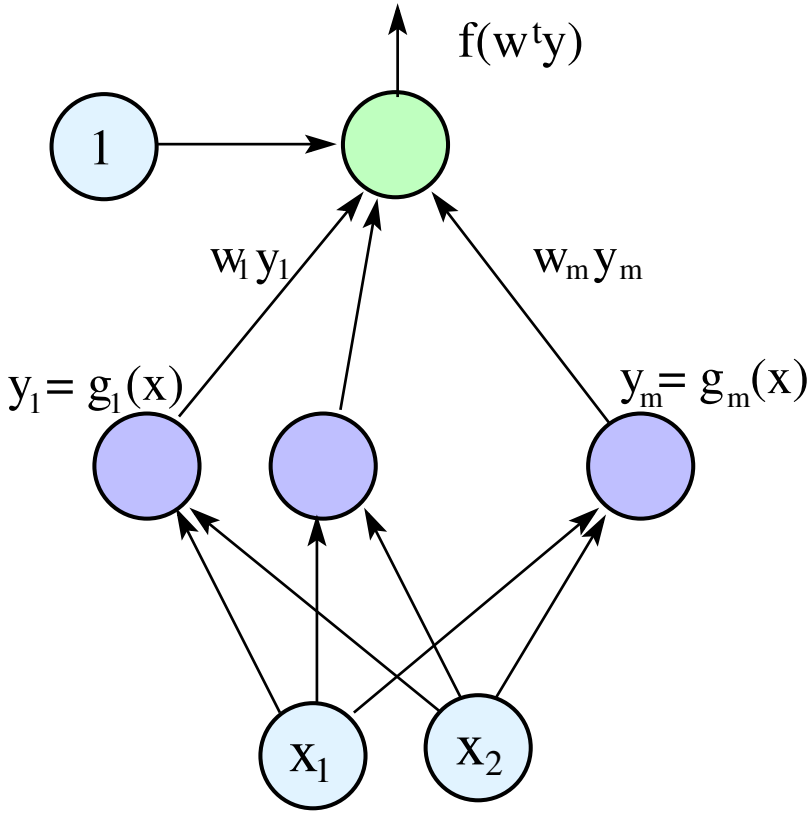
$$g_k(\boldsymbol{x}) = \exp\left(-\frac{1}{2\sigma^2}\|\boldsymbol{x} - \boldsymbol{x}_k\|^2\right)$$

measuring the similarity to the prototypes $\boldsymbol{x}_k$.

- The variance $\sigma^2$ controls how quickly the basis function vanishes as a function of the distance to the prototype.
- **Training examples themselves could serve as prototypes.**

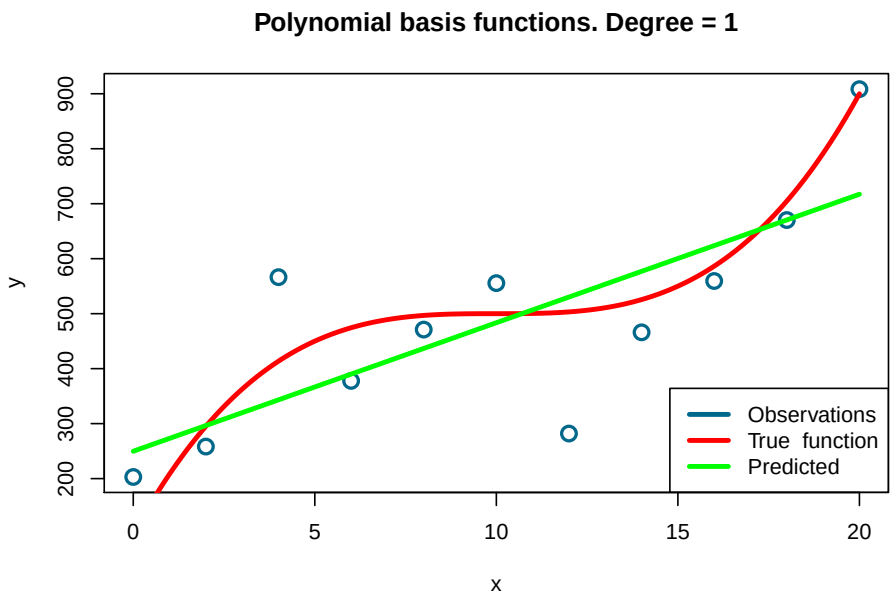
# Additive models cont'd

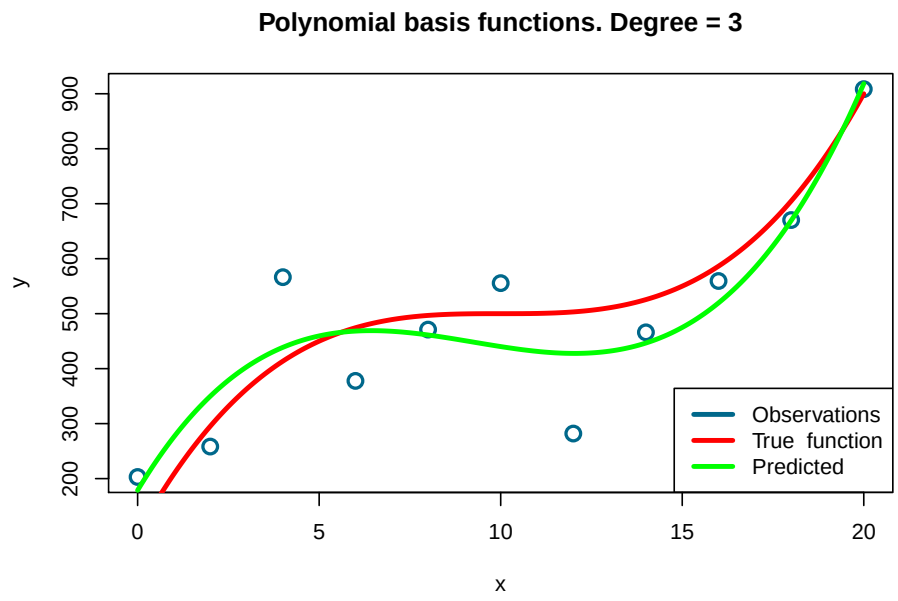
Can view additive models graphically in terms of **units** and **weights**.

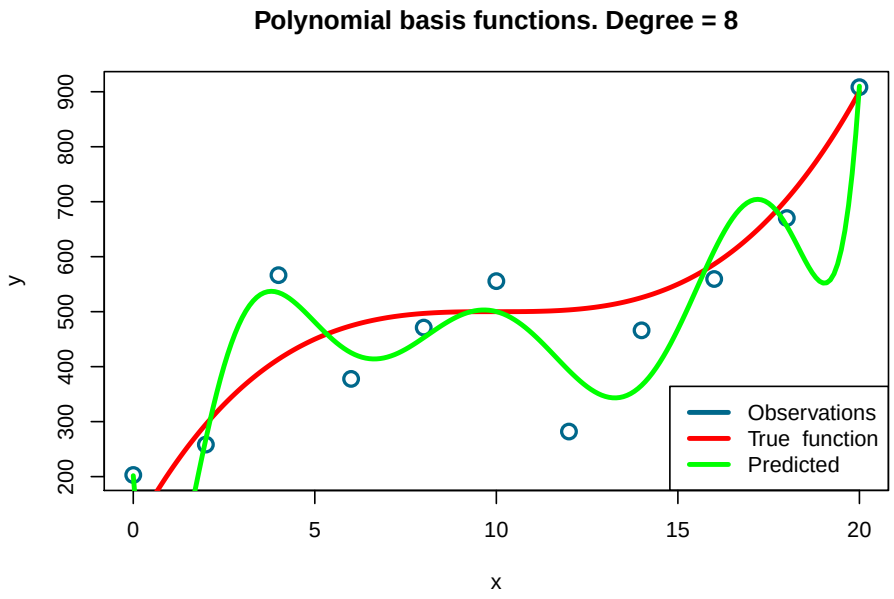


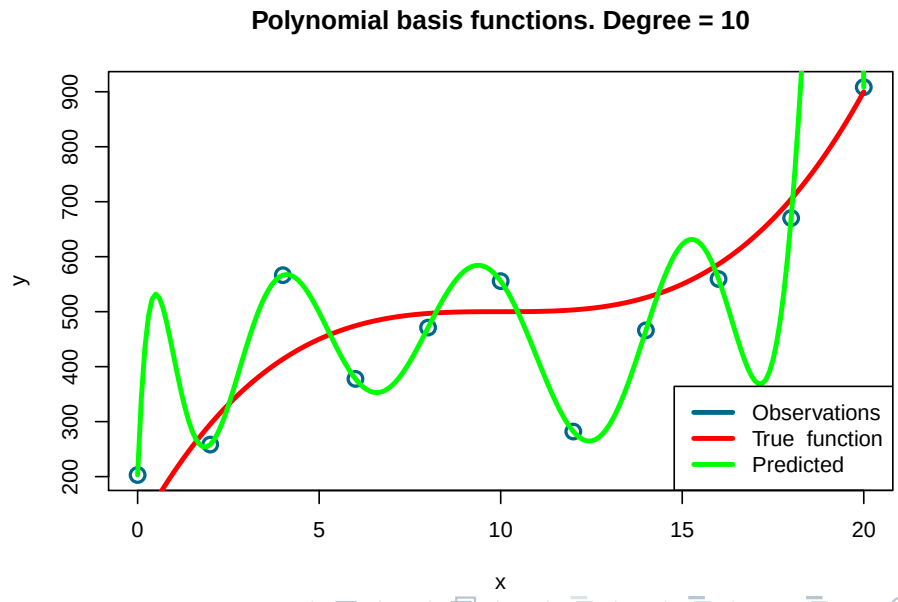

In **neural networks** the basis functions have adjustable parameters.

# Example: Polynomial regression



# Complexity and overfitting

With limited training examples our polynomial regression model may achieve zero training error but nevertheless has a large expected error.

$$\text{training} \qquad \frac{1}{n}\sum_{i=1}^{n}(y_i - f(\boldsymbol{x}_i; \hat{\boldsymbol{w}})^2 \approx 0$$

$$\text{expectation} \qquad E_{(\boldsymbol{x},y)\sim p}\,(y - f(\boldsymbol{x}; \hat{\boldsymbol{w}})^2 \gg 0$$

We suffer from **over-fitting**
$\rightsquigarrow$ should reconsider our model $\rightsquigarrow$ **model selection.**

We will discuss model selection from a **Bayesian perspective** first.
A frequentist approach will follow later in the chapter on **statistical learning theory.**

Subsection 1

## Bayesian Regression

# Bayesian interpretation: priors

- Suppose our generative model takes an input $\boldsymbol{x} \in \mathbb{R}^d$ and maps it to a real valued output $y$ according to
$$p(y|\boldsymbol{x}, \boldsymbol{w}, \sigma^2) = N(y|\boldsymbol{w}^t\boldsymbol{x}, \sigma^2)$$
- We will keep $\sigma^2$ fixed and only try to estimate $\boldsymbol{w}$.
- Given data $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}$, the **likelihood function** is
$$L(\boldsymbol{w}; \mathcal{D}) = \prod_{i=1}^{n} N(y_i|\boldsymbol{w}^t\boldsymbol{x}_i, \sigma^2) = \prod_{i=1}^{n} \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}(y_i - \boldsymbol{w}^t\boldsymbol{x}_i)^2\right).$$
- In classical regression we used the maximizing parameters $\hat{\boldsymbol{w}}$.
- **In Bayesian analysis we keep all regression functions**, just weighted by their ability to explain the data.
- Our knowledge about $\boldsymbol{w}$ after seeing the data is defined by the **posterior distribution** $p(\boldsymbol{w}|\mathcal{D})$.

# Bayesian regression: Prior and posterior

- We specify our **prior belief** about the parameter values as $p(\boldsymbol{w})$. For instance, we could prefer small parameter values:

$$p(\boldsymbol{w}) = N\left(\boldsymbol{w}|0, \tau^2 I\right)$$

  The smaller $\tau^2$ is, the smaller values of $\boldsymbol{w}$ we prefer **prior to seeing the data**.

- **Posterior** proportional to prior $p(\boldsymbol{w})$ times likelihood:

$$p(\boldsymbol{w}|\mathcal{D}) \propto L(\boldsymbol{w}; \mathcal{D}) p(\boldsymbol{w})$$

- Here: posterior is **Gaussian** $p(\boldsymbol{w}|\mathcal{D}, \sigma^2) = N(\boldsymbol{w}|\boldsymbol{w}_N, V_N)$ with mean $\boldsymbol{w}_N$ and covariance $V_N$ given by

$$\boldsymbol{w}_N = (X^t X + \lambda I)^{-1} X^t \boldsymbol{y}, \quad V_N = \sigma^2 (X^t X + \lambda I)^{-1},$$

  with $\lambda = \frac{\sigma^2}{\tau^2}$.

# Bayesian regression: Posterior computation

Given variables $\boldsymbol{x} \in \mathbb{R}^{d_x}$ and $\boldsymbol{y} \in \mathbb{R}^{d_y}$, assume **linear Gaussian system:**

$$p(\boldsymbol{x}) = N(\boldsymbol{x}|\boldsymbol{\mu}_x, \Sigma_x) \quad (\rightsquigarrow \text{ prior})$$
$$p(\boldsymbol{y}|\boldsymbol{x}) = N(\boldsymbol{y}|A\boldsymbol{x} + \boldsymbol{b}, \Sigma_y) \quad (\rightsquigarrow \text{ likelihood})$$

- **The posterior is also Gaussian:**

$$p(\boldsymbol{x}|\boldsymbol{y}) = N(\boldsymbol{x}|\boldsymbol{\mu}_{x|y}, \Sigma_{x|y})$$
$$\Sigma_{x|y}^{-1} = \Sigma_x^{-1} + A^t \Sigma_y^{-1} A$$
$$\boldsymbol{\mu}_{x|y} = \Sigma_{x|y} \left( A^t \Sigma_y^{-1} (\boldsymbol{y} - \boldsymbol{b}) + \Sigma_x^{-1} \boldsymbol{\mu}_x \right).$$

  **Gaussian likelihood and Gaussian prior form a conjugate pair.**

- The normalization constant (denominator in Bayes formula) is

$$p(\boldsymbol{y}) = N(\boldsymbol{y}|A\boldsymbol{\mu}_x + \boldsymbol{b}, \Sigma_y + A\Sigma_x A^t).$$

# Bayesian regression: Posterior predictive

- Prediction of $y$ for new $\boldsymbol{x}$: use posterior as weights for predictions based on individual $\boldsymbol{w}$'s $\rightsquigarrow$ **Posterior predictive:**

$$
\begin{aligned}
p(y|\boldsymbol{x}, \mathcal{D}, \sigma^2) &= \int p(y|\boldsymbol{x}, \boldsymbol{w}, \sigma^2) p(\boldsymbol{w}|\mathcal{D})\, d\boldsymbol{w} \\
&= \int N(y|\boldsymbol{x}^t \boldsymbol{w}, \sigma^2) N(\boldsymbol{w}|\boldsymbol{w}_N, V_N) \\
&= N(y|\boldsymbol{w}_N^t \boldsymbol{x}, \sigma_N^2(\boldsymbol{x})), \text{ with} \\
\sigma_N^2(\boldsymbol{x}) &= \sigma^2 + \boldsymbol{x}^t V_N \boldsymbol{x}.
\end{aligned}
$$

- The variance in this prediction, $\sigma_N^2(\boldsymbol{x})$, depends on two terms:
  - the variance of the observation noise, $\sigma^2$
  - the variance in the parameters, $V_N$
    $\rightsquigarrow$ depends on how close $\boldsymbol{x}$ is to training data $\mathcal{D}$
    $\rightsquigarrow$ error bars get larger as we move away from training points.

# Bayesian regression: Posterior predictive

- By contrast, the **plugin approximation** uses only the ML-parameter estimate with the degenerate distribution $p(\boldsymbol{w}|\mathcal{D}, \sigma^2) = \delta_{\hat{\boldsymbol{w}}}(\boldsymbol{w})$:
$p(\boldsymbol{y}|\boldsymbol{x}, \mathcal{D}, \sigma^2) \approx \int p(y|\boldsymbol{x}, \boldsymbol{w}, \sigma^2)\delta_{\hat{\boldsymbol{w}}}(\boldsymbol{w})\, d\boldsymbol{w} = p(y|\boldsymbol{x}, \hat{\boldsymbol{w}}, \sigma^2) = N(y|\boldsymbol{x}^t\hat{\boldsymbol{w}}, \sigma^2)$.

