Advanced probabilistic methods

Lecture 4: Sparse Bayesian linear models

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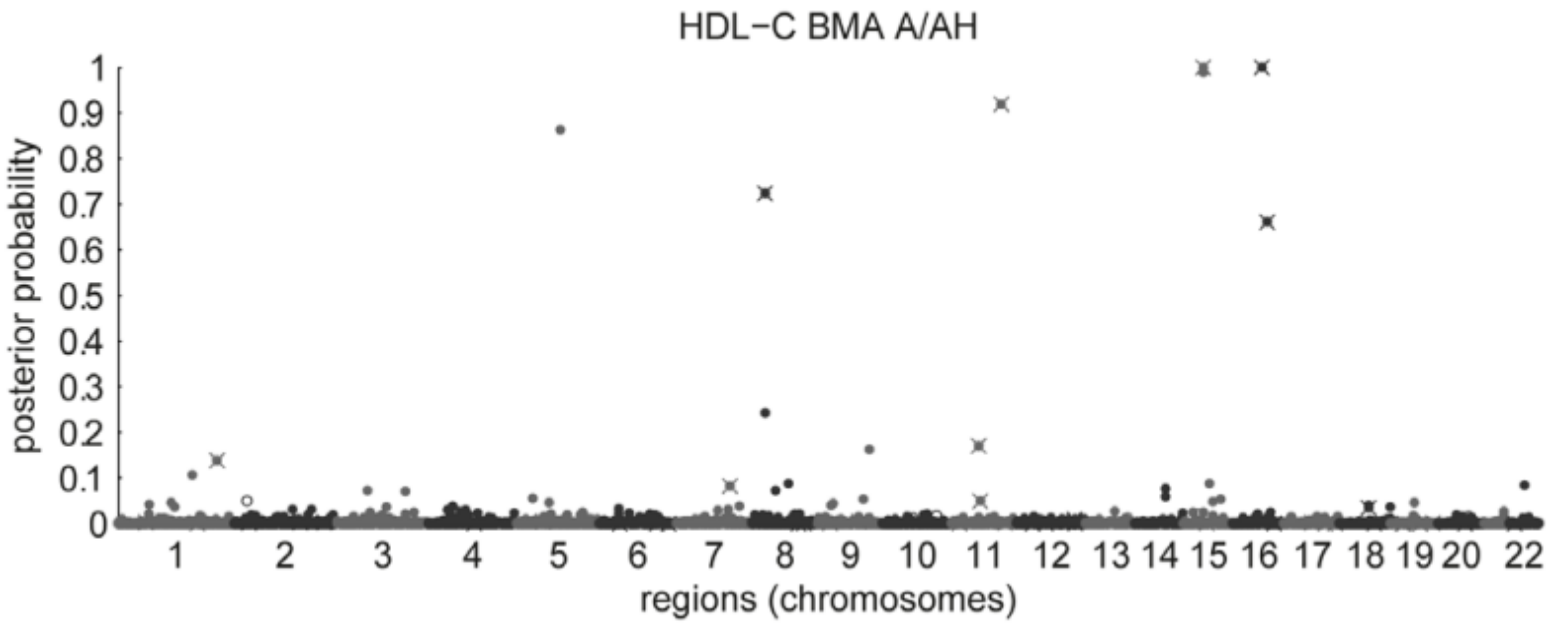
Lecture 4 overview[1]

- Bayesian Linear Parameter Models (LPMs)
  - Posterior computation (given fixed hyperparameters)
  - Determining hyperparameters
  - Example using radial basis functions
- Logistic regression for classification
  - Laplace approximation
- Barber, Ch. 18

[1] These slides build upon the book *Bayesian Reasoning and Machine Learning* and the associated teaching materials. The book and the demos can be downloaded from *www.cs.ucl.ac.uk/staff/D.Barber/brml.*

Example: genetic association studies

- Analysis of $\sim 1,000,000$ genetic polymorphisms in $\sim 50,000$ genomic regions (Peltola et al., 2012, *PLoS ONE*).
- *Spike-and-slab* prior on regression weights



Regression with Gaussian noise

- **Data** $\mathcal{D} = \{(\mathbf{x}_i, y_i), i = 1, \ldots, N\}$
  - $\mathbf{x}_i$: the input
  - y_i: the output
- **Model**:

$$y = \underbrace{f(\mathbf{w}, \mathbf{x})}_{\text{clean output}} + \underbrace{\eta}_{\text{noise}}, \quad \eta \sim N(0, \beta^{-1})$$

- In the simplest case

$$\begin{aligned} f(\mathbf{w}, \mathbf{x}) &= \mathbf{w}^T \mathbf{x} \\ &= w_1 x_1 + \ldots + w_D x_D \end{aligned}$$

- The *parameters* w_i are also called the *weights*

Bayesian linear parameter models

- A prior distribution $p(\mathbf{w}|\alpha)$ is placed on the weights $\mathbf{w}$.
- The posterior distribution $p(\mathbf{w}|\mathcal{D}, \Gamma)$ can be computed, and reflects the uncertainty of the parameters.

