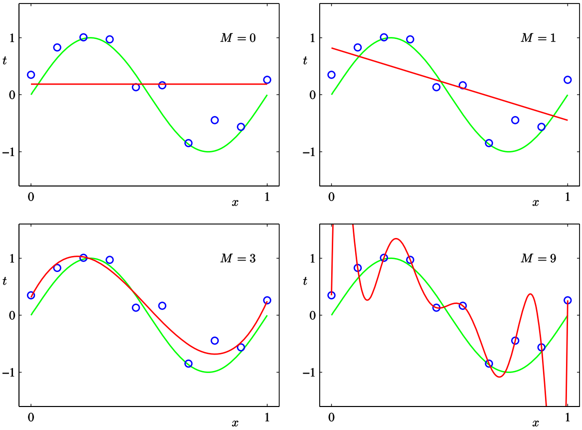
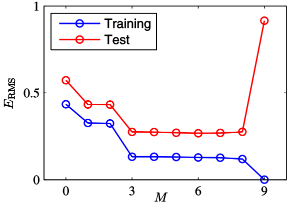
AI4ER 0: Bayesian Linear Regression

Rich Turner
(with thanks to Miguel Hernandez Lobato for the slides)

Motivation

A large number of basis functions can lead to **over-fitting** of the maximum likelihood estimate: the model fits the **training data** well but it performs poorly on new **test data**.





	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Instead, favor **smooth solutions** by using Bayes rule with **priors** that enforce $\mathbf{w}$ to be small.

Figures and table: C. Bishop. *Pattern Recognition and Machine Learning*, 2006.

Bayesian inference

Given data $\mathcal{D} = \{(\widetilde{\mathbf{x}}_n, y_n)\}_{n=1}^N$, we assume the linear regression model

$$y_n = \mathbf{w}^\mathsf{T}\widetilde{\mathbf{x}}_n + \epsilon_n\,, \quad \epsilon_n \sim \mathcal{N}(0, \sigma^2)\,,$$

with unknown $\mathbf{w}$. We assume σ^2 **is known** to simplify inference.

We also assume a **prior distribution** $p(\mathbf{w})$ on the model coefficients.

The **posterior distribution** for $\mathbf{w}$ given $\mathcal{D}$ is obtained by Bayes rule:

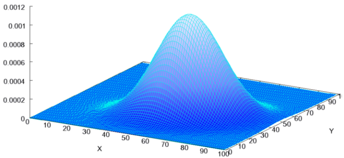
$$p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}}) = \frac{p(\mathbf{y}|\widetilde{\mathbf{X}}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{y}|\widetilde{\mathbf{X}})}\,. \qquad \textbf{Model}$$

The **predictive distribution** for $y_\star$ given a new corresponding $\mathbf{x}_\star$ is

$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}, \widetilde{\mathbf{X}}) = \int p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w})p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}})\,d\mathbf{w}\,. \qquad \textbf{Inference}$$

Exact inference is possible if prior and noise distributions are **Gaussian**.

Multivariate Gaussian distribution



The density of a D-dimensional vector $\mathbf{x}$ is

$$\mathcal{N}(\mathbf{x}|\mathbf{m},\mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^{\mathsf{T}}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\}.$$

The density is proportional to the **exponential of a quadratic function** of $\mathbf{x}$:

$$\mathcal{N}(\mathbf{x}|\mathbf{m},\mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}\mathbf{x}\mathbf{V}^{-1}\mathbf{x}^T + \mathbf{m}^{\mathsf{T}}\mathbf{V}^{-1}\mathbf{x} - \frac{1}{2}\mathbf{m}\mathbf{V}^{-1}\mathbf{m}^T\right\}$$

$$\propto \exp\left\{-\frac{1}{2}\mathbf{x}^{\mathsf{T}}\mathbf{V}^{-1}\mathbf{x} + \mathbf{m}^{\mathsf{T}}\mathbf{V}^{-1}\mathbf{x}\right\}, \qquad (1)$$

with **normalization constant** $\sqrt{(2\pi)^D|\mathbf{V}|}\exp\{1/2\mathbf{m}^{\mathsf{T}}\mathbf{V}^{-1}\mathbf{m}\}$.