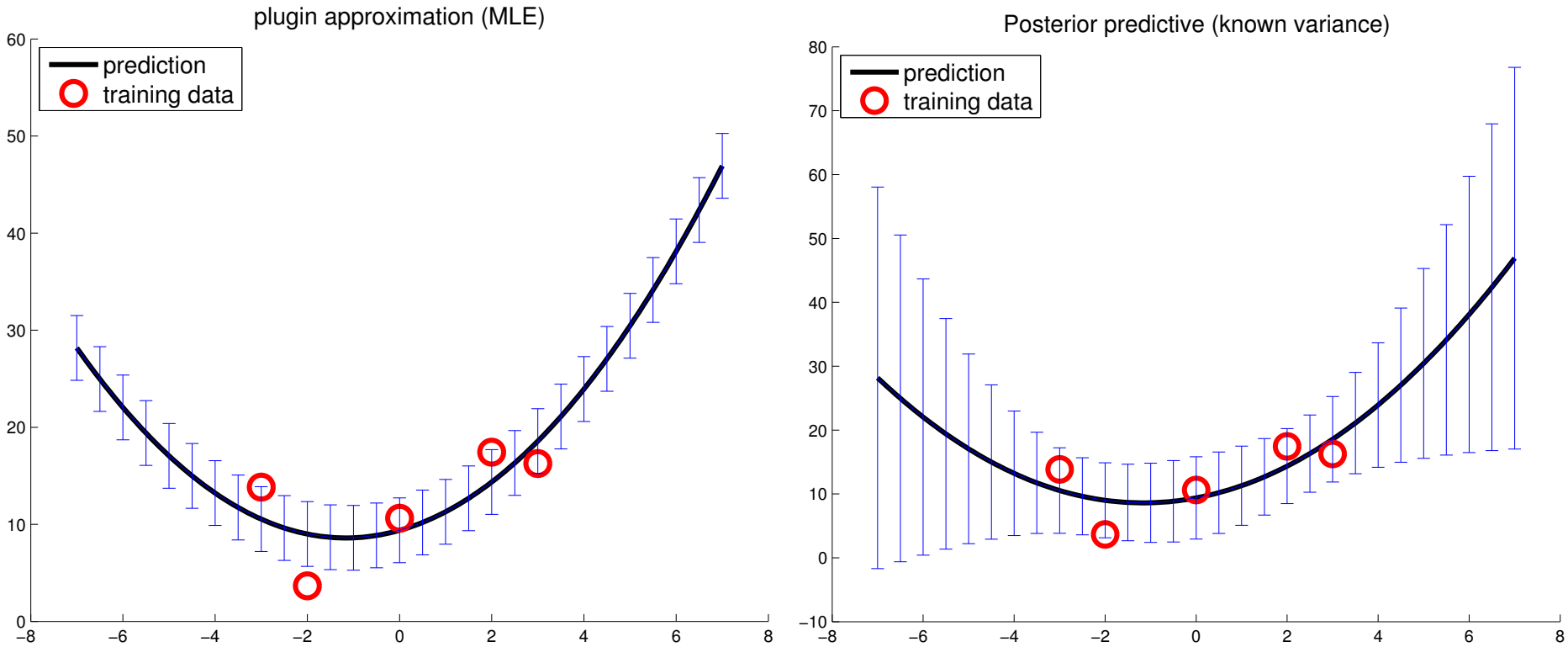



Fig. 7.12 in (K. Murphy). Example with quadratic basis functions: posterior predictive distribution (mean and $\pm 1\sigma$).

# Sampling from posterior predictive

Left: plugin approximation: $f(y) = \phi(\boldsymbol{x})^t \hat{\boldsymbol{w}}$,
where $\phi(\boldsymbol{x})$ is the expanded input vector $(1, x, x^2)^t$.
Right: sampled functions $\phi(\boldsymbol{x})^t \boldsymbol{w}^{(s)}$, where $w^{(s)}$ are samples from the posterior

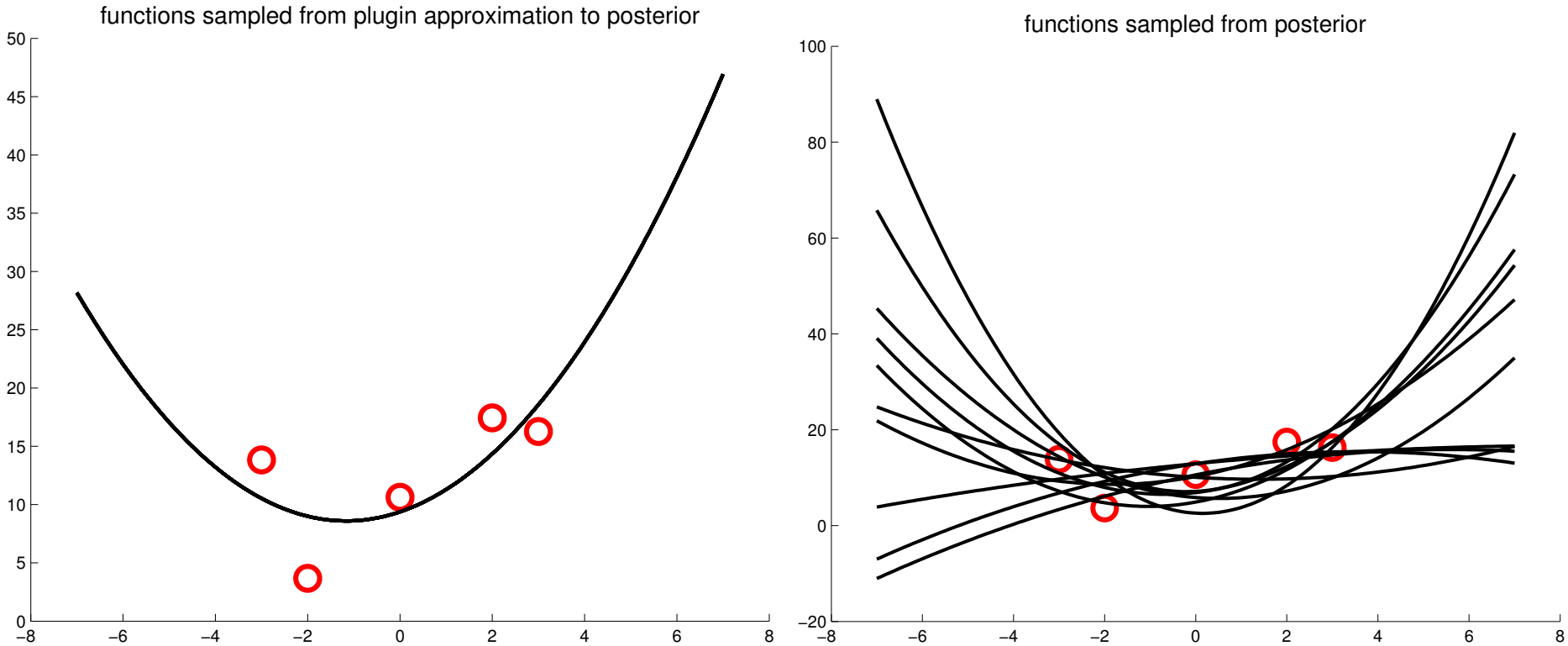



Fig. 7.12 in (K. Murphy)

# MAP approximation and ridge regression

- Posterior proportional to prior $p(\boldsymbol{w}) = N\left(\boldsymbol{w}|0, \tau^2 I\right)$ times likelihood.
- The MAP estimate is

$$\begin{aligned}
\boldsymbol{w}_{\text{MAP}} &= \arg\max\{\log[L(\boldsymbol{w}; \mathcal{D})] + \log[p(\boldsymbol{w})]\} \\
&= \arg\min\{-\log[L(\boldsymbol{w}; \mathcal{D})] - \log[p(\boldsymbol{w})]\} \\
&= \arg\min\{\frac{1}{2\sigma^2}\sum_i (y_i - \boldsymbol{w}^t \boldsymbol{x}_i)^2 + \frac{1}{2\tau^2}\boldsymbol{w}^t\boldsymbol{w}\} \\
&= \arg\min\{\sum_i (y_i - \boldsymbol{w}^t \boldsymbol{x}_i)^2 + \frac{\sigma^2}{\tau^2}\boldsymbol{w}^t\boldsymbol{w}\} \\
&= \arg\min\{\sum_i (y_i - \boldsymbol{w}^t \boldsymbol{x}_i)^2 + \lambda\boldsymbol{w}^t\boldsymbol{w}\}
\end{aligned}$$

- In classical statistics, this is called **ridge regression:**

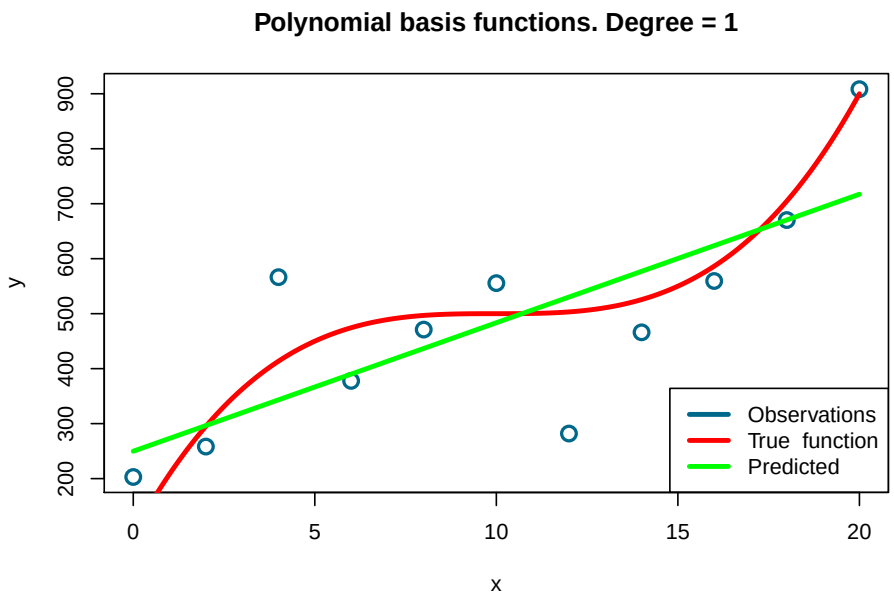
$$\boldsymbol{w}_{\text{MAP}} = \boldsymbol{w}_{\text{ridge}} = (X^t X + \lambda I)^{-1} X^t \boldsymbol{y}.$$

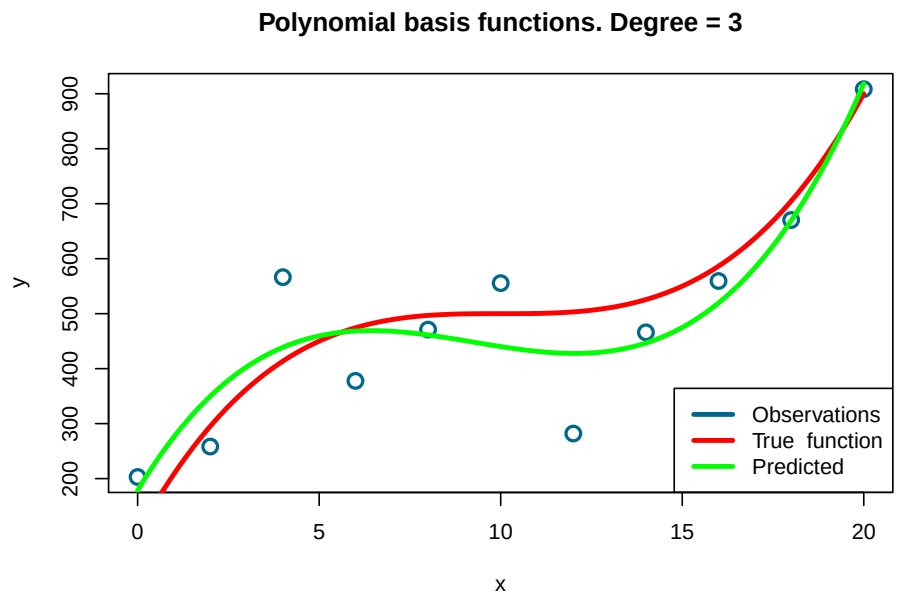
- In regularization theory, this is an example of **Tikhonov Regularization.**

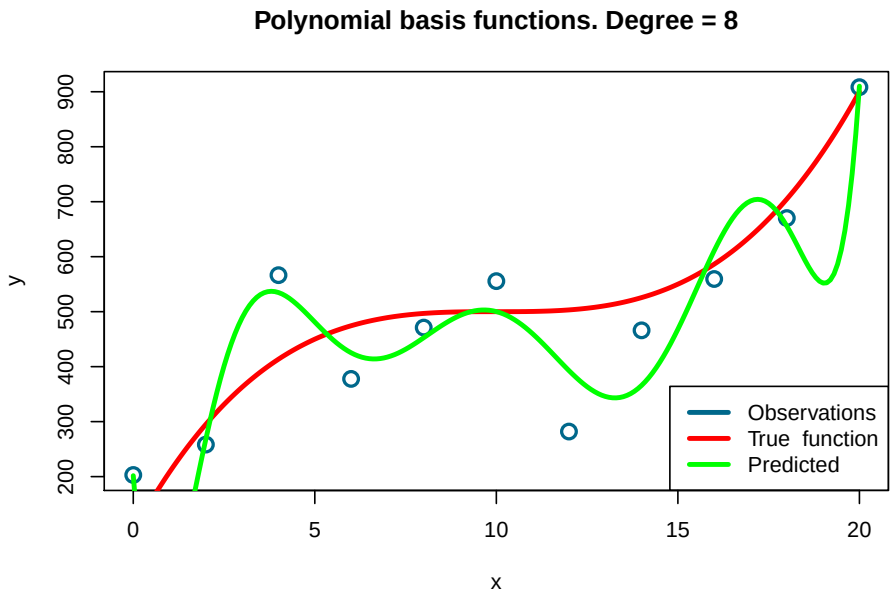
Subsection 2

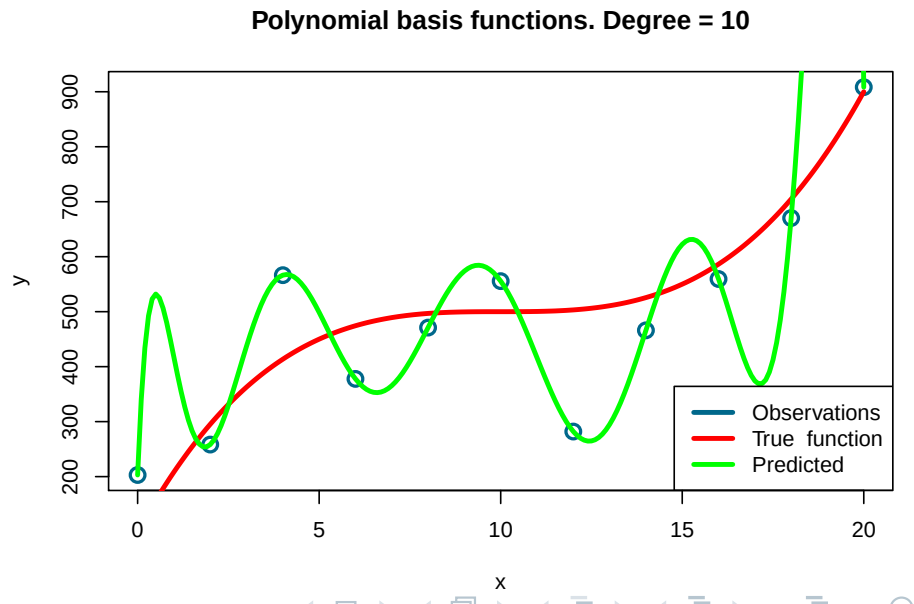
## Bayesian model selection

# Example: Polynomial regression



# Bayesian regression (again)

- Suppose our parametrized model $\mathcal{F}_{\boldsymbol{\theta}}$ takes an input $\boldsymbol{x} \in \mathbb{R}^d$ and maps it to a real valued output $y$ according to

$$p(y|\boldsymbol{x}, \boldsymbol{\theta}, \sigma^2) = N(y; \boldsymbol{\theta}^t \boldsymbol{x}, \sigma^2)$$

- We will keep $\sigma^2$ fixed and only try to estimate $\boldsymbol{\theta}$.
- Given data $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}$, define likelihood

$$L(\boldsymbol{\theta}; \mathcal{D}) = \prod_{i=1}^{n} N(y_i; \boldsymbol{\theta}^t \boldsymbol{x}_i, \sigma^2) = \prod_{i=1}^{n} \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2}(y_i - \boldsymbol{\theta}^t \boldsymbol{x}_i)^2\right).$$

- In classical regression we used the maximizing parameters $\hat{\boldsymbol{\theta}}$.
- In Bayesian analysis we keep **all regression functions**, just weighted by their ability to explain the data.
- Knowledge about $\boldsymbol{\theta}$ after seeing the data defined by posterior $p(\boldsymbol{\theta}|\mathcal{D})$.