Prior distribution

- A Gaussian prior distribution may placed on $\mathbf{w}$:

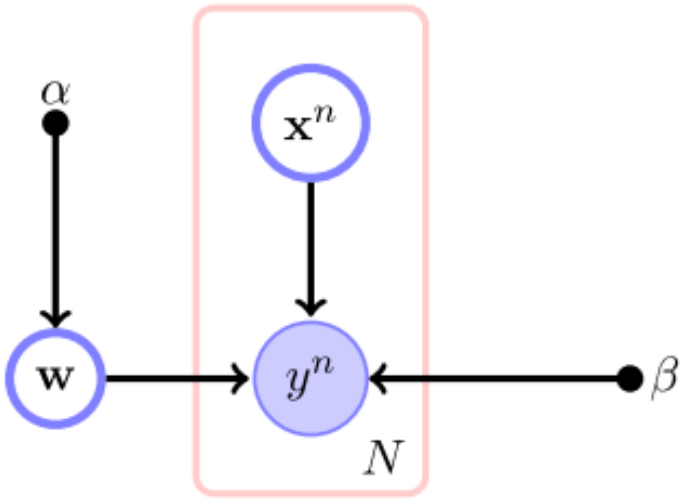
$$p(\mathbf{w}|\alpha) = N(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$$

$$= \prod_{i=1}^{D} N(w_i|0, \alpha^{-1}) = \left(\frac{\alpha}{2\pi}\right)^{\frac{D}{2}} e^{-\frac{\alpha}{2}\sum_i w_i^2}$$

- Posterior

$$\log p(\mathbf{w}|\Gamma, \mathcal{D}) = -\frac{\beta}{2}\sum_{i=1}^{N}\left[y_i - \mathbf{w}^T\mathbf{x}_i\right]^2 - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const}$$

Hyperparameters



- α: *precision* of the *regression weights*
  - determines the amount of regularization
  - large precision $\longrightarrow$ small variance $\longrightarrow$ weights are close to zero
- β: *precision* of the noise
- $\Gamma = \{\alpha, \beta\}$ are called the **hyperparameters** (in the course book...)

Posterior distribution

- Posterior distribution is obtained by completing the square (left as an exercise):

$$p(\mathbf{w}|\Gamma, \mathcal{D}) = N(\mathbf{w}|\mathbf{m}, S)$$

where

$$S = \left(\alpha I + \beta \sum_{i=1}^{N} \mathbf{x}_i {\mathbf{x}_i}^T\right)^{-1}, \qquad \mathbf{m} = \beta S \sum_{i=1}^{N} y_i \mathbf{x}_i$$

- Mean prediction

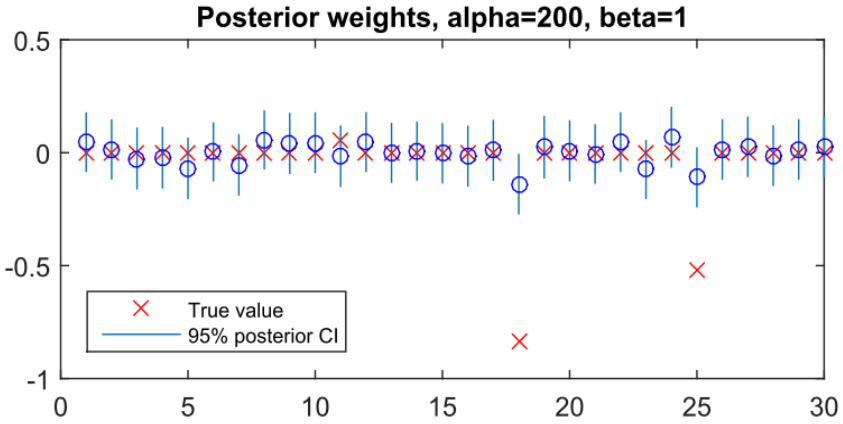
$$\widetilde{y} = \int \mathbf{w}^T \mathbf{x} \times p(\mathbf{w}|\Gamma, \mathcal{D}) d\mathbf{w} = \mathbf{m}^T \mathbf{x}$$

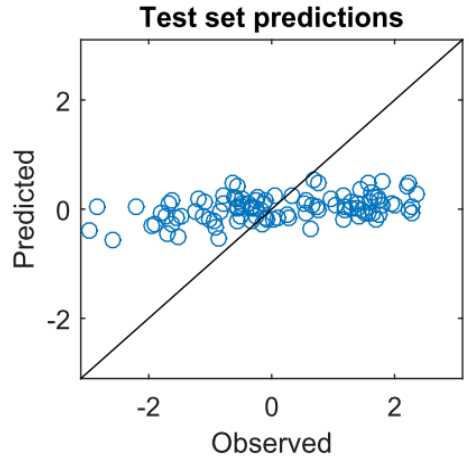
Example, impact of hyperparameters (1/3)

- Setup: simulate $y = \mathbf{w}_{true}^T \mathbf{x} + \epsilon$, where $\epsilon \sim N(0, \beta^{-1})$ and $\beta = 1$
- The goal is to investigate how hyperparameter α affects the posterior distribution of the parameters $\mathbf{w}$

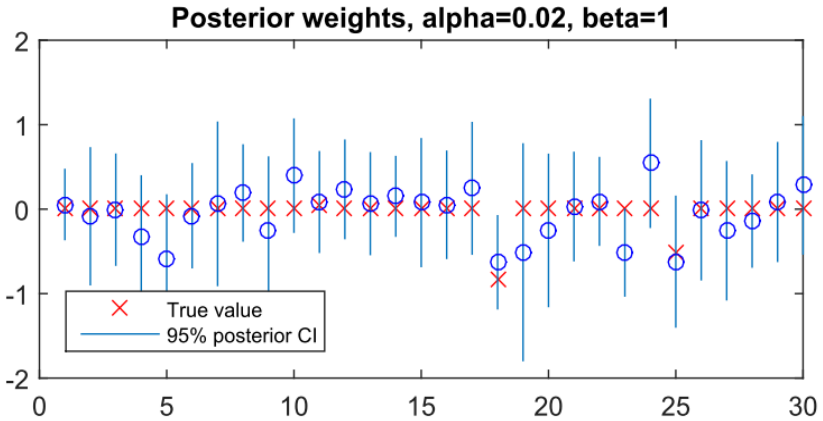
Example, impact of hyperparameters (2/3)