$\mathbf{m}$ is the D-dimensional mean vector and $\mathbf{V}$ is the $D \times D$ covariance matrix:

$$\mathbf{m} = \mathbf{E}[\mathbf{x}], \qquad \mathbf{V} = \mathbf{E}[(\mathbf{x}-\mathbf{m})(\mathbf{x}-\mathbf{m})^{\mathsf{T}}] = \mathbf{E}[\mathbf{x}\mathbf{x}^{\mathsf{T}}] - \mathbf{m}\mathbf{m}^{\mathsf{T}}.$$

$\hat{\mathbf{x}} \sim \mathcal{N}(\mathbf{x}|\mathbf{m},\mathbf{V})$ can be obtained using the **matrix square root** $\mathbf{V} = \mathbf{V}^{1/2}(\mathbf{V}^{1/2})^{\mathsf{T}}$:

$$\hat{\mathbf{x}} = \mathbf{m} + \mathbf{V}^{1/2}\mathbf{z}, \qquad \mathbf{z} \sim \mathcal{N}(\mathbf{0},\mathbf{I}).$$

Effect of parameters on density function

Assuming

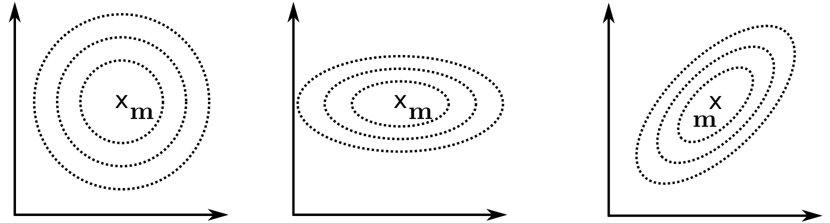
$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\} .$$

The parameter $\mathbf{m}$ determines **mode location** and $\mathbf{V}$ **scales and rotates** the space.

What can you say about

$$\mathbf{V} = \begin{bmatrix} v_1 & \mathrm{cov} \\ \mathrm{cov} & v_2 \end{bmatrix}$$

given the following contour plots of $p(\mathbf{x})$?



Effect of parameters on density function

Assuming

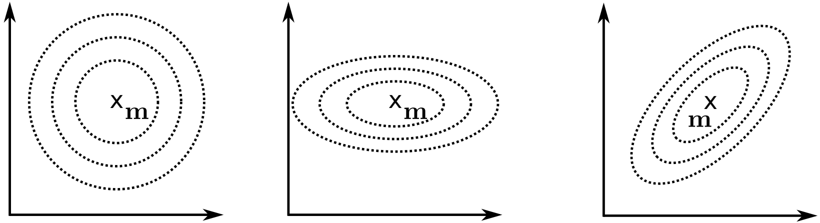
$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^{\mathsf{T}}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\}.$$

The parameter **m** determines **mode location** and **V** **scales and rotates** the space.

What can you say about

$$\mathbf{V} = \begin{bmatrix} v_1 & \text{cov} \\ \text{cov} & v_2 \end{bmatrix}$$

given the following contour plots of $p(\mathbf{x})$?



$v_1 = v_2$, cov $= 0$.

Effect of parameters on density function

Assuming

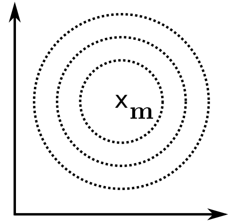
$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\}.$$

The parameter $\mathbf{m}$ determines **mode location** and $\mathbf{V}$ **scales and rotates** the space.

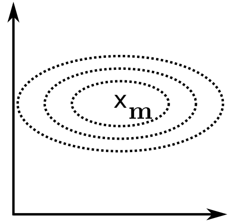
What can you say about

$$\mathbf{V} = \begin{bmatrix} v_1 & \text{cov} \\ \text{cov} & v_2 \end{bmatrix}$$

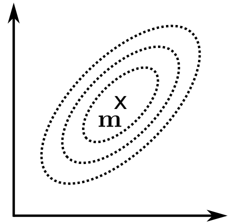
given the following contour plots of $p(\mathbf{x})$?



$v_1 = v_2$, cov $= 0$.



$v_1 > v_2$, cov $= 0$.



Effect of parameters on density function

Assuming

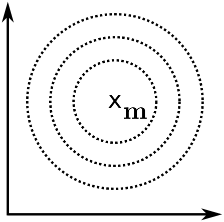
$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\}.$$

The parameter $\mathbf{m}$ determines **mode location** and $\mathbf{V}$ **scales and rotates** the space.