# Bayesian regression (again)

- We specify our **prior belief** about the parameter values as $p(\boldsymbol{\theta})$. For instance, we could prefer small parameter values:

  $$p(\boldsymbol{\theta}) = N(\boldsymbol{\theta}; 0, \tau^2 I)$$

  Small $\tau^2 \rightsquigarrow$ small $\boldsymbol{\theta}$ preferred **prior to seeing data.**
- Posterior proportional to prior $p(\boldsymbol{\theta})$ times likelihood:

  $$p(\boldsymbol{\theta}|\mathcal{D}) \propto L(\boldsymbol{\theta}; \mathcal{D}) p(\boldsymbol{\theta})$$
- Normalization constant, a.k.a. **marginal likelihood**:

  $$p(\boldsymbol{y}|\mathcal{F}, X) = \int \underbrace{L(\boldsymbol{\theta}; \mathcal{D})}_{p(\boldsymbol{y}|\boldsymbol{\theta}, X)} p(\boldsymbol{\theta}|\mathcal{F}) d\boldsymbol{\theta},$$

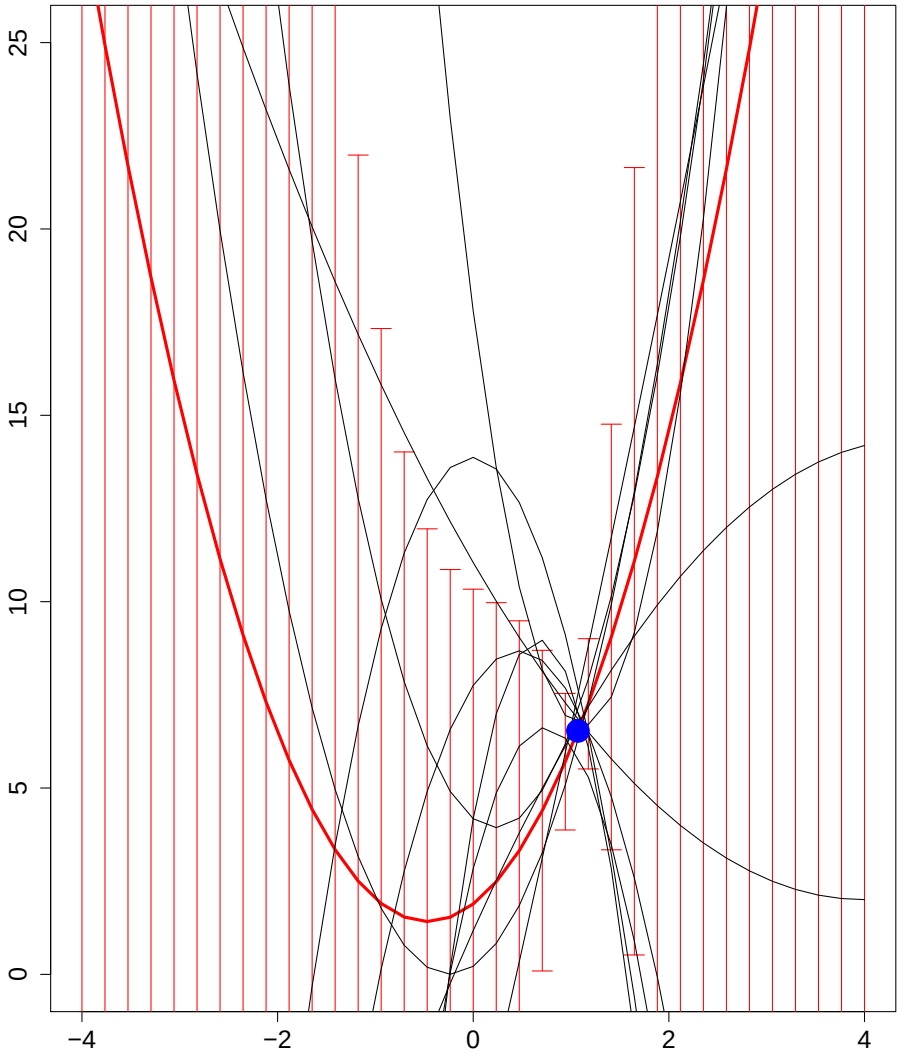
  depends on model + data but **not on specific parameter values.**

# Example: Bayesian regression

- Goal: choose among regression model families, specified by different feature mappings $\boldsymbol{x} \to \phi(\boldsymbol{x})$.
- Example: linear $\phi_1(\boldsymbol{x})$ and quadratic $\phi_2(\boldsymbol{x})$.
- The model families we compare are:

$$\begin{aligned} \mathcal{F}_1 &: p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}_1, \sigma^2) = N(\boldsymbol{y}|\boldsymbol{\theta}_1^t \phi_1(\boldsymbol{x}), \sigma^2) \\ \mathcal{F}_2 &: p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}_2, \sigma^2) = N(\boldsymbol{y}|\boldsymbol{\theta}_2^t \phi_2(\boldsymbol{x}), \sigma^2). \end{aligned}$$