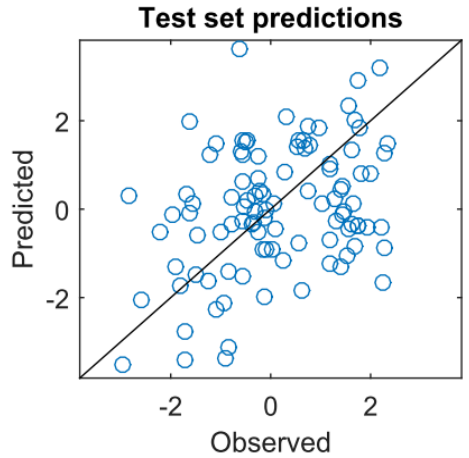
- Too large α, $Var(y - \widetilde{y}) = 1.54$ (Original $Var(y) = 1.75$)





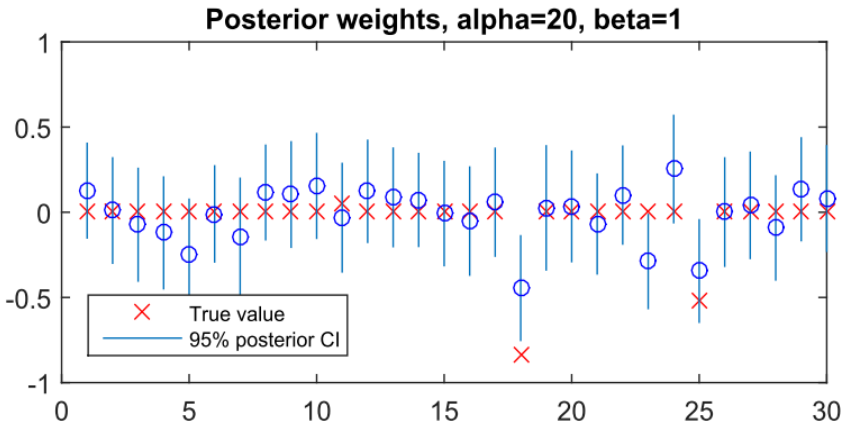
- Too small α, $Var(y - \widetilde{y}) = 2.48$

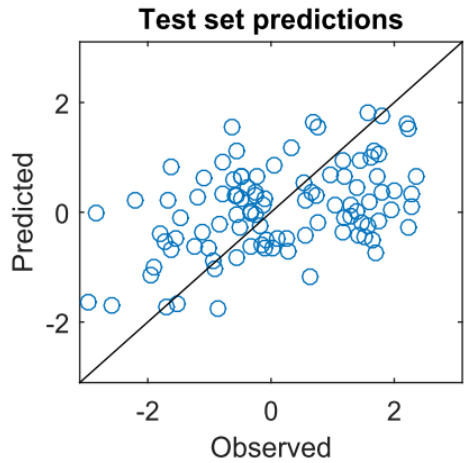




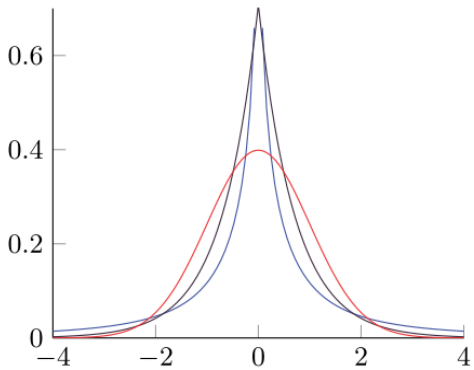
Example, impact of hyperparameters (3/3)

- About good α, $Var(y - \widetilde{y}) = 1.46$
- A compromise between bias and variance