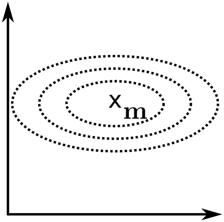
What can you say about

$$\mathbf{V} = \begin{bmatrix} v_1 & \mathrm{cov} \\ \mathrm{cov} & v_2 \end{bmatrix}$$

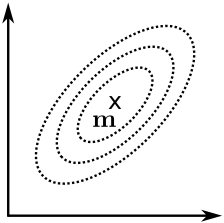
given the following contour plots of $p(\mathbf{x})$?



$v_1 = v_2$, $\mathrm{cov} = 0$.

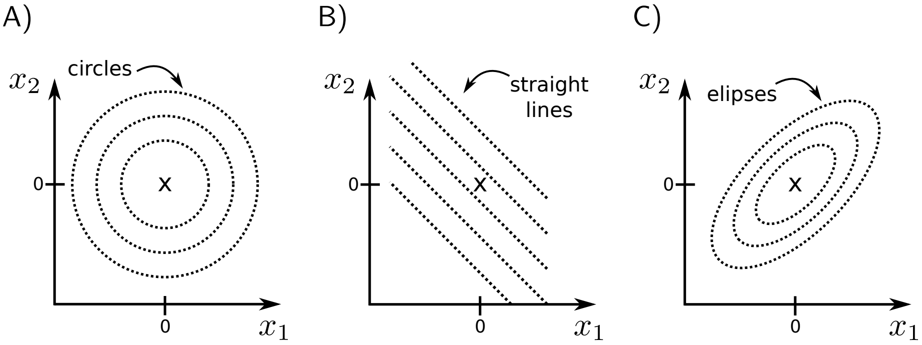


$v_1 > v_2$, $\mathrm{cov} = 0$.



$\mathrm{cov} > 0$.

Gaussian quiz



Match each exponential of quadratic function with its contour plot.

$$i)\quad \exp\left\{-\frac{1}{2}x_1^2 a - \frac{1}{2}x_2^2 a\right\},$$

$$ii)\quad \exp\left\{-\frac{1}{2}x_1^2 a - \frac{1}{2}x_2^2 b + x_1 x_2 c\right\},$$

$$iii)\quad \exp\left\{-\frac{1}{2}(y - x_1 - x_2)^2\right\},$$

Linear combination of Gaussian random variables

Let $p(\mathbf{x}) = \mathbf{N}(\mathbf{x}|\mathbf{0}, \mathbf{V}_1)$ and $p(\mathbf{e}) = \mathbf{N}(\mathbf{x}|\mathbf{0}, \mathbf{V}_2)$ and assume that, for a matrix $\mathbf{W}$,

$$\mathbf{y} = \mathbf{W}\mathbf{x} + \mathbf{e}\,.$$

What is $p(\mathbf{y})$? Linear combinations of Gaussian random variables are Gaussian.

Therefore, $p(\mathbf{y})$ is Gaussian with mean vector

$$\mathbf{m}_3 = \mathbf{E}[\mathbf{y}] = \mathbf{E}[\mathbf{W}\mathbf{x} + \mathbf{e}] = \mathbf{W}\mathbf{E}[\mathbf{x}] + \mathbf{E}[\mathbf{e}] = \mathbf{0}$$

and covariance matrix

$$\begin{aligned}
\mathbf{V}_3 &= \mathbf{E}[\mathbf{y}\mathbf{y}^\mathsf{T}] - \mathbf{E}[\mathbf{y}]\mathbf{E}[\mathbf{y}]^\mathsf{T} \\
&= \mathbf{E}[\mathbf{y}\mathbf{y}^\mathsf{T}] \\
&= \mathbf{E}[(\mathbf{W}\mathbf{x} + \mathbf{e})(\mathbf{W}\mathbf{x} + \mathbf{e})^\mathsf{T}] \\
&= \mathbf{E}[\mathbf{W}\mathbf{x}\mathbf{x}^\mathsf{T}\mathbf{W}^\mathsf{T} + \mathbf{e}\mathbf{x}^\mathsf{T}\mathbf{W}^\mathsf{T} + \mathbf{W}\mathbf{x}\mathbf{e}^\mathsf{T} + \mathbf{e}\mathbf{e}^\mathsf{T}] \\
&= \mathbf{W}\mathbf{V}_1\mathbf{W}^\mathsf{T} + \mathbf{V}_2\,.
\end{aligned}$$

What if $p(\mathbf{x}) = \mathbf{N}(\mathbf{x}|\mathbf{m}_1, \mathbf{V}_1)$?