- Focusing on $p(\boldsymbol{y}|\mathcal{F}, X) = \int L(\boldsymbol{\theta}; \mathcal{D}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$, two possibilities:
  - $\mathcal{F}$ **too flexible:** posterior $p(\boldsymbol{\theta}|\mathcal{D})$ requires many training examples before it focuses on useful parameter values;
  - $\mathcal{F}$ **too simple:** posterior concentrates quickly but the predictions remain poor.
- Pragmatic choice: Select the family whose **marginal likelihood** (a.k.a. **Bayesian score**) is larger.
- After seeing data $\mathcal{D}$ we would select model $\mathcal{F}_1$ if $p(\boldsymbol{y}|\mathcal{F}_1, X) > p(\boldsymbol{y}|\mathcal{F}_2, X)$.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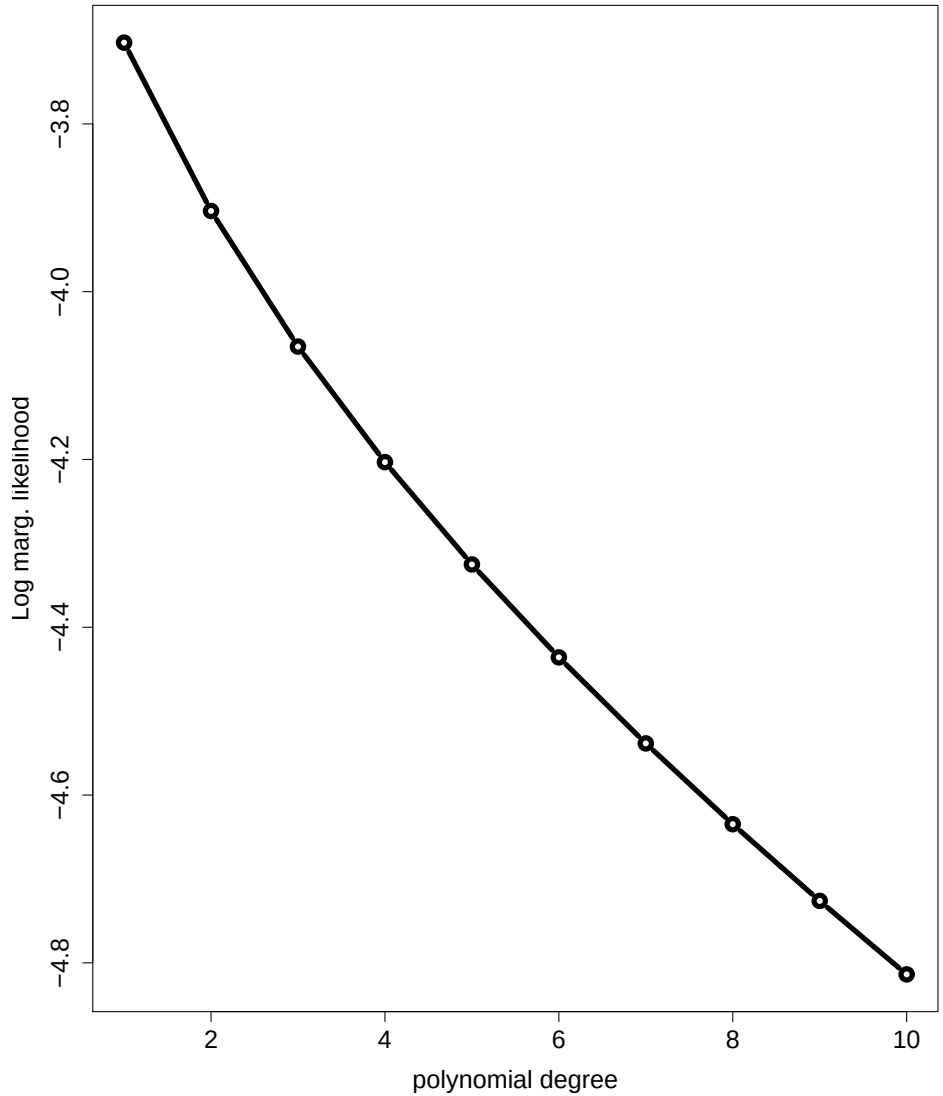
Log marg. likelihood
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−4.0
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−4.4
−4.6
−4.8
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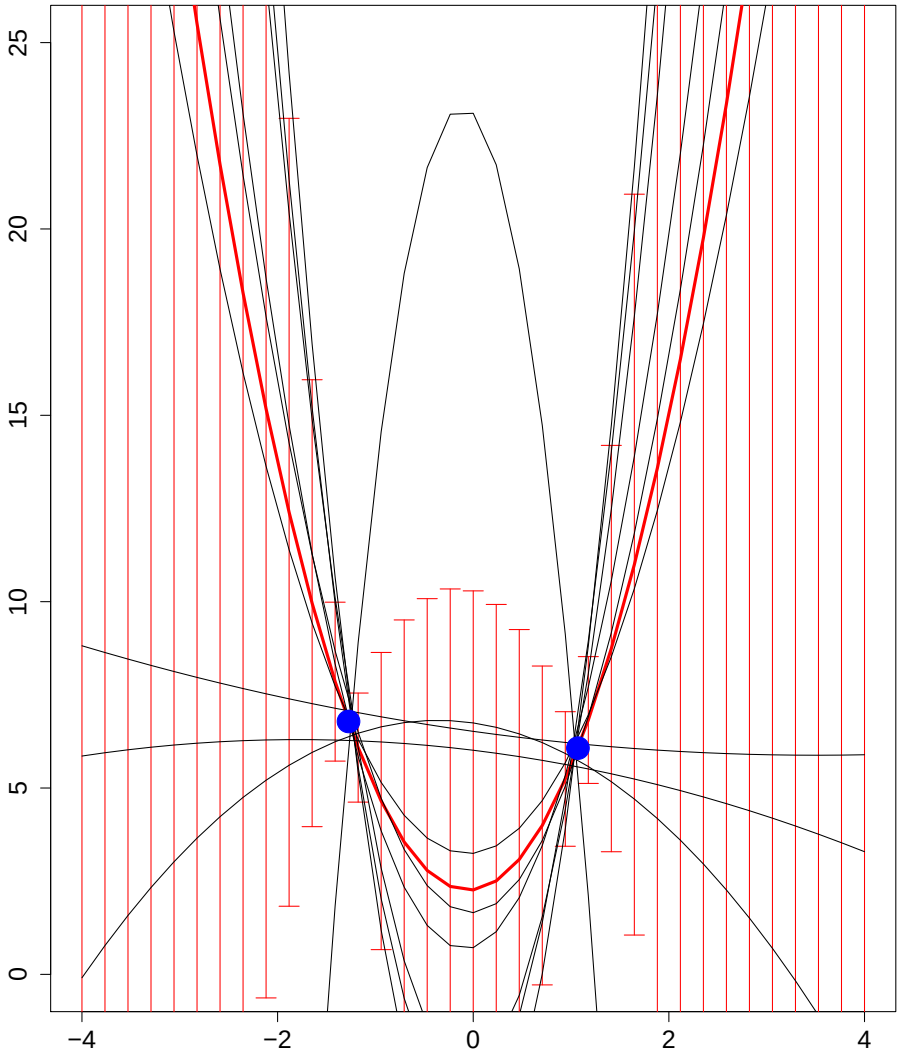
10
polynomial degree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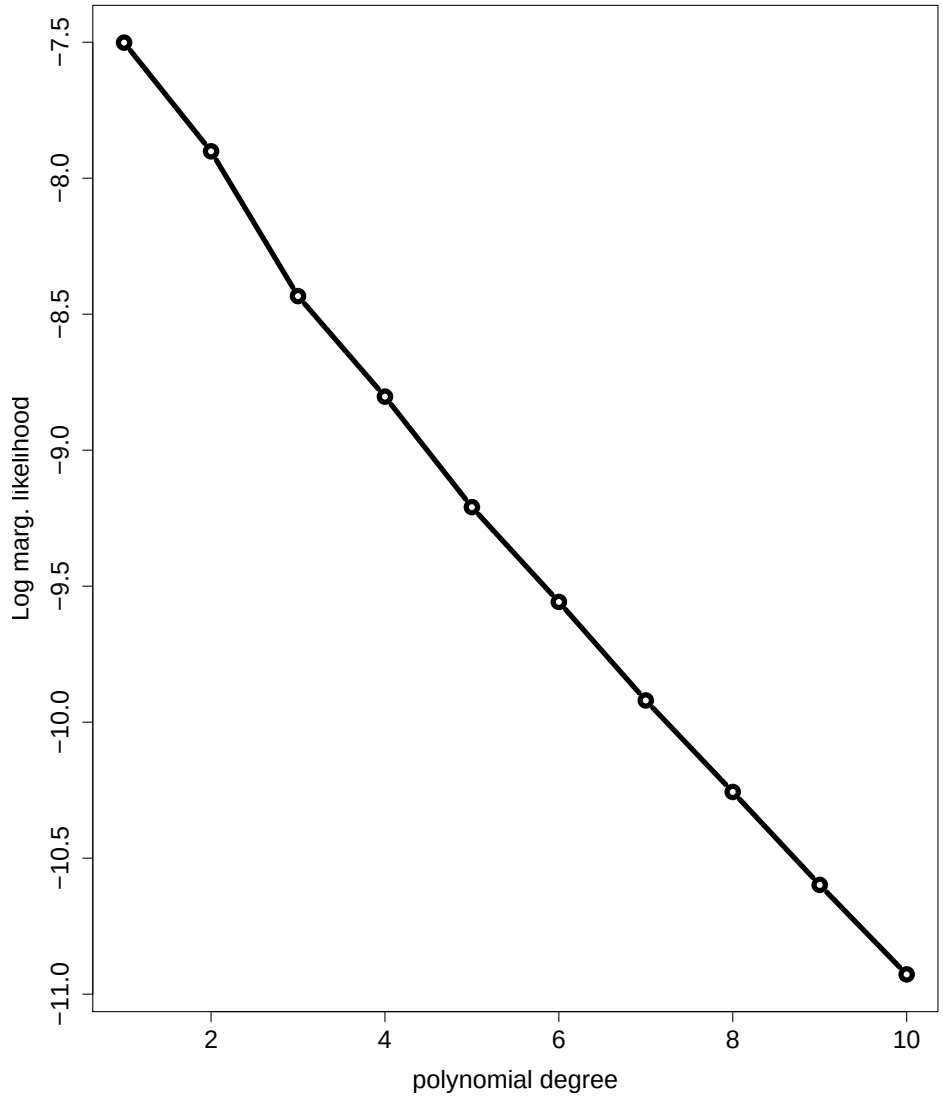
Log marg. likelihood
−7.5
−8.0
−8.5
−9.0
−9.5
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−10.5
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8
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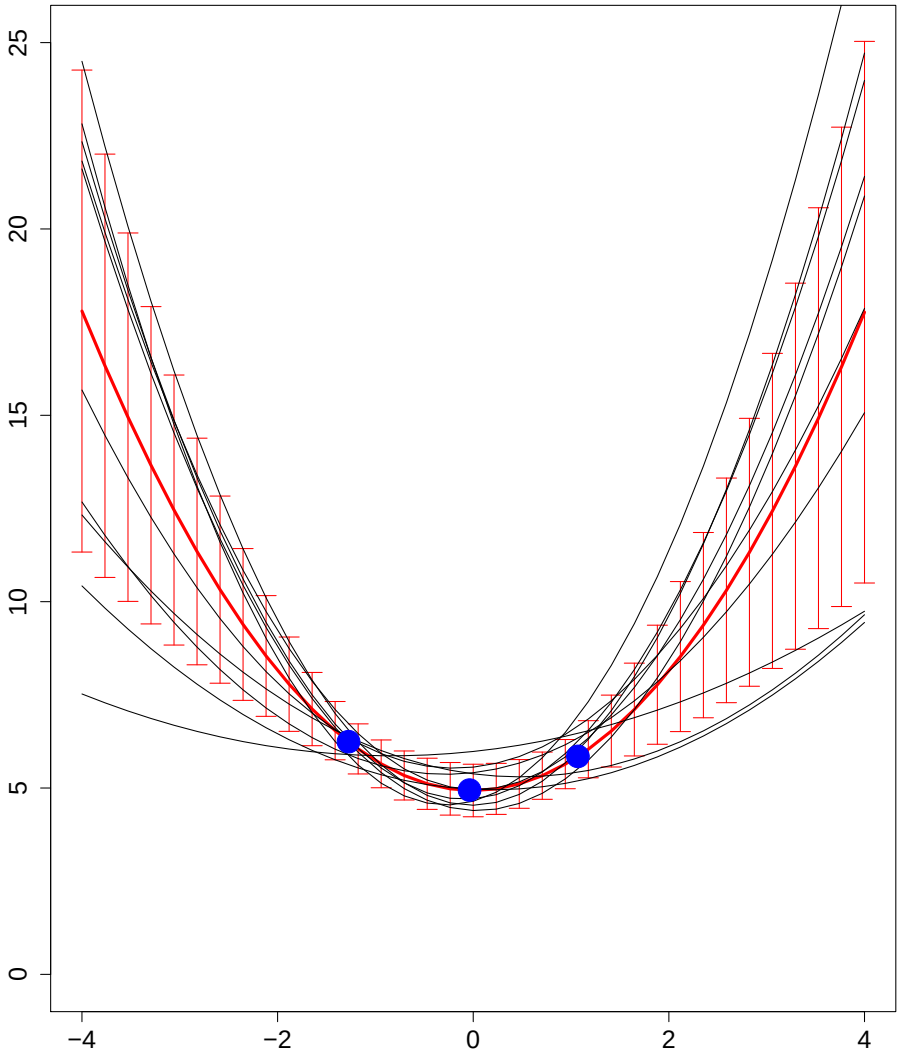
polynomial degree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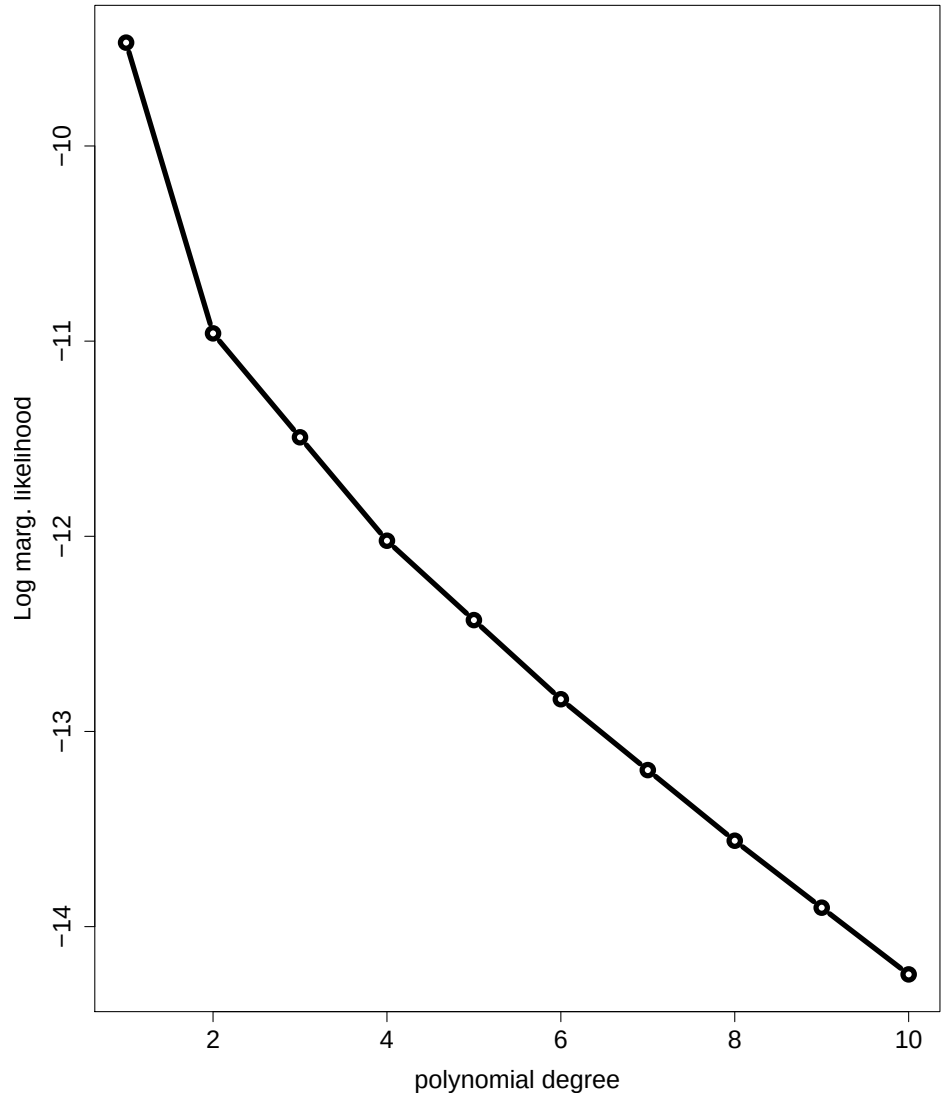
Log marg. likelihood
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−11
−12
−13
−14
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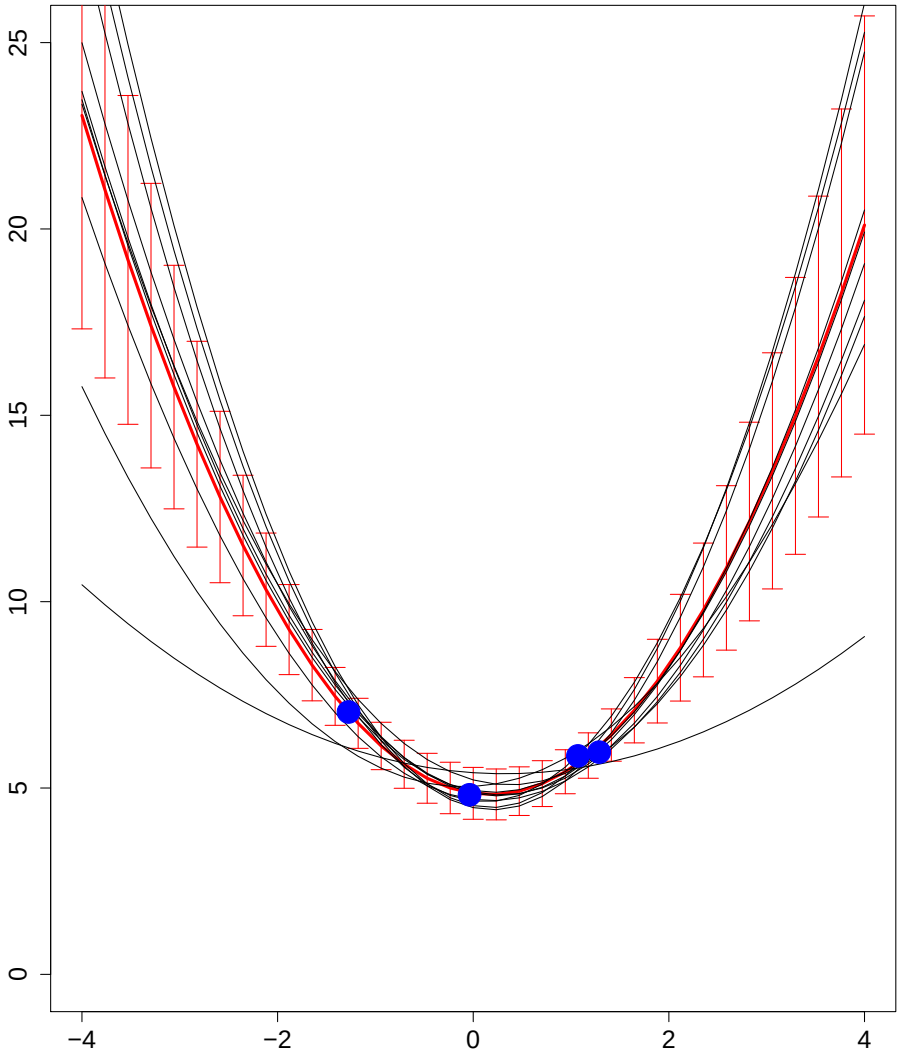
polynomial degree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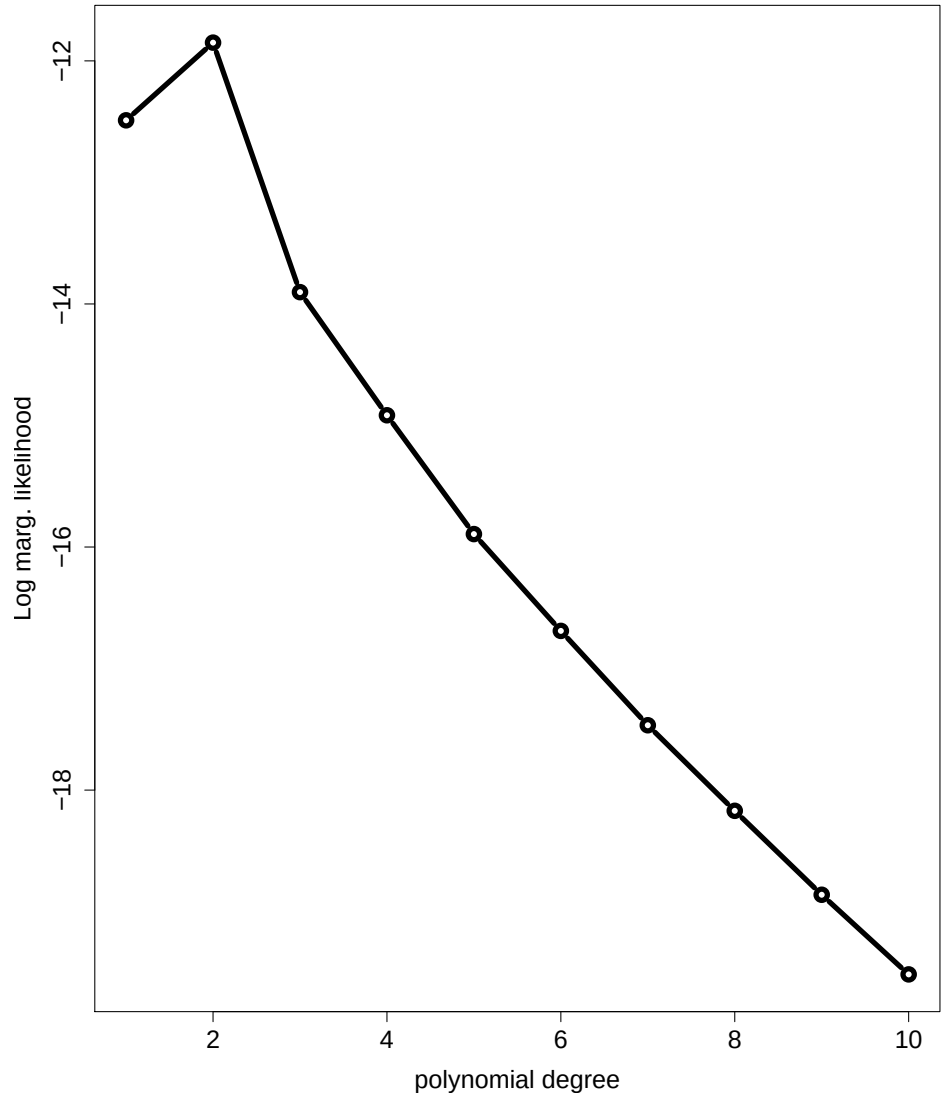
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Log marg. likelihood
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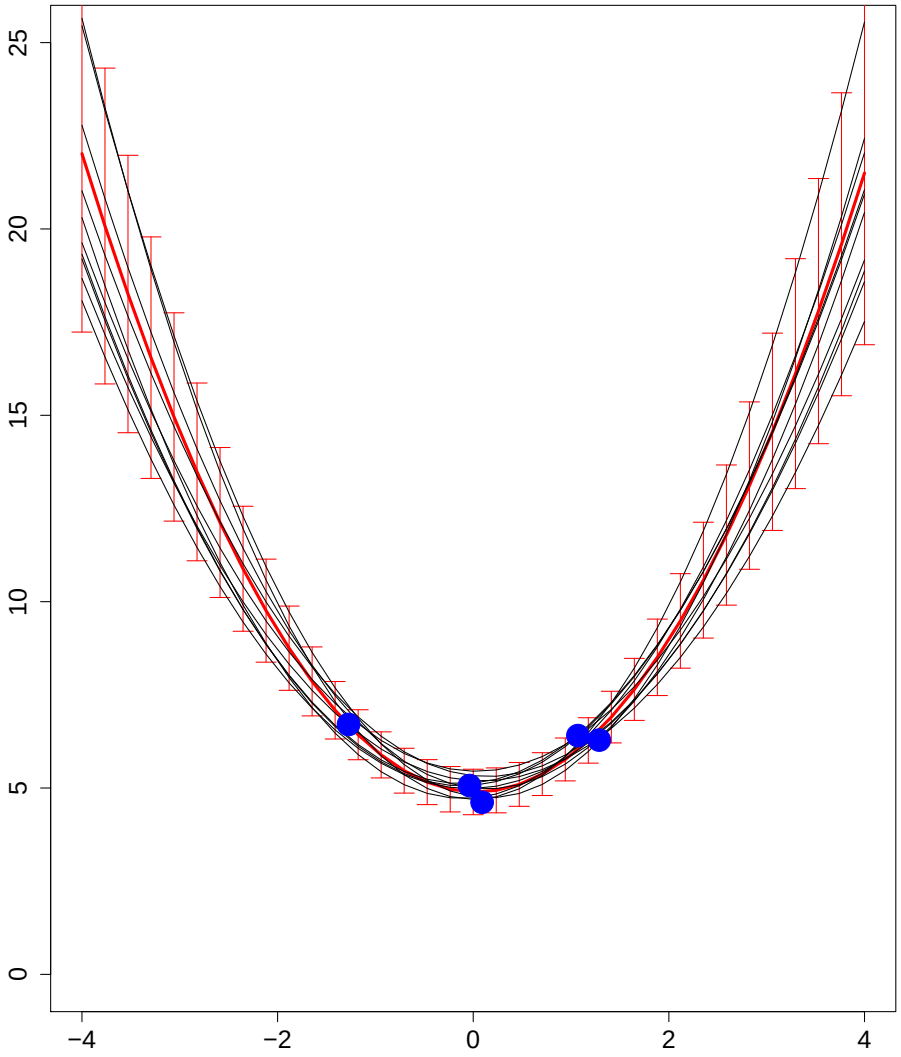
polynomial degree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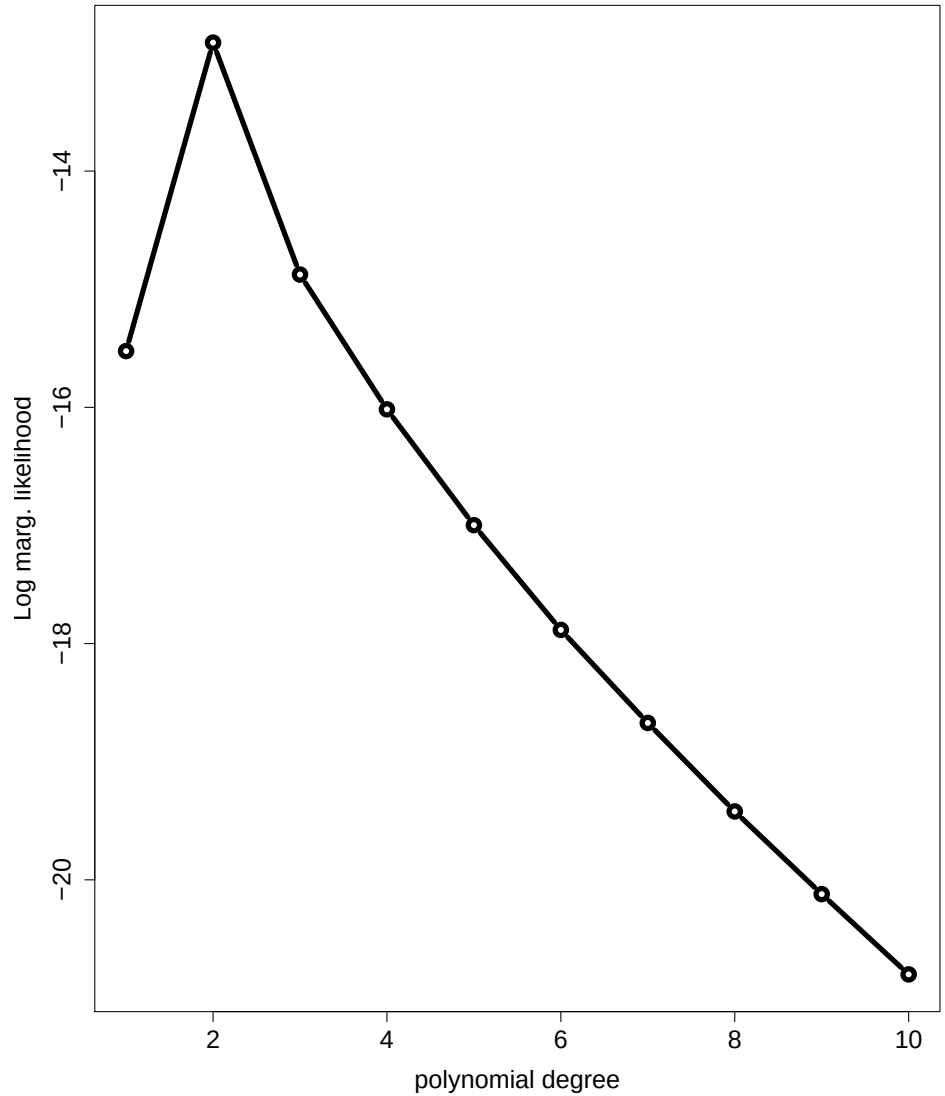
Log marg. likelihood
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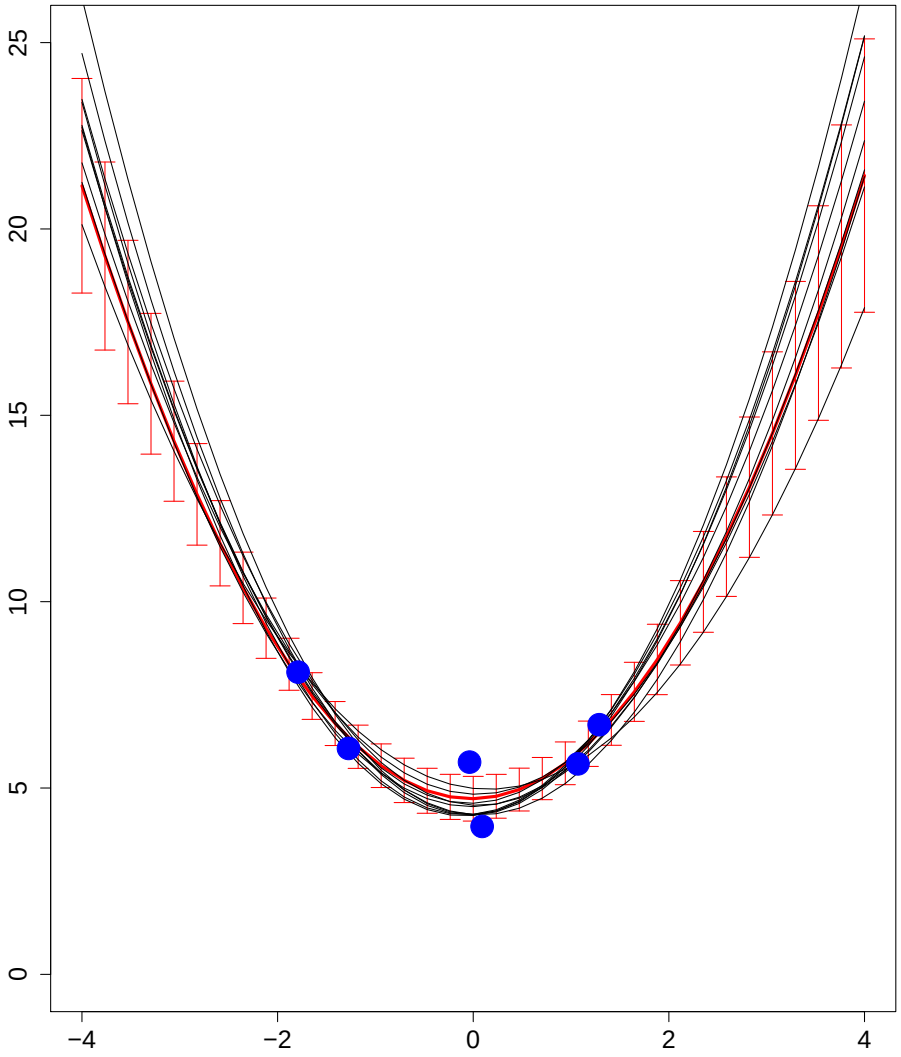
polynomial degree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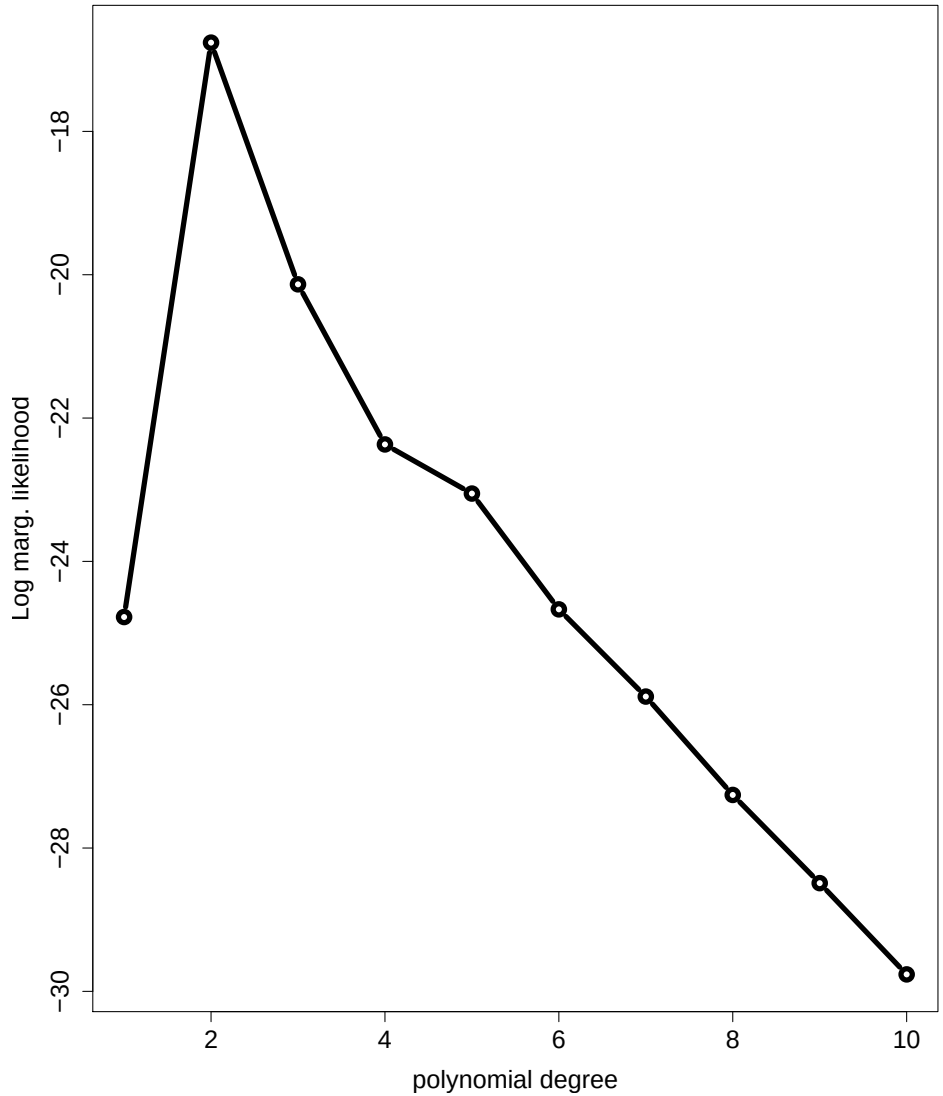
Log marg. likelihood
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−20
−22
−24
−26
−28
−30
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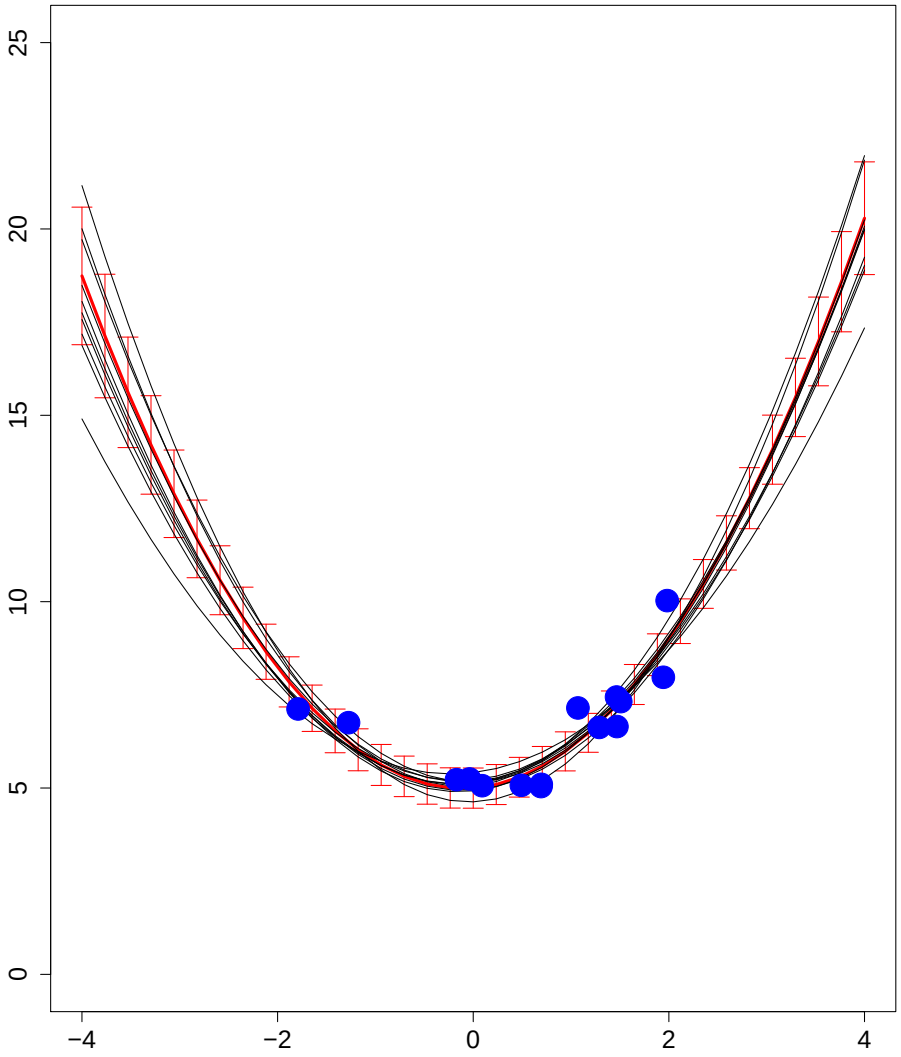
polynomial degree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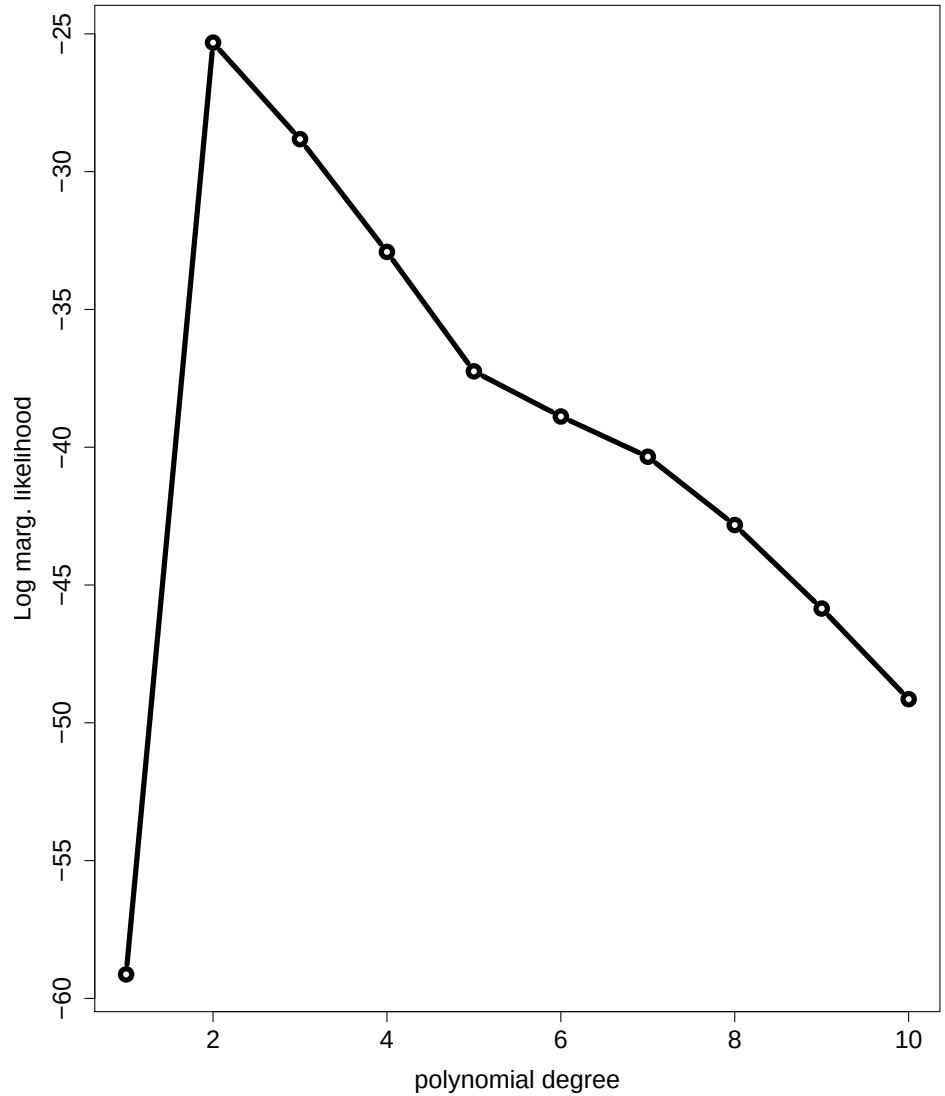
Log marg. likelihood
−25
−30
−35
−40
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−50
−55
−60
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4
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polynomial degree