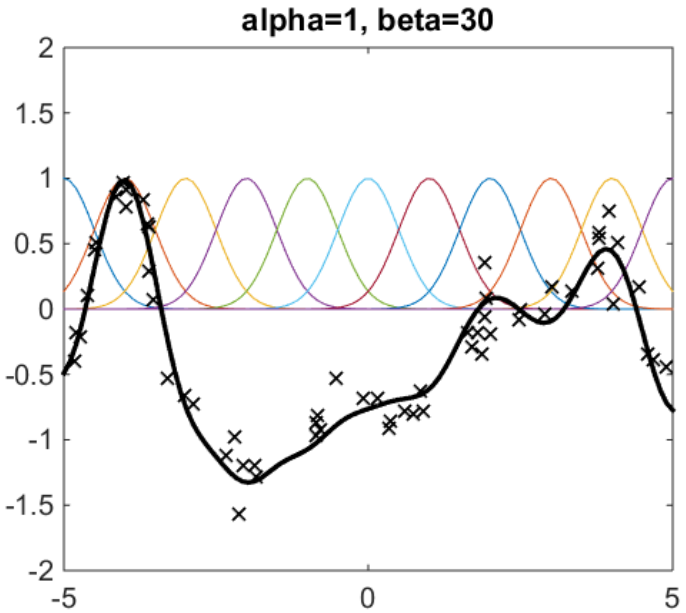


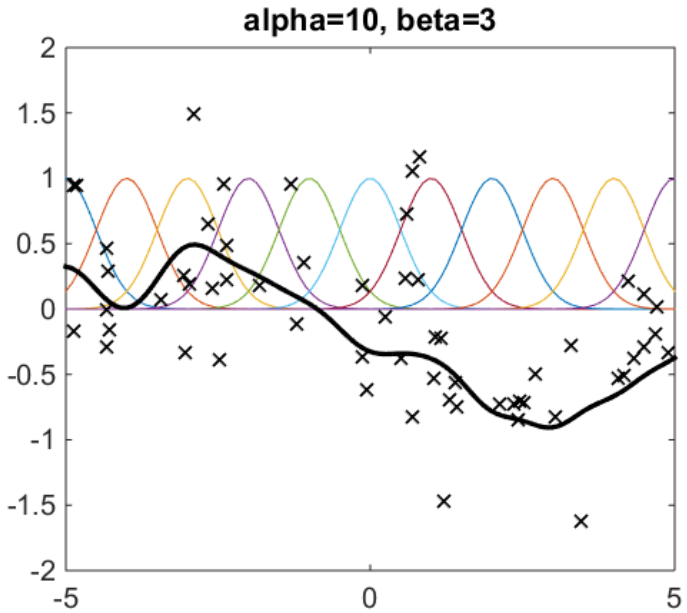
- Other sparse priors (e.g., Laplace, horse-shoe, spike-and-slab):



Non-linear transformation of the inputs

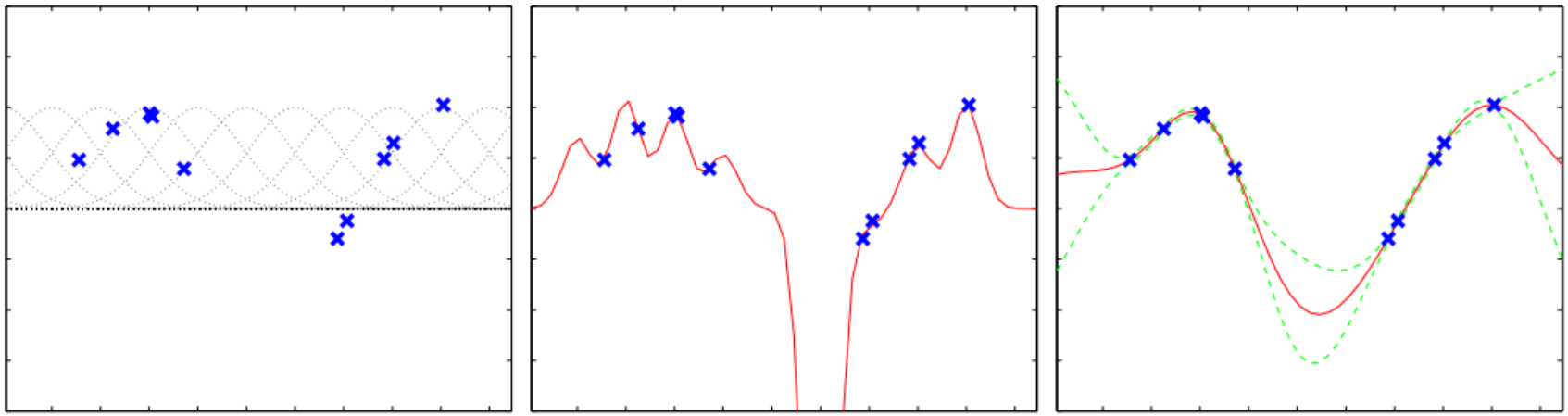
- Select $f(\mathbf{w}, \mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$
- $\phi(\mathbf{x})$ are the *basis functions*
- Example
  - weights drawn from $N(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$; β is the noise precision.
  - $\mathbf{w} = (-0.7, 1.1, -0.8, -1.1, -0.8, -0.6, -0.6, 0.2, -0.2, 0.6, -0.9)$ for basis functions ordered from left to right (left panel)





Importance of learning hyperparameters

- (a): raw data and 15 radial basis functions $\phi_i(x) = \exp\left(-0.5(x - c_i)^2/\lambda^2\right)$ with $\lambda = 0.03^2$ and c_i spread evenly over the input space
- (b): predictions with $\beta = 100$ and $\alpha = 1$ (severe overfitting)
- (c): predictions with ML-II fitted hyperparameter values



Determining hyperparameters

- The hyperparameter posterior distribution is

$$p(\Gamma|\mathcal{D}) \propto p(\mathcal{D}|\Gamma)p(\Gamma)$$

- If $p(\Gamma) \approx const$ this is equivalent to

$$\Gamma^* = \arg\max_{\Gamma} p(\mathcal{D}|\Gamma),$$

where the **marginal likelihood**

$$p(\mathcal{D}|\Gamma) = \int p(\mathcal{D}|\Gamma, \mathbf{w})p(\mathbf{w}|\Gamma)d\mathbf{w}$$

- Selecting hyperparameters that maximize the marginal likelihood is called ML-II approach (in the book...)