Completing the square

Let

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}, \mathbf{V}) = \frac{1}{\sqrt{(2\pi)^D |\mathbf{V}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{m})^\mathsf{T}\mathbf{V}^{-1}(\mathbf{x}-\mathbf{m})\right\},$$

$$q(\mathbf{x}) = \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\mathbf{P}\mathbf{x} + \mathbf{a}^\mathsf{T}\mathbf{x}\right\}.$$

Assume that $p(\mathbf{x}) \propto q(\mathbf{x})$.

Write $\mathbf{m}$ and $\mathbf{V}$ in terms of $\mathbf{P}$ and $\mathbf{a}$.

We have that

$$p(\mathbf{x}) \propto \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\mathbf{V}^{-1}\mathbf{x} + \mathbf{m}^\mathsf{T}\mathbf{V}^{-1}\mathbf{x}\right\} \quad \text{from equation (1)},$$

$$q(\mathbf{x}) = \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\mathbf{P}\mathbf{x} + \mathbf{a}^\mathsf{T}\mathbf{x}\right\}.$$

Therefore, $\mathbf{V} = \mathbf{P}^{-1}$ and $\mathbf{m} = \mathbf{V}\mathbf{a}$.

What is the normalization constant of $q(\mathbf{x})$?

Product of Gaussian densities

Let $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}_1, \mathbf{V}_1)$ and $q(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{m}_2, \mathbf{V}_2)$. What is $t(\mathbf{x}) \propto p(\mathbf{x})q(\mathbf{x})$?

$t(\mathbf{x})$ is Gaussian $\mathcal{N}(\mathbf{x}|\mathbf{m}_3, \mathbf{V}_3)$ because the product of exponentials of quadratic functions is also the exponential of a quadratic function. What are $\mathbf{m}_3$ and $\mathbf{V}_3$?

$$
\begin{aligned}
p(x)q(x) &= \mathcal{N}(\mathbf{x}|\mathbf{m}_1, \mathbf{V}_1)\mathcal{N}(\mathbf{x}|\mathbf{m}_2, \mathbf{V}_2) \\
&= \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}_1|}} \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\mathbf{V}_1^{-1}\mathbf{x} + \mathbf{m}_1^\mathsf{T}\mathbf{V}_1^{-1}\mathbf{x} - \frac{1}{2}\mathbf{m}_1^\mathsf{T}\mathbf{V}_1^{-1}\mathbf{m}_1\right\} \\
&\quad \frac{1}{\sqrt{(2\pi)^D|\mathbf{V}_2|}} \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\mathbf{V}_2^{-1}\mathbf{x} + \mathbf{m}_2^\mathsf{T}\mathbf{V}_2^{-1}\mathbf{x} - \frac{1}{2}\mathbf{m}_2^\mathsf{T}\mathbf{V}_2^{-1}\mathbf{m}_2\right\} \\
&\propto \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\underbrace{\left(\mathbf{V}_1^{-1} + \mathbf{V}_2^{-1}\right)}_{\mathbf{V}_3^{-1}}\mathbf{x} + \underbrace{\left(\mathbf{m}_1^\mathsf{T}\mathbf{V}_1^{-1} + \mathbf{m}_2^\mathsf{T}\mathbf{V}_2^{-1}\right)}_{\mathbf{m}_3^\mathsf{T}\mathbf{V}_3^{-1}}\mathbf{x}\right\}.
\end{aligned}
$$

Therefore, $\mathbf{V}_3 = (\mathbf{V}_1^{-1} + \mathbf{V}_2^{-1})^{-1}$ and $\mathbf{m}_3 = \mathbf{V}_3(\mathbf{m}_1^\mathsf{T}\mathbf{V}_1^{-1} + \mathbf{m}_2^\mathsf{T}\mathbf{V}_2^{-1})^\mathsf{T}$.