# Approximating the marginal likelihood

- Problem: In most cases we cannot compute the marginal likelihood in closed form $\rightsquigarrow$ approximations are needed.
- A specific approximation will lead to the **Bayesian Information Criterion (BIC)**.
- Key insight: when computing

$$p(\boldsymbol{y}|\mathcal{F}, X) = \int p(\boldsymbol{y}|\boldsymbol{\theta}, X) p(\boldsymbol{\theta}|\mathcal{F}) d\boldsymbol{\theta},$$

  the integrand is a product of two densities $\rightsquigarrow$ integrand itself is an unnormalized density.
- Laplace's approximation uses a clever trick to approximate such integrals...

# Approximation details: Laplace's Method

- Assume unnormalized density $p^*(\theta)$ has peak at $\hat{\theta}$. Goal: calculate normalizing constant

$$Z_p = \int p^*(\theta) d\theta$$

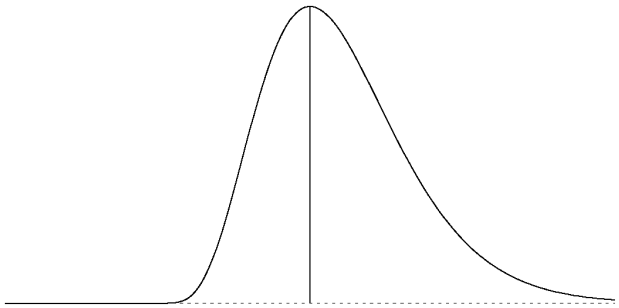
- Taylor-expand logarithm around $\hat{\theta}$:

$$\ln p^*(\theta) \approx \ln p^*(\hat{\theta}) - \frac{c}{2}(\theta - \hat{\theta})^2 + \cdots,$$

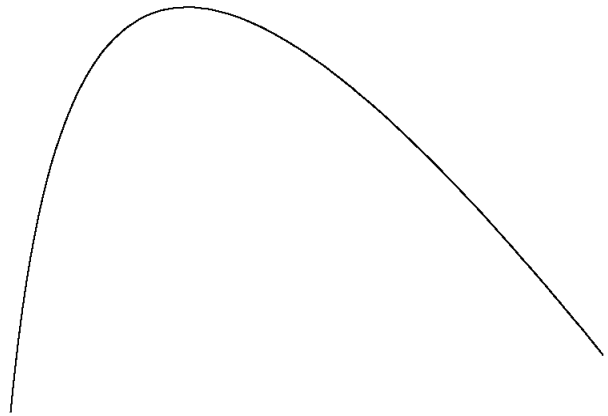
where

$$c := -\frac{\partial^2}{\partial \theta^2} \ln p^*(\theta)\big|_{\theta=\hat{\theta}}.$$

(note that first order term vanishes)



$p^*(\theta)$



$\ln p^*(\theta)$

# Laplace's Method (cont'd)

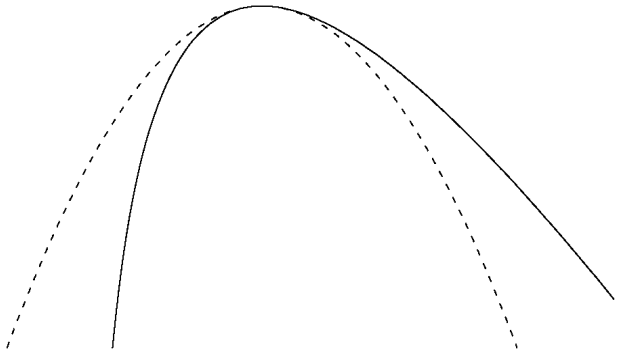
- Approximate $p^*(\theta)$ by unnormalized Gaussian

$$Q^*(\theta) := p^*(\hat{\theta}) \exp\left[-c/2 \cdot (\theta - \hat{\theta})^2\right]$$

- A normalized Gaussian would be:

$$Q(\theta \mid \mu = \hat{\theta}, \sigma^2) = \frac{1}{Z_Q} \exp\left[-\frac{(\theta - \hat{\theta})^2}{2\sigma^2}\right],$$

with $Z_Q = \sqrt{2\pi\sigma^2} = \int \exp\left[-\frac{(\theta-\hat{\theta})^2}{2\sigma^2}\right] d\theta$



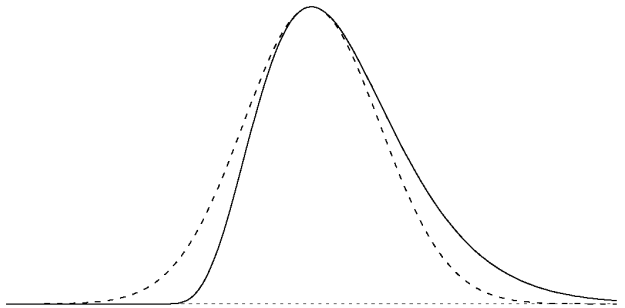
$\ln p^*(\theta)$ & $\ln Q^*(\theta)$

- Approximate $Z_p = \int p^*(\theta)\, d\theta$ by

$$Z_p \approx \int Q^*(\theta)\, d\theta$$

$$= p^*(\hat{\theta}) \int \exp\left[-c/2 \cdot (\theta - \hat{\theta})^2\right] d\theta$$

$$= p^*(\hat{\theta}) \sqrt{2\pi/c} \quad \rightsquigarrow c \text{ is the inverse variance}$$



$p^*(\theta)$ & $Q^*(\theta)$

# Laplace's Method (cont'd)

- Multivariate generalization in $d$ dimensions:
  second derivative $\rightsquigarrow$ **Hessian matrix**

$$H_{ij} = \left. \frac{\partial^2 \ln p^*(\boldsymbol{\theta})}{\partial\theta_i \partial\theta_j} \right|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

$$Z_p \approx p^*(\hat{\boldsymbol{\theta}}) \int \exp\left[-\frac{1}{2}(\boldsymbol{\theta}-\hat{\boldsymbol{\theta}})^t H (\boldsymbol{\theta}-\hat{\boldsymbol{\theta}})\right] d\boldsymbol{\theta}$$

$$= p^*(\hat{\boldsymbol{\theta}}) \sqrt{\frac{(2\pi)^d}{|H|}} = p^*(\hat{\boldsymbol{\theta}}) \left|\frac{H}{2\pi}\right|^{-\frac{1}{2}},$$

  where the last equation follows from the properties of the determinant: $|aM| = a^d |M|$ for $M \in \mathbb{R}^{d\times d}$, $a \in \mathbb{R}$.