ML vs. ML-II

- In **maximum likelihood**, we select parameter values $\mathbf{w}$ that maximize the log-likelihood

$$\log p(y|\mathbf{w}, \mathbf{x}) = \sum_{i=1}^{N} \log N(y_i|\mathbf{w}^T \phi(\mathbf{x}_i), \beta^{-1})$$

$$\widehat{\mathbf{w}} = \arg\max_{\mathbf{w}} \{\log p(y|\mathbf{w}, \mathbf{x})\} \quad \text{(does not depend on } \beta)$$

- In **ML-II**, we select hyperparameter values α and β that *maximize the (log-)marginal likelihood* (parameters $\mathbf{w}$ integrated out)

$$p(y|\Gamma, \mathbf{x}) = \int p(y|\Gamma, \mathbf{w}, \mathbf{x}) p(\mathbf{w}|\Gamma) d\mathbf{w}$$

$$\Gamma^* = \arg\max_{\Gamma} \{\log p(y|\Gamma, x)\}$$

Hyperparameter optimization in practice

- EM-algorithm
- using the gradient
- compute log-marginal likelihood over a grid of values and choose the best value
- use some standard optimization routine (e.g. *fminunc*)

Alternative to ML-II: validation data (1/2)*

- Set the hyperparameters Γ to the value that minimizes the prediction error in the validation data

$$\{\mathcal{X}_{val}, \mathcal{Y}_{val}\} = \left\{(\mathbf{x}_j^{val}, y_j^{val}), j = 1, \ldots, M\right\}.$$

- Mean squared error (MSE)

$$\text{MSE}(\Gamma) = \frac{1}{M}\sum_{j=1}^{M}(y_j^{val} - \widetilde{y}_j^{val})^2,$$

where

$$\widetilde{y}_j^{val} = \mathbf{m}^T\phi(\mathbf{x}_j^{val}), \qquad \mathbf{m} = E(\mathbf{w}|\Gamma, \mathcal{X}_{train}, \mathcal{Y}_{train})$$

Alternative to ML-II: validation data (2/2)*

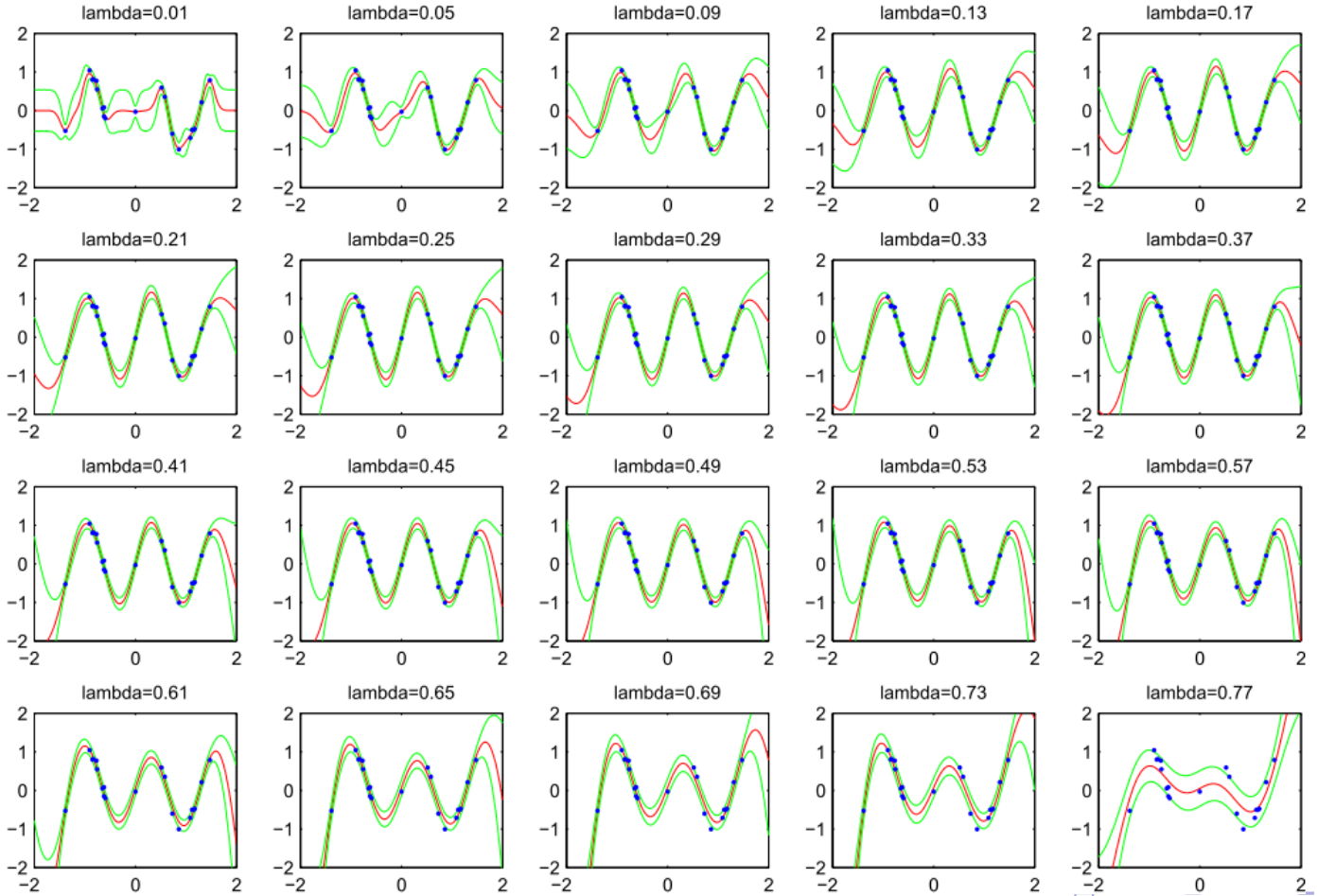
- Or by maximizing the validation data marginal likelihood

$$p(\mathcal{Y}_{val}|\Gamma, \mathcal{D}_{train}, \mathcal{X}_{val}) = \int_{\mathbf{w}} p(\mathcal{Y}_{val}|\mathbf{w}, \mathcal{X}_{val}, \Gamma) p(\mathbf{w}|\Gamma, \mathcal{X}_{train}, \mathcal{Y}_{train}) d\mathbf{w}$$