What is the normalization constant of $p(\mathbf{x})q(\mathbf{x})$?

Bayesian linear regression

Consider a regression model in which σ^2 is known: the only unknown is $\mathbf{w}$.

Recall that the likelihood function under Gaussian noise is

$$p(\mathbf{y}|\widetilde{\mathbf{X}}, \mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}(y_n|\mathbf{w}^\mathsf{T}\widetilde{\mathbf{x}}_n, \sigma^2) \propto \exp\left\{-\frac{\mathbf{w}^\mathsf{T}\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}\mathbf{w}}{2\sigma^2} + \frac{\mathbf{y}^\mathsf{T}\widetilde{\mathbf{X}}\mathbf{w}}{\sigma^2}\right\}.$$

We choose the prior for $\mathbf{w}$ to be a zero-mean isotropic Gaussian:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}) \propto \exp\left\{-\frac{1}{2}\mathbf{x}^\mathsf{T}\lambda\mathbf{I}\mathbf{x}\right\}.$$

The posterior is then Gaussian:

$$\begin{aligned} p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}}, \sigma^2) &\propto p(\mathbf{y}|\widetilde{\mathbf{X}}, \mathbf{w})p(\mathbf{w}) \\ &\propto \exp\left\{-\frac{1}{2}\mathbf{w}^\mathsf{T}\underbrace{\left(\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}\sigma^{-2} + \lambda\mathbf{I}\right)}_{\mathbf{V}^{-1}}\mathbf{w} + \underbrace{\mathbf{y}^\mathsf{T}\widetilde{\mathbf{X}}\sigma^{-2}}_{\mathbf{m}^\mathsf{T}\mathbf{V}^{-1}}\mathbf{w}\right\}. \end{aligned}$$

Therefore, $p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}}, \sigma^2) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{V})$ where

$$\mathbf{V} = (\widetilde{\mathbf{X}}^\mathsf{T}\widetilde{\mathbf{X}}\sigma^{-2} + \lambda\mathbf{I})^{-1}, \qquad \mathbf{m} = \mathbf{V}\sigma^{-2}\widetilde{\mathbf{X}}^\mathsf{T}\mathbf{y}.$$

The Bayesian predictive distribution

The predictive distribution for the $y_\star$ of a given new corresponding $\widetilde{\mathbf{x}}_\star$ is

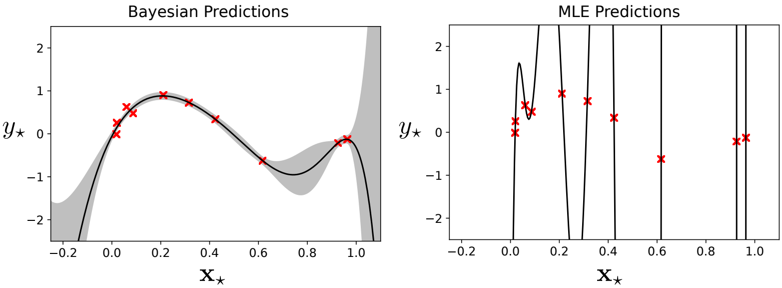
$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}, \widetilde{\mathbf{X}}) = \int p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w}) p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}})\, d\mathbf{w} = \int \mathcal{N}(y_\star|\mathbf{w}^\mathsf{T}\widetilde{\mathbf{x}}_\star, \sigma^2)\mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{V})\, d\mathbf{w}\,.$$

We have that $y_\star = \mathbf{w}^\mathsf{T}\widetilde{\mathbf{x}}_\star + e_\star$, where $\mathbf{w} \sim \mathcal{N}(\mathbf{m}, \mathbf{V})$ and $e_\star \sim \mathcal{N}(0, \sigma^2)$. Thus,

$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}, \widetilde{\mathbf{X}}) = \mathcal{N}(y_\star|m_\star, v_\star)\,,$$

where $m_\star = \mathbf{m}^\mathsf{T}\widetilde{\mathbf{x}}_\star$ and $v_\star = \widetilde{\mathbf{x}}_\star^\mathsf{T}\mathbf{V}\widetilde{\mathbf{x}}_\star + \sigma^2$.