- Another interpretation: complicated distribution $p(\boldsymbol{\theta})$ is approximated by Gaussian centered at the mode $\hat{\boldsymbol{\theta}}$:

$$p(\boldsymbol{\theta}) \approx \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\mu} = \hat{\boldsymbol{\theta}}, \Sigma = H^{-1}).$$

# Example: Bayesian logistic regression

- Linear logistic regression: model parameters are simply the weights $\boldsymbol{w}$.
- Likelihood: $p(y|\boldsymbol{x}, \boldsymbol{w}) = \text{Ber}(y|\text{sigm}(\boldsymbol{w}^t \boldsymbol{x}))$
- Unfortunately, there is no convenient conjugate prior. Let's use a standard Gaussian prior: $p(\boldsymbol{w}) = N(\boldsymbol{w}|\boldsymbol{0}, V_0)$
- Laplace's approximation of posterior:

$$p(\boldsymbol{w}|\mathcal{D}) \approx N(\boldsymbol{w}|\boldsymbol{w}^*, H^{-1})$$

$$\boldsymbol{w}^* = \arg\max J[\boldsymbol{w}], \quad J[\boldsymbol{w}] = \log \underbrace{p(y|\boldsymbol{x}, \boldsymbol{w})}_{\text{likelihood}} + \log \underbrace{p(\boldsymbol{w})}_{\text{prior}}$$

$$H = \nabla^2 J(\boldsymbol{w})\Big|_{\boldsymbol{w}^*}$$

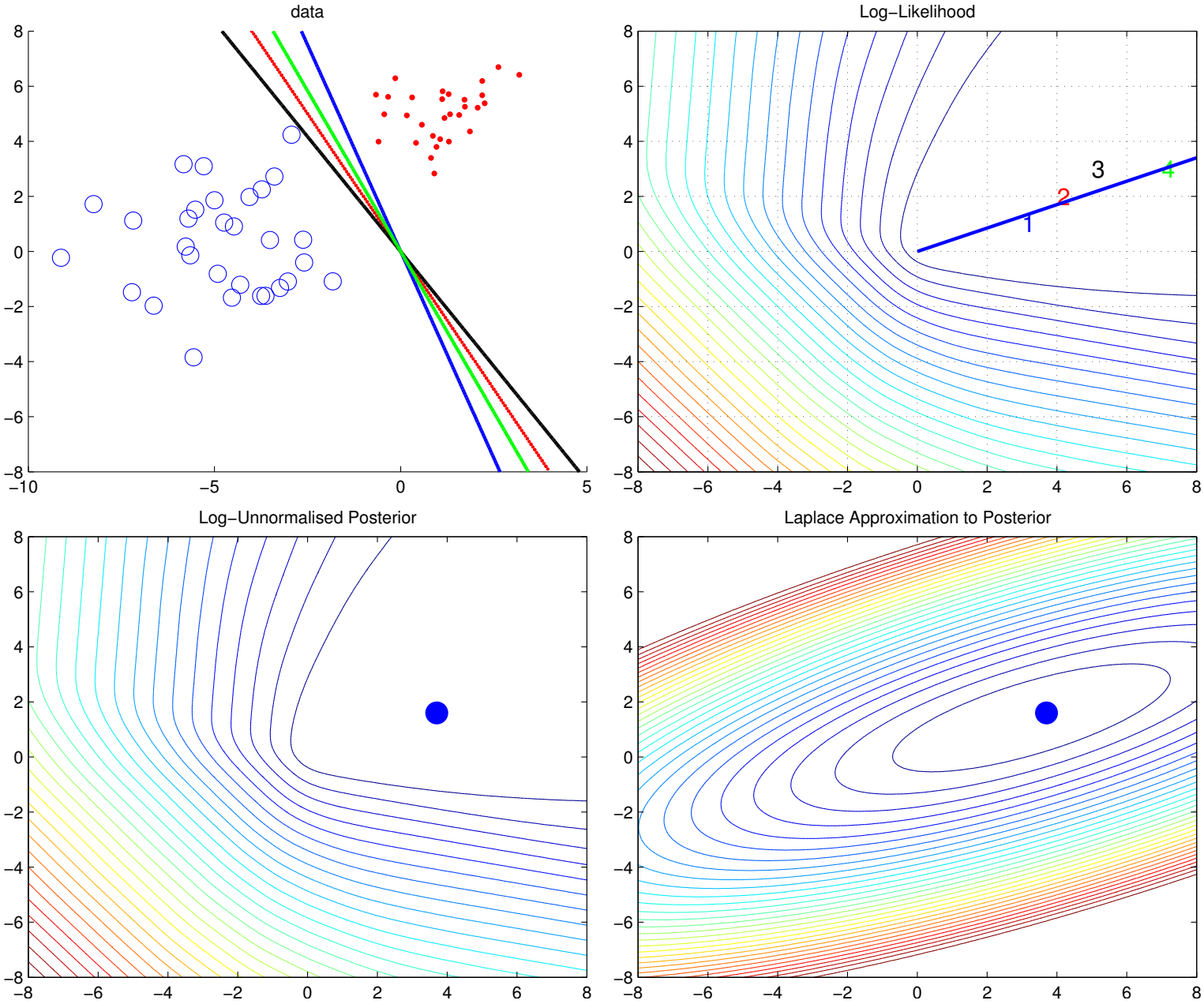



Fig 8.5 in K.Murphy

# Bayesian LOGREG: Approximating the posterior predictive

- Posterior $\rightsquigarrow$ can compute credible intervals etc.
- But in machine learning, interest usually focuses on **prediction.**
- The **posterior predictive distribution** has the form

$$p(y|\boldsymbol{x}, \mathcal{D}) = \int p(y|\boldsymbol{x}, \boldsymbol{w}) p(\boldsymbol{w}|\mathcal{D}) \, d\boldsymbol{w}.$$

  Here (and in most cases), this integral is intractable.
- The simplest approximation is the plug-in approximation

$$p(y = 1|\boldsymbol{x}, \mathcal{D}) \approx p(y = 1|\boldsymbol{x}, \boldsymbol{w}^*)$$

- But such a plug-in estimate underestimates the uncertainty.
- Better: **Monte Carlo approximation**

$$p(y|\boldsymbol{x}, \mathcal{D}) \approx \frac{1}{S} \sum_{s=1}^{S} \text{sigm}((\boldsymbol{w}^s)^t \boldsymbol{x}),$$

  where $\boldsymbol{w}^s \sim p(\boldsymbol{w}|\mathcal{D})$ are samples from the Gaussian approximation to the posterior.

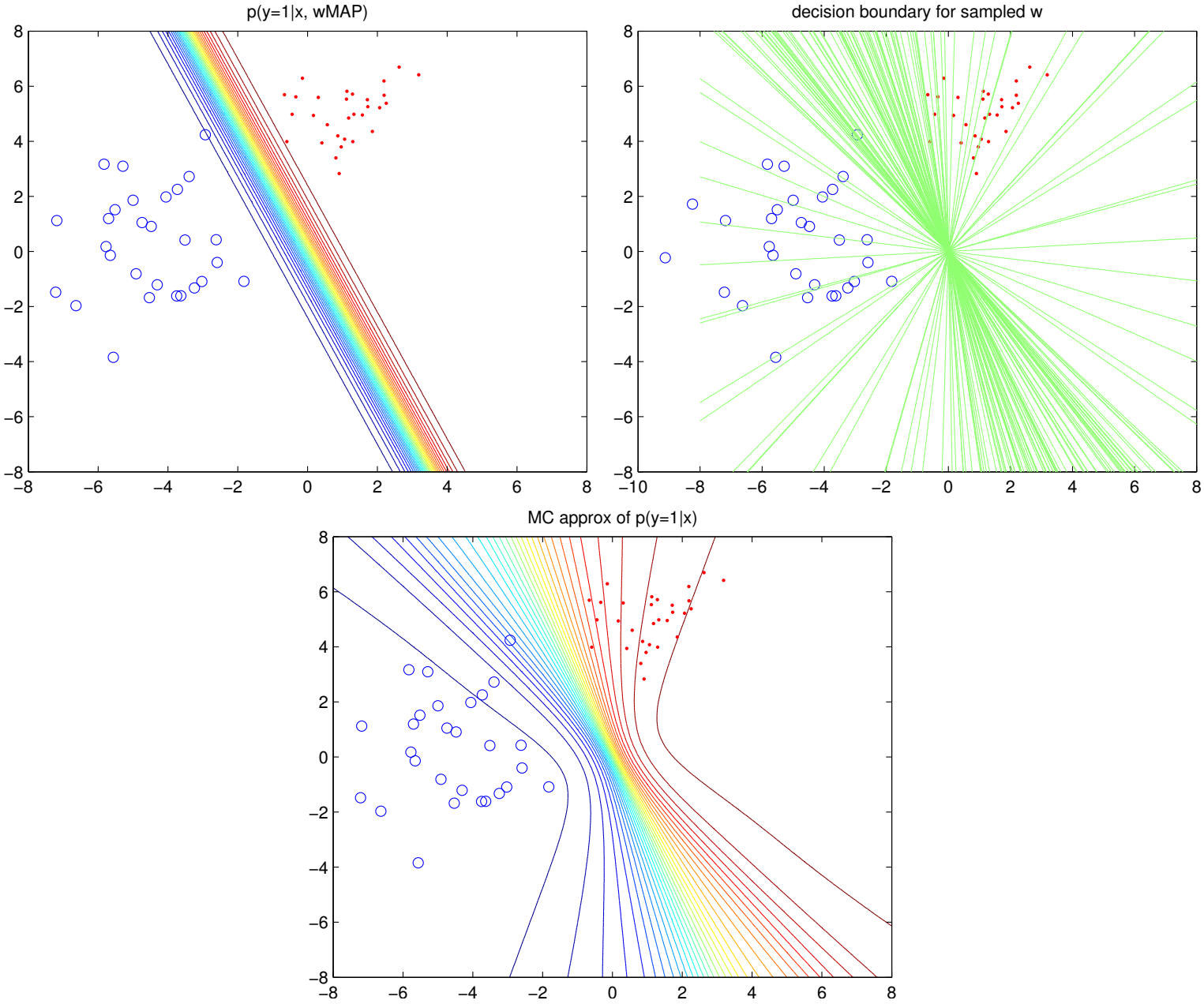



Fig 8.6 in K.Murphy

# Approximating the marginal likelihood

$$
\begin{aligned}
p(\mathcal{D}|\mathcal{F}) &= \int p(\mathcal{D}|\boldsymbol{\theta}) \cdot p(\boldsymbol{\theta}|\mathcal{F}) d\boldsymbol{\theta} \\
&\approx p(\mathcal{D}|\boldsymbol{\theta}^*) \cdot p(\boldsymbol{\theta}^*|\mathcal{F}) |H/(2\pi)|^{-\frac{1}{2}} \overset{\text{flat prior}}{\approx} p(\mathcal{D}|\hat{\boldsymbol{\theta}}) |H/(2\pi)|^{-\frac{1}{2}} \\
\log p(\mathcal{D}|\mathcal{F}) &\approx \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}) - \frac{1}{2} \log |H| + C, \quad \text{with} \quad \hat{\boldsymbol{\theta}} = \boldsymbol{\theta}_{MLE} \text{ in } \mathcal{F}.
\end{aligned}
$$

- Focus on last term:

$$H = \sum_{i=1}^{n} H_i, \quad \text{with} \quad H_i = \nabla_{\boldsymbol{\theta}} \nabla_{\boldsymbol{\theta}} \log p(\mathcal{D}_i|\boldsymbol{\theta}).$$

  Let's approximate each $H_i$ with a **fixed** matrix $H'$

$$\log |H| = \log |nH'| = \log(n^d |H'|) = d \log n + \log(|H'|).$$

- For model selection, last term can be dropped, because it is independent of $\mathcal{F}$ and $n$.

$$\log p(\mathcal{D}|\mathcal{F}) \approx \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}) - \frac{d}{2} \log n + C = \text{BIC}(\mathcal{F}, n|\mathcal{D}) + C.$$

# Intuitive interpretation of BIC

- The **Shannon information content** of a specific outcome $a$ of a random experiment is

$$h(a) = -\log_2 P(a) = \log \frac{1}{P(a)}.$$

It measures the "surprise" (in bits):
**Outcomes that are less probable have larger values of surprise.**

- **Information theory:** Can find a code so that the **number of bits** used to encode each symbol $a \in \mathcal{A}$ is essentially $-\log_2 P(a)$.
- Here:

$$-\text{BIC}(\mathcal{F}, n|\mathcal{D}) = \overbrace{\sum_{i=1}^{n} \left( \underbrace{-\log_2 p(y_i|\boldsymbol{x}_i, \hat{\boldsymbol{w}})}_{\text{surprise of } y_i} \right)}^{\text{DL of observations given model}} + \frac{d}{2} \log_2(n)$$

- The sum of surprises of all observations is the **description length** of the observations given the (most probable) model in $\mathcal{F}$.