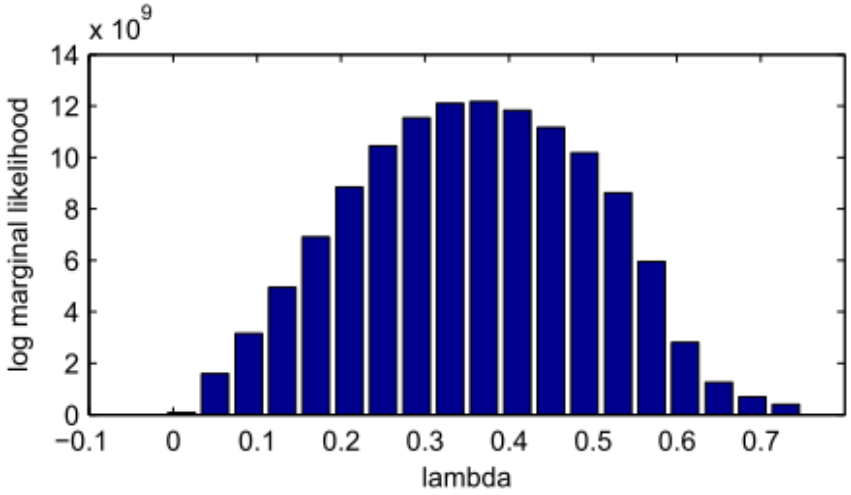
- Possible extension: *cross-validation*

Learning radial basis function width (1/2)

- A set of 10 evenly spaced radial basis functions is used
  $\phi_i(x) = \exp\left(-0.5(x - c_i)^2 / \lambda^2\right)$
- $\Gamma = (\alpha, \beta)$ optimized for different width parameters λ



Learning radial basis function width (2/2)



- The log marginal likelihood

$$\log p(\mathcal{D}|\lambda, \alpha^*(\lambda), \beta^*(\lambda))$$

  having optimized α and β using ML-II. These values depend on λ.
- The best model corresponds to $\lambda = 0.37$.

Linear parameter models for classification

- Binary classification problem: $\mathcal{D} = \{(\mathbf{x}_i, c_i), i = 1, \ldots, N\}$, where the output $c \in \{0, 1\}$.
- Let p denote the probability that $p(c = 1|\mathbf{x})$
- Logistic (linear) regression

$$\log \frac{p}{1-p} = \mathbf{w}^T \mathbf{x}$$

- Or, equivalently

$$p(c = 1|\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x}),$$

where $\sigma(\cdot)$ is the so-called *logistic sigmoid*

$$\sigma(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$$

Logistic regression for classification

- When used for classification, the decision boundary is defined by $p(c = 1|\mathbf{x}) = p(c = 0|\mathbf{x}) = 0.5$. This corresponds to a hyperplane

$$\mathbf{w}^T\mathbf{x} = 0.$$

Classification rule

$$\mathbf{w}^T\mathbf{x} > 0 \rightarrow c = 1$$
$$\mathbf{w}^T\mathbf{x} < 0 \rightarrow c = 0$$

- Note: $\mathbf{x}$ can include a constant term, $\mathbf{x} = (1, x_1, \ldots, x_D)$, such that the *intercept* is automatically included

$$\mathbf{w}^T\mathbf{x} = w_0 + w_1 x_1 + \ldots + w_D x_D$$

Logistic regression, interpretation of parameters*

$$\log\left(\frac{p}{1-p}\right) = w_0 + w_1 x$$
$$\Leftrightarrow \frac{p}{1-p} = \exp(w_0 + w_1 x)$$

- Interpretation: when x increases by one unit, the **odds** $\frac{p}{1-p}$ of belonging in class 1 increases by a factor equal to e^{w_1}.
- If x is binary itself, $x \in \{0, 1\}$, then e^{w_1} is the **odds ratio** between classes $x = 1$ and $x = 0$.
  - a common term in medical literature, e.g., X='smoking', C='cancer'.

Prior for logistic regression

- Gaussian prior

$$p(\mathbf{w}|\alpha) = N_D(\mathbf{w}|\mathbf{0},\alpha^{-1}\mathbf{I}) = \alpha^{\frac{D}{2}}(2\pi)^{-\frac{D}{2}} e^{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}}$$

  where α is the precision.