Example with polynomial basis functions, $M = 10$, $\lambda = 10^{-5}$, $\sigma^2 = 0.005$:

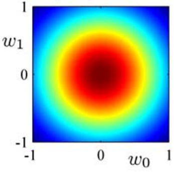


We reduce **overfitting** and obtain **confidence bands** $m_\star \pm v_\star^{1/2}$ in our predictions!

Example

Prior

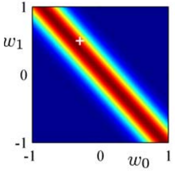
$p(\mathbf{w})$



$\times$

Likelihood

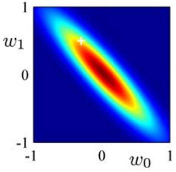
$p(y_1|\widetilde{\mathbf{x}}_1, \mathbf{w})$



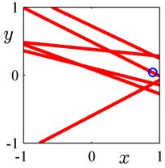
$\propto$

Posterior

$p(\mathbf{w}|y_1, \widetilde{\mathbf{x}}_1)$



Predictions of posterior samples



Another example with Gaussian basis functions

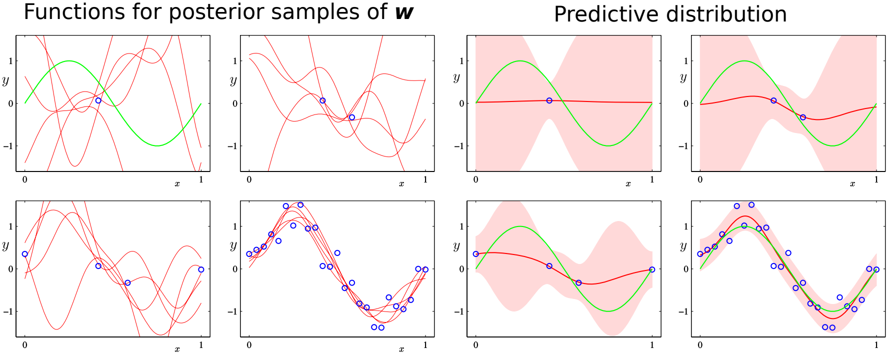
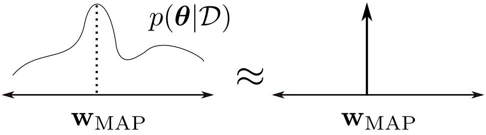


Figure: C. Bishop. *Pattern Recognition and Machine Learning*, 2006.

Maximum a posteriori (MAP) inference

Assumes that the posterior is well approximated by a point mass at its mode:



$$= \delta(\mathbf{w} - \mathbf{w}_{\text{MAP}})$$

In particular,

$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}, \widetilde{\mathbf{X}}) = \int p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w})p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}})\, d\mathbf{w}$$

$$p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{y}, \widetilde{\mathbf{X}}) \approx \int p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w})\delta(\mathbf{w} - \mathbf{w}_{\text{MAP}})\, d\mathbf{w}$$

$$\approx p(y_\star|\widetilde{\mathbf{x}}_\star, \mathbf{w}_{\text{MAP}}),$$

$$\begin{aligned} \mathbf{w}_{\text{MAP}} &= \arg\max_{\mathbf{w}} \, p(\mathbf{w}|\mathbf{y}, \widetilde{\mathbf{X}}) \\ &= \arg\max_{\mathbf{w}} \, p(\mathbf{y}|\mathbf{w}, \widetilde{\mathbf{X}})p(\mathbf{w}) \\ &= \arg\max_{\mathbf{w}} \, \left\{ \log p(\mathbf{y}|\mathbf{w}, \widetilde{\mathbf{X}}) + \log p(\mathbf{w}) \right\}. \end{aligned}$$

MAP inference is a form of **regularized** MLE. For $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I})$, we obtain

$$\mathbf{w}_{\text{MAP}} = \arg\max_{\mathbf{w}} \left\{ \log p(\mathbf{y}|\mathbf{w}, \widetilde{\mathbf{X}}) - \frac{\lambda}{2}\mathbf{w}^{\mathsf{T}}\mathbf{w} \right\} = (\widetilde{\mathbf{X}}^{\mathsf{T}}\widetilde{\mathbf{X}}\sigma^{-2} + \lambda\mathbf{I})^{-1}\sigma^{-2}\widetilde{\mathbf{X}}^{\mathsf{T}}\mathbf{y}.$$

MAP inference fails to generate **confidence bands** in the resulting predictions!