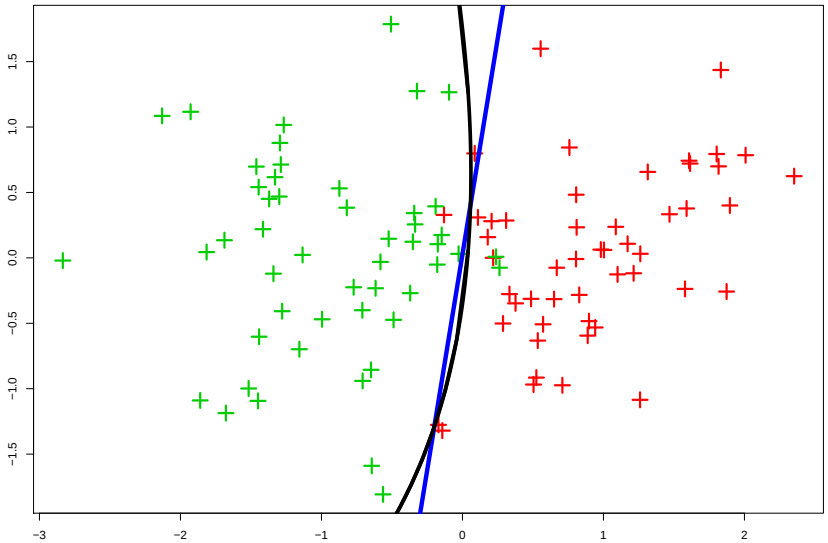
# Intuitive interpretation of BIC

- Second term: description length of the model. Intuitive explanation:
  - The model, i.e. $\hat{\boldsymbol{w}} \in \mathbb{R}^d$, was estimated based on $n$ samples.
  - Can quantize every component into $\sqrt{n}$ levels. Why?
  - Remember the **standard parametric rate:**
    $1/\sqrt{n}$ represents the magnitude of the estimation error
    $\rightsquigarrow$ **no need for encoding with greater precision.**
  - Grid of $(\sqrt{n})^d$ possible values for describing a model.
  - We need $\log_2((\sqrt{n})^d) = \log_2 n^{(d/2)} = (d/2)\log_2 n$ bits to encode $\hat{\boldsymbol{w}}$.
- In summary: -BIC = DL(data|model) + DL(model).
- Maximizing BIC = minimizing joint DL of data and model
  $\rightsquigarrow$ **Minimum Description Length principle.**

# Example: Bayesian logistic regression

Example: polynomial logistic regression, $n = 100$.
$\phi_1(\boldsymbol{x}) = (1, x_1, x_2)^t$, $\phi_2(\boldsymbol{x}) = (1, x_1, x_2, (x_1 + x_2)^2)^t$.

$$-\text{BIC} = \sum_{i=1}^{n} (-\log_2 p(y_i|\boldsymbol{x}_i, \hat{\boldsymbol{w}})) + \frac{d}{2} \log_2(n)$$

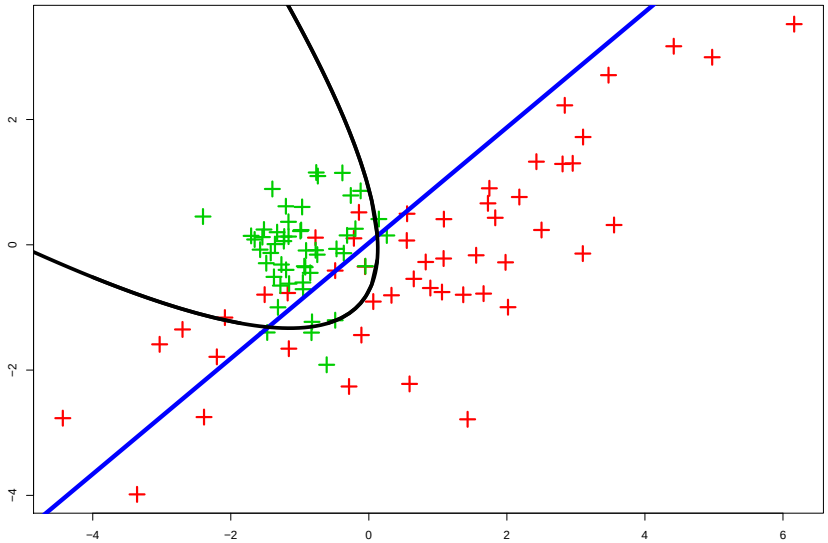


| degree | #(param) | DL(data) | DL(model) | BIC score |
|---|---|---|---|---|
| 1 | 3 | 16.36 bits | 9.97 bits | **-26.33** |
| 2 | 4 | 15.77 bits | 13.29 bits | -29.06 |

# Example: Bayesian logistic regression

Example: polynomial logistic regression, $n = 100$.
$\phi_1(\boldsymbol{x}) = (1, x_1, x_2)^t$, $\phi_2(\boldsymbol{x}) = (1, x_1, x_2, (x_1 + x_2)^2)^t$.

$$-\text{BIC} = \sum_{i=1}^{n} (-\log_2 p(y_i|\boldsymbol{x}_i, \hat{\boldsymbol{w}})) + \frac{d}{2} \log_2(n)$$




| degree | #(param) | DL(data) | DL(model) | BIC score |
|---|---|---|---|---|
| 1 | 3 | 58.56 bits | 9.97 bits | -68.53 |
| 2 | 4 | 38.05 bits | 13.29 bits | **-51.34** |

Subsection 3

## Sparse models

# Sparse Models

- Sometimes, we have many more dimensions $d$ than training cases $n$.
- Corresponding design matrix $X$ is "short and fat", rather than "tall and skinny".
- This is called **small $n$ , large $d$ problem**.
- For example, with **gene microarrays**, it is common to measure the expression levels of $d \approx 20,000$ genes, but to only get $n \approx 100$ samples (for instance, from 100 patients).
- Q: what is the **smallest set of features** that can accurately predict the response in order to **prevent overfitting**, to **reduce the cost** of building a diagnostic device, or to help with **scientific insight** into the problem?

# Bayesian variable selection

- Let $\gamma_j = 1$ if feature $j$ is **relevant**, and let $\gamma_j = 0$ otherwise.
- Our goal is to compute the posterior over models

$$p(\boldsymbol{\gamma}|\mathcal{D}) = \frac{\exp(-f(\boldsymbol{\gamma}))}{\sum_{\boldsymbol{\gamma}'} \exp(-f(\boldsymbol{\gamma}'))},$$

  where $f(\boldsymbol{\gamma})$ is the cost function:

$$f(\boldsymbol{\gamma}) = -[\log p(\mathcal{D}|\boldsymbol{\gamma}) + \log p(\boldsymbol{\gamma})].$$

- For example, suppose we generate $n = 20$ samples from a $d = 10$ dimensional linear regression model, $y_i \sim N(w^t x_i, \sigma^2)$, in which $K = 5$ elements of $w$ are non-zero.
- Enumerate all $2^{10} = 1024$ models and compute $p(\boldsymbol{\gamma}|\mathcal{D})$ for each one.

# Bayesian variable selection

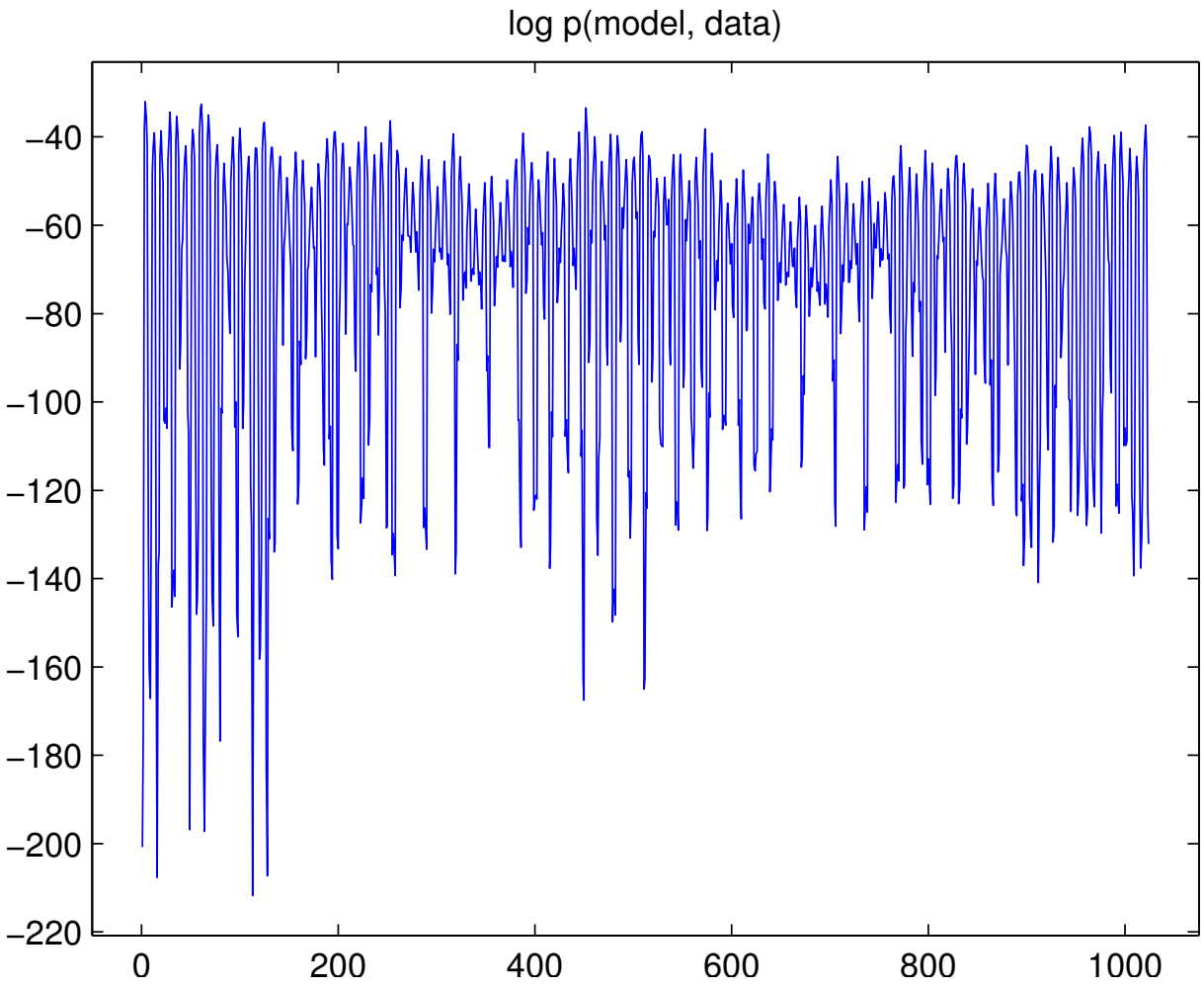



Fig 13.1 in K. Murphy: Score function $f(\gamma)$ for all possible models.

# Bayesian variable selection

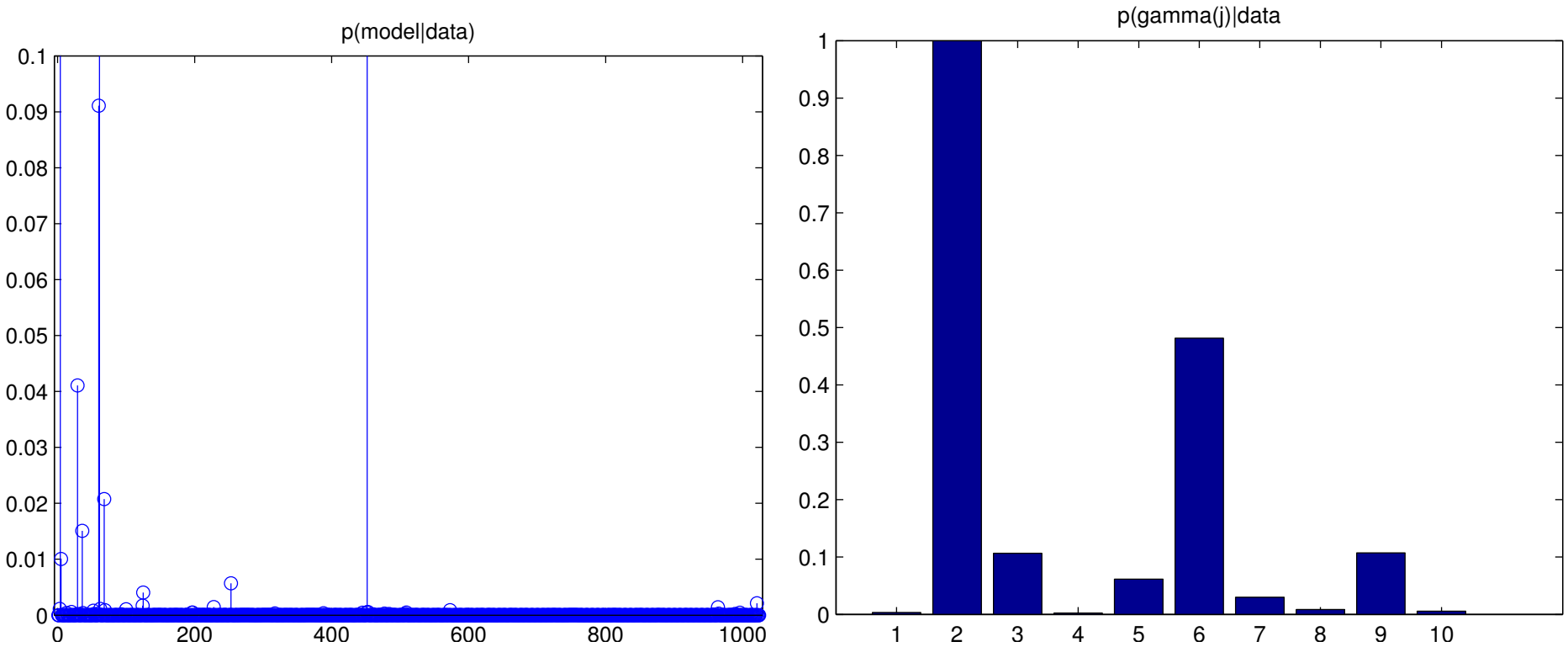



Fig 13.1 in K. Murphy. Left: Posterior over all 1024 models. Vertical scale has been truncated at 0.1 for clarity. Right: Marginal inclusion probabilities $p(\gamma_j = 1|\mathcal{D})$. The true model is $\{2, 3, 6, 8, 9\}$

# Bayesian variable selection

- Interpreting the posterior over a large number of models is difficult $\rightsquigarrow$ seek **summary statistics**.
- A natural one is the **posterior mode**, or MAP estimate

$$\hat{\boldsymbol{\gamma}} = \arg\max p(\boldsymbol{\gamma}|\mathcal{D}) = \arg\min f(\boldsymbol{\gamma}).$$

- However, the mode is often not representative of the full posterior mass. A better summary is the **median model**, computed using

$$\hat{\boldsymbol{\gamma}} = \{j : p(\gamma_j = 1|\mathcal{D}) > 0.5\}$$

This requires computing the **posterior marginal inclusion probabilities** $p(\gamma_j = 1|\mathcal{D})$.

# Bayesian variable selection

- The above example illustrates the **gold standard** for variable selection: the problem was small ($d = 10$)
  $\rightsquigarrow$ we were able to **compute the full posterior exactly**.
- Of course, variable selection is most useful in the cases where the number of dimensions is **large**.
- There are $2^d$ possible models (bit vectors) $\rightsquigarrow$ **impossible** to compute the full posterior in general.
- Even finding summaries (MAP, or marginal inclusion probabilities) is **intractable**
  $\rightsquigarrow$ **algorithmic speedups** necessary.
- But first, focus on the computation of $p(\boldsymbol{\gamma}|\mathcal{D})$.

# The spike and slab model

- The posterior is given by

$$p(\boldsymbol{\gamma}|\mathcal{D}) \propto p(\boldsymbol{\gamma})p(\mathcal{D}|\boldsymbol{\gamma})$$

- It is common to use the following prior:

$$\begin{aligned} p(\boldsymbol{\gamma}) &= \prod_{j=1}^{d} Ber(\gamma_j|\pi_0) = \pi_0^{\|\boldsymbol{\gamma}\|_0}(1-\pi_0)^{d-\|\boldsymbol{\gamma}\|_0}, \\ \log p(\boldsymbol{\gamma}|\pi_0) &= -\lambda\|\boldsymbol{\gamma}\|_0 + const., \end{aligned}$$

where $\pi_0$ is the probability that a feature is relevant, and $\|\boldsymbol{\gamma}\|_0 = \sum_{j=1}^{d} \gamma_j$ is the $\ell_0$ pseudo-norm, i.e., the **number of non-zero elements**.

- $\lambda = \log \frac{1-\pi_0}{\pi_0}$ controls the **sparsity** of the model.
- Setting $\sigma^2 = 1$, we can write the likelihood as follows:

$$p(\mathcal{D}|\boldsymbol{\gamma}) = p(\boldsymbol{y}|X, \boldsymbol{\gamma}) = \int p(\boldsymbol{y}|X, \boldsymbol{w}, \boldsymbol{\gamma})p(\boldsymbol{w}|\boldsymbol{\gamma})\, d\boldsymbol{w}$$

# The spike and slab model

- Prior $p(\boldsymbol{w}|\boldsymbol{\gamma})$. If $\gamma_j = 0$, feature $j$ is **irrelevant**, so we expect $w_j = 0$. If $\gamma_j = 1$, we expect $w_j$ to be non-zero.
- Standardized inputs $\rightsquigarrow$ reasonable **prior** is $N(0, \sigma_w^2)$, where $\sigma_w^2$ reflects our expectation of the coefficients associated with the **relevant variables**:

$$p(w_j|\gamma_j) = \begin{cases} \delta_0(w_j) & , \text{ if } \gamma_j = 0 \\ N(w_j|0, \sigma_w^2) & , \text{ else} \end{cases}$$

- The first term is a **spike** at the origin.
- As $\sigma_w^2 \to \infty$, the distribution $p(w_j|\gamma_j = 1)$ approaches a **uniform** distribution $\rightsquigarrow$ **slab** of constant height.
- **Spike and slab model** (Mitchell and Beauchamp 1988).
- Full Bayesian treatment is computationally challenging!

# Simplifying the model

- Assume $\sigma_w^2 \to \infty$ ($\rightsquigarrow$ uniform prior $p(w_j|\gamma_j)$ over nonzero components) and approximate the likelihood using **BIC**:

$$\log p(\mathcal{D}|\gamma) = \int p(\boldsymbol{y}|X, \boldsymbol{w}, \gamma) p(\boldsymbol{w}|\gamma)\, d\boldsymbol{w}$$

$$\approx \log p(\boldsymbol{y}|X, \hat{\boldsymbol{w}}_\gamma) - \frac{1}{2} \underbrace{\|\hat{\boldsymbol{w}}_\gamma\|_0}_{\text{degrees of freedom}} \log n,$$

  where $\hat{\boldsymbol{w}}_\gamma$ is the ML estimate.