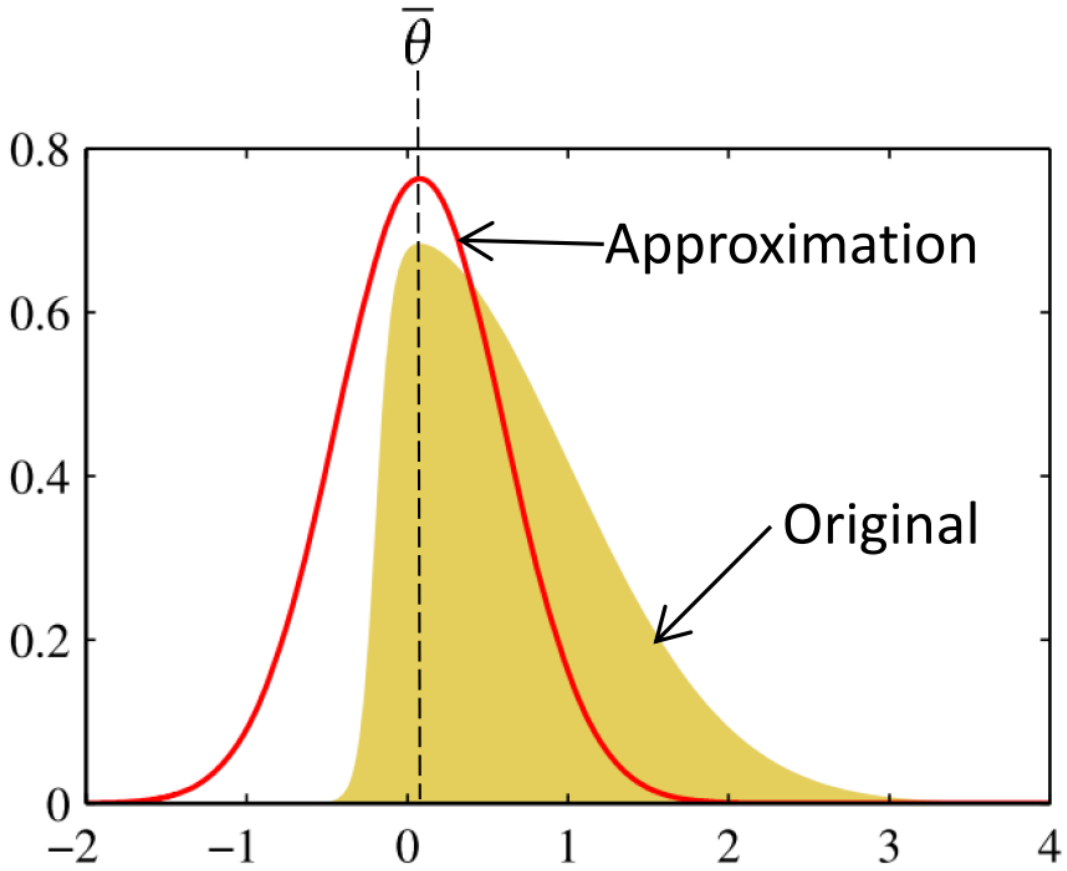
- Given $\mathcal{D} = \{(\mathbf{x}_i, c_i), i = 1, \ldots, N\}$ the posterior equals

$$p(\mathbf{w}|\alpha, \mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w}, \alpha)p(\mathbf{w}|\alpha)}{p(\mathcal{D}|\alpha)} = \frac{1}{p(\mathcal{D}|\alpha)} p(\mathbf{w}|\alpha) \prod_{i=1}^{N} p(c_i|\mathbf{x}_i, \mathbf{w})$$

  (not of standard form, Laplace approximation is feasible to compute).

Laplace approximation

- Gaussian approximation at the mode



modified from Bishop, Fig. 4.14

Laplace approximation to the posterior

- In general,

$$p(\mathbf{w}|\alpha, \mathcal{D}) \propto \exp(-E(\mathbf{w})), \quad E(\mathbf{w}) = -\log p(\mathbf{w}|\alpha, \mathcal{D}).$$

- For logistic regression,

$$E(\mathbf{w}) = \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{N} \log \sigma(\mathbf{w}^T\mathbf{h}_i), \quad \mathbf{h}_i \equiv (2c_i - 1)\mathbf{x}_i.$$

1. approximate $E(\mathbf{w})$ by a quadratic function $\widetilde{E}(\mathbf{w})$ around the minimum $\overline{\mathbf{w}}$

$$\widetilde{E}(\mathbf{w}) = E(\overline{\mathbf{w}}) + \frac{1}{2}(\mathbf{w}-\overline{\mathbf{w}})^T H_{\overline{\mathbf{w}}}(\mathbf{w}-\overline{\mathbf{w}})$$

2. obtain a Gaussian approximation $q(\mathbf{w}|\alpha, \mathcal{D}) \propto \exp(-\widetilde{E}(\mathbf{w}))$ to $p(\mathbf{w}|\alpha, \mathcal{D})$

Laplace approximation in practice

- In practice:
  - Find the minimum $\overline{\mathbf{w}}$ of $E(\mathbf{w})$ analytically (root of the derivative), or by numerical optimization, e.g. Newton's method:

$$\mathbf{w}^{new} = \mathbf{w} - \mathbf{H}_w^{-1} \nabla E$$

  - When converged, compute the Hessian $H_{\overline{\mathbf{w}}}$ of $E(\mathbf{w})$ at $\overline{\mathbf{w}}$.
  - The posterior approximation is

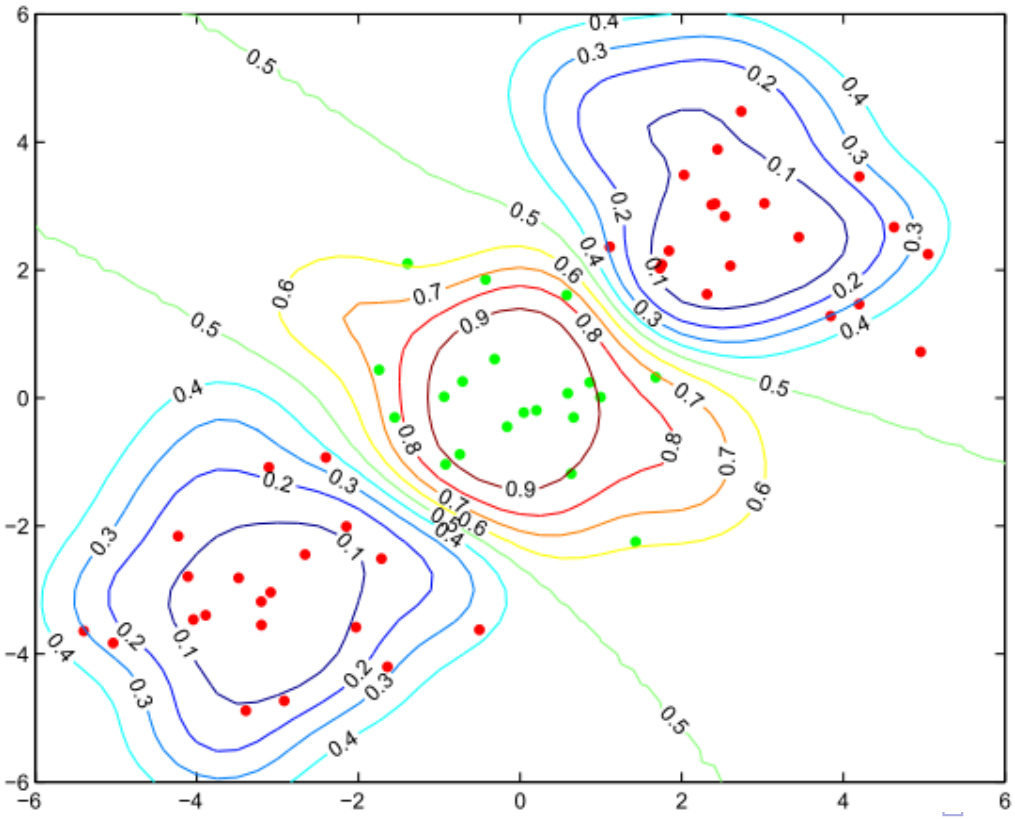
$$q(\mathbf{w}|\alpha, \mathcal{D}) = N(\mathbf{w}|\mathbf{m}, \mathbf{S}), \quad \mathbf{m} = \overline{\mathbf{w}}, \quad \mathbf{S} = \mathbf{H}_{\overline{\mathbf{w}}}^{-1}.$$

- Reminder: if $f \equiv f(x_1, \ldots, x_n)$

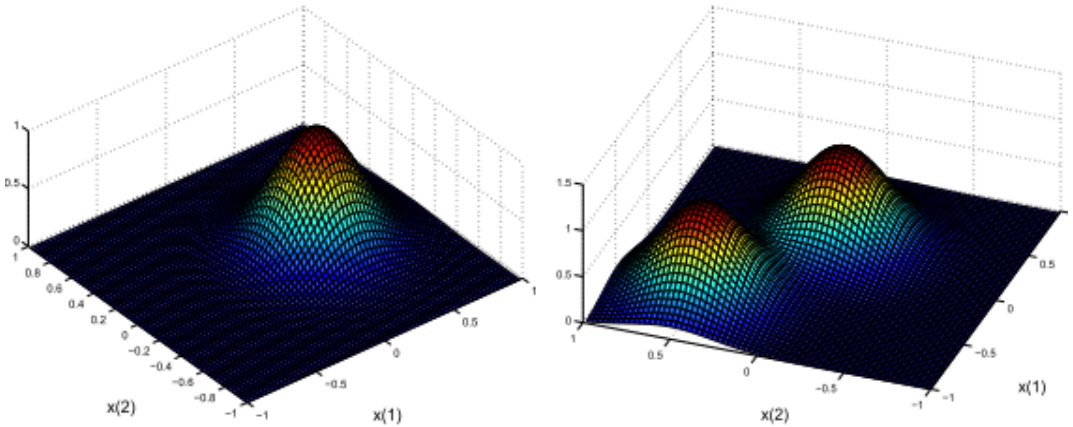
$$H_f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

Example

- Bayesian logistic regression with RBF functions $\phi_i(\mathbf{x}) = \exp(-\lambda(\mathbf{x} - \mathbf{m}_i)^2)$.
- $\mathbf{m}_i$ placed on a subset of training points, λ set to 2
- Hyperparameter α optimized as with the Bayesian linear regression by maximizing the approximated marginal likelihood ($\rightarrow \alpha = 0.45$).



Curse of dimensionality



- In the 1-dimensional example, we used 10 radial basis functions
- To cover 2D region with same resolution, we would need 10^2 basis functions
- **Curse of dimensionality**: the number of basis functions required scales exponentially w.r.t. the dimension

General comments on usage

- Curse of dimensionality limits the use of RBFs to low-dimensional cases
  - Possible remedy: place basis functions on observations
  - Alternatives: kernel methods, Gaussian processes
- With sparse priors, standard linear models can be used with very large D
  - $y = \sum_{i=1}^{D} w_i x_i + \epsilon$

Important points

- By placing a Gaussian prior on the parameters of linear regression, the posterior is also Gaussian.
- In classification, no closed form solution is available for logistic regression and approximations, e.g., the Laplace approximation, are needed.
- Hyperparameters can be set by maximizing the marginal likelihood (either exact or approximate).