- Another view of this model: minimize the negative log likelihood under a $\ell_0$ constraint (or penalty in the Lagrangian form)

$$\text{minimize} \quad -\log p(\boldsymbol{y}|X, \boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_0.$$

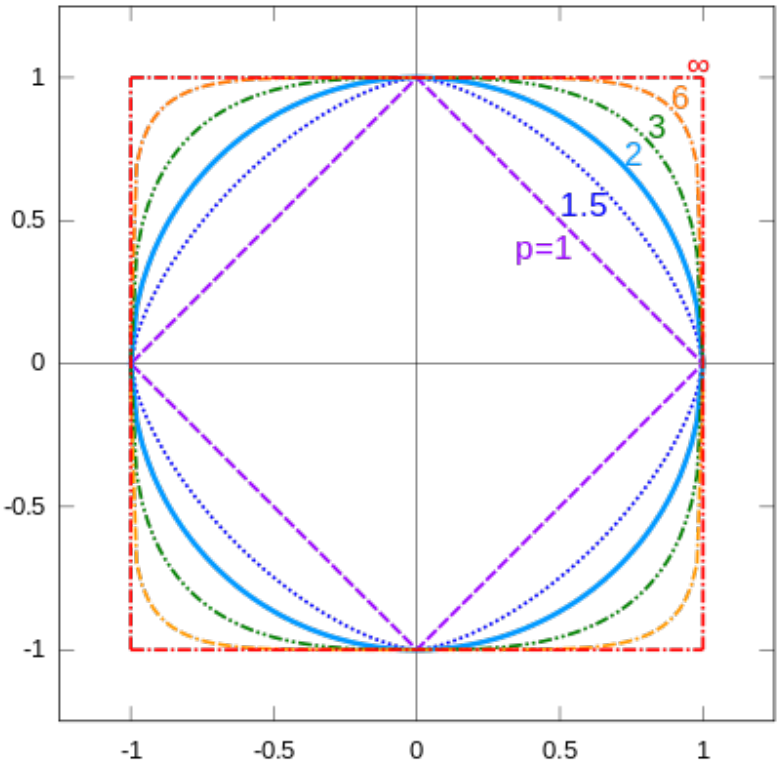
- Practical problem: $\ell_0$ is highly non-convex!

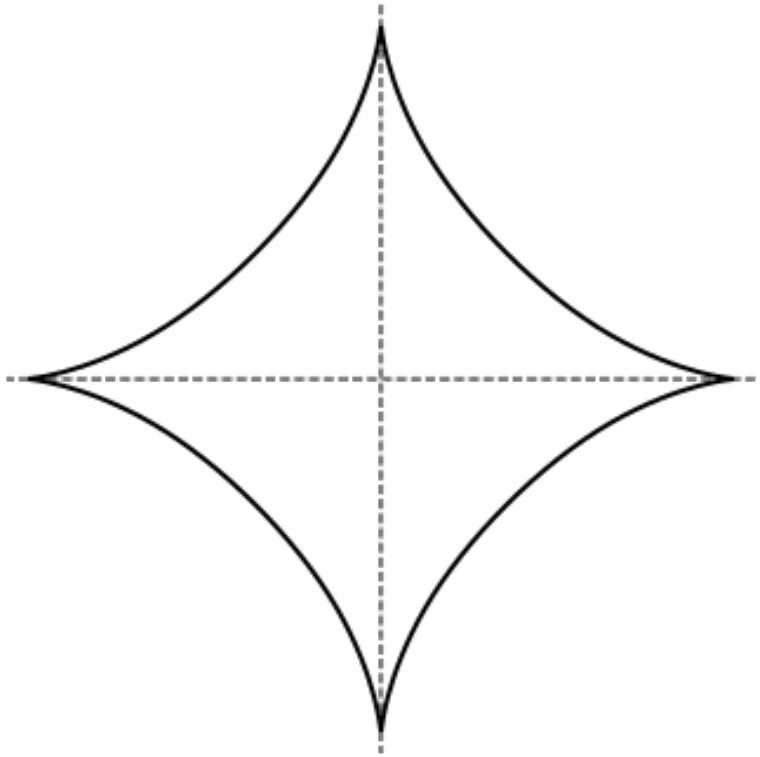
# Vector norms

The **vector $p$-norms ($\ell_p$ norms)** are defined by

$$\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}, \quad 1 \le p \le \infty,$$

$$\|\boldsymbol{x}\|_\infty = \max(|x_1|, \cdots |x_n|).$$



# Simplifying the model further

- When we have many variables, it is computationally difficult to find the posterior mode
- Idea: replace discrete variables with continuous ones. Use continuous priors that "encourage" $w_j = 0$ by putting a lot of probability density near the origin, such as a zero-mean Laplace distribution.

$$p(\boldsymbol{w}|\lambda) = \prod_{j=1}^{d} Lap(w_j|0, 1/\lambda) \propto \prod_{j=1}^{d} \exp(-\lambda|w_j|)$$

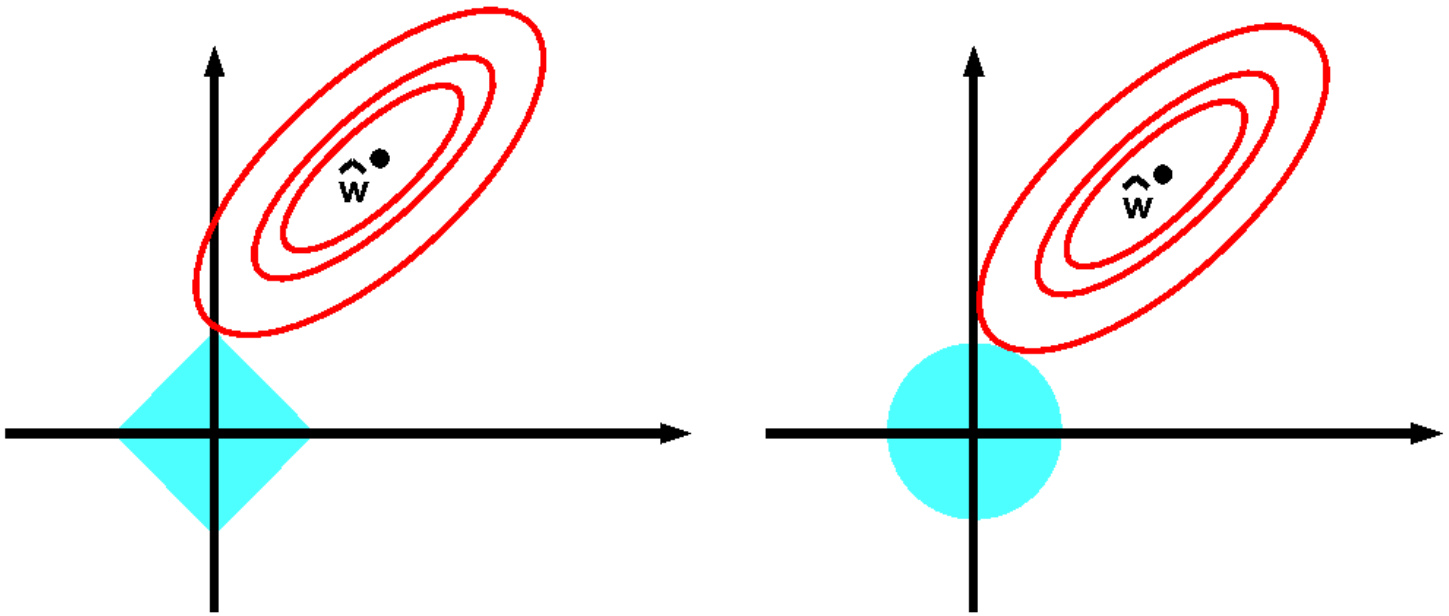
- Let us perform MAP estimation with this prior:

$$f(\boldsymbol{w}) = -\log p(\mathcal{D}|\boldsymbol{w}) - \log p(\boldsymbol{w}|\lambda) = NLL(\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_1.$$

where $\|\boldsymbol{w}\|_1 = \sum_{j=1}^{d} |w_j|$ is the $\ell_1$ norm of $\boldsymbol{w}$ and $NNL$ means **negative log-likelihood**.

# The Lasso

- For suitably large $\lambda$, the estimate $\hat{\boldsymbol{w}}$ will be sparse.
- Can be thought of as a convex approximation to the non-convex $\ell_0$ objective.
- This model has the colorful name **least absolute shrinkage and selection operator**.
- For linear regression, $NLL(\boldsymbol{w}) = RSS(\boldsymbol{w})$, a.k.a. **basis pursuit denoising** (Chen et al. 1998).



# The Lasso

- Unfortunately, the $\|\boldsymbol{w}\|_1$ term is not differentiable at 0
  $\rightsquigarrow$ non-smooth optimization problem.
- The **subderivative or subgradient** of a (convex) function $f : \mathcal{I} \to \mathbb{R}$ at a point $x_0$ is a scalar $c$ such that

$$f(x) - f(x_0) \geq c(x - x_0), \ \forall x \in \mathcal{I}$$

where $\mathcal{I}$ is some interval containing $x_0$.
Note that $c$ is a **linear lower bound** to $f$ at $x_0$.

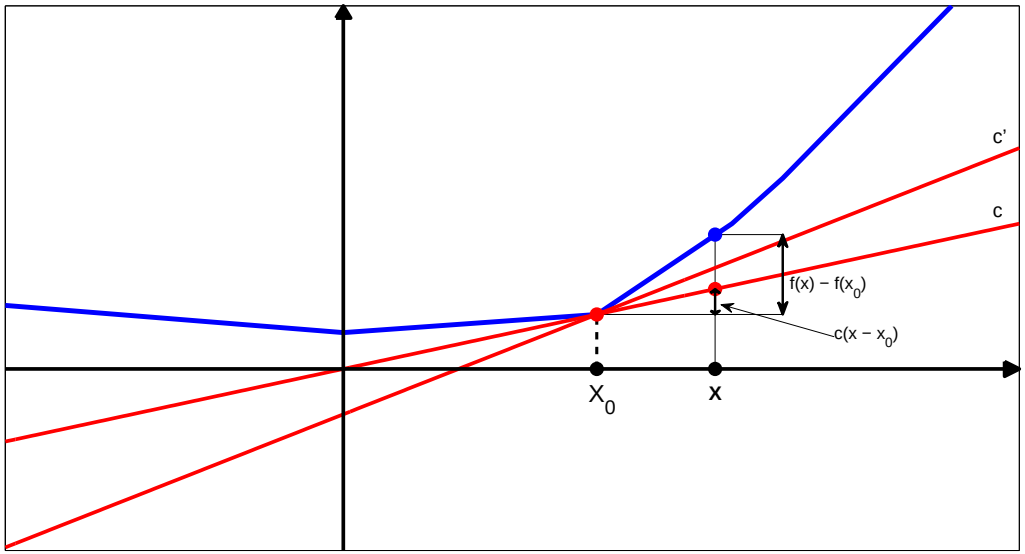



Fig. 13.4 in (K. Murphy)

# The Lasso

- The set of all subderivatives is called the **subdifferential**
- For the **absolute value function** $f(x) = |x|$:

$$\partial f(x) = \begin{cases} -1 & , \text{ if } x < 0 \\ [-1, 1] & , \text{ if } x = 0 \\ +1 & , \text{ if } x > 0 \end{cases}$$

- For least-squares regression, it is easy to show that

$$\begin{aligned} \frac{\partial}{\partial w_j} RSS(\boldsymbol{w}) &= a_j w_j - c_j \\ a_j &= 2 \sum_{i=1}^{n} x_{ij}^2 \\ c_j &= 2 \sum_{i=1}^{n} x_{ij} (y_i - \boldsymbol{w}_{-j}^t \boldsymbol{x}_{i,-j}). \end{aligned}$$

where $\boldsymbol{w}_{-j}$ is $\boldsymbol{w}$ without component $j$.

# The Lasso

- $c_j$ is (proportional to) the correlation between the $j$'th feature $\boldsymbol{x}_j$ and the residual due to other features, $r_{-j} = y - \boldsymbol{x}_{-j}^t \boldsymbol{w}_{-j}$.
- The magnitude of $c_j$ is an indication of **how relevant** feature $j$ is for predicting $y$.
- Adding the $\ell_1$ penalty term:

$$\begin{aligned}
\partial_{w_j} f(\boldsymbol{w}) &= (a_j w_j - c_j) + \lambda \partial_{w_j} \|\boldsymbol{w}\|_1 \\
&= \begin{cases} a_j w_j - c_j - \lambda & , \text{if } w_j < 0 \\ [-c_j - \lambda, -c_j + \lambda] & , \text{if } w_j = 0 \\ a_j w_j - c_j + \lambda & , \text{if } w_j > 0 \end{cases}
\end{aligned}$$

# The Lasso

- Depending on the value of $c_j$, the solution to $\partial_{w_j} f(\boldsymbol{w}) = 0$ can occur at 3 different values of $w_j$:

$$\hat{w}_j = \begin{cases} (c_j + \lambda)/a_j & , \text{ if } c_j < -\lambda \\ 0 & , \text{ if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j & , \text{ if } c_j > \lambda \end{cases}$$

- We can write this as follows:

$$\hat{w}_j = \text{soft}\left(\frac{c_j}{a_j}; \frac{\lambda}{a_j}\right),$$

where $\text{soft}(a; \delta) = \text{sign}(a)(|a| - \delta)_+$ and $x_+ = \max(x, 0)$ is the positive part of $x$.

- This is called **soft thresholding.**

# The Lasso

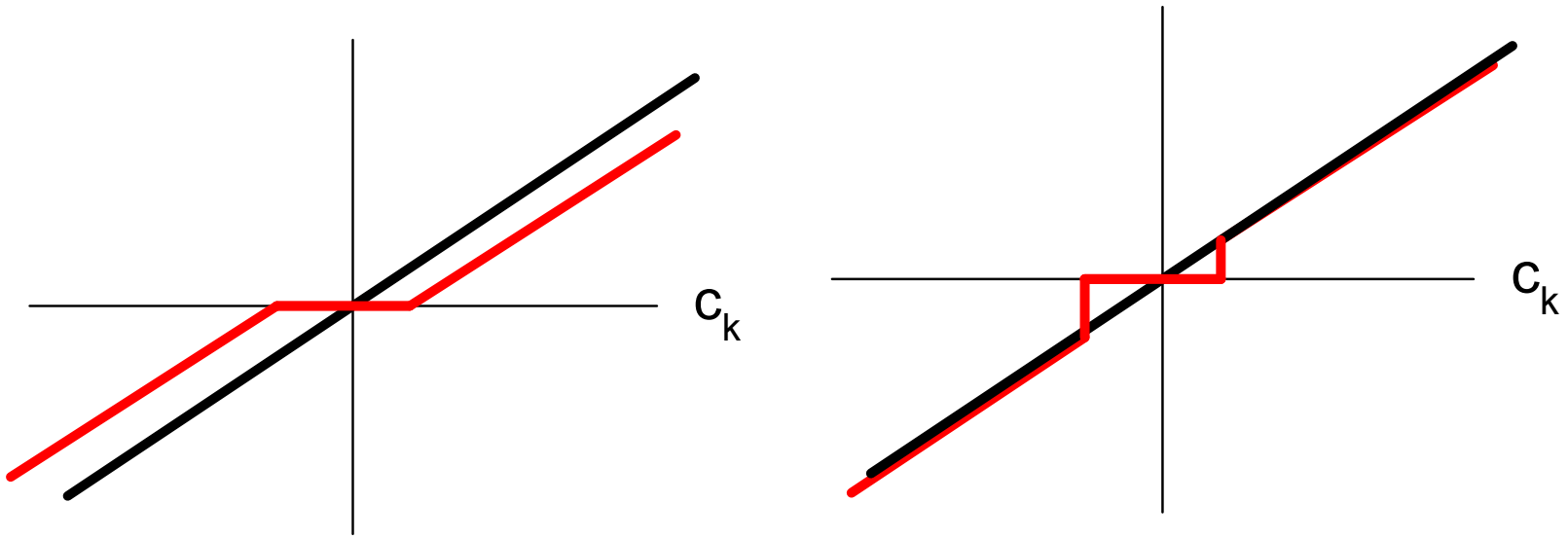



Fig. 13.5 in (K. Murphy). Black line: **Least squares fit** $w_k = c_k/a_k$.
The red line (the regularized estimate) $\hat{w}_k(c_k)$, shifts the black line down (or up) by $\lambda$, except when $-\lambda \leq c_k \leq \lambda$, in which case it sets $w_k = 0$.
By contrast, **hard thresholding** sets values of $w_k$ to 0 if $-\lambda \leq c_k \leq \lambda$,
but it **does not shrink the values of $w_k$ outside of this interval.**

# Lasso Algorithms: Coordinate-wise Descent

Sometimes it is hard to optimize all variables simultaneously, but it is easy to optimize them one by one.
Can solve for $j$-th coefficient $w_j$ with all other coefficients held fixed:

$$\hat{w}_j = \arg\min_z f(\boldsymbol{w} + z\boldsymbol{e}_j),$$

where $\boldsymbol{e}_j$ is the $j$-th unit vector. Cycle (potentially many times) through these component-wise updates:
**for** $j = 1, \ldots, d$ **do:**

$$\begin{aligned} a_j &= 2\sum_{i=1}^{n} x_{ij}^2 \\ c_j &= 2\sum_{i=1}^{n} x_{ij}(y_i - \boldsymbol{w}_{-j}^t \boldsymbol{x}_{i,-j}) \\ w_j &= \text{soft}\left(\frac{c_j}{a_j}; \frac{\lambda}{a_j}\right). \end{aligned}$$