Session 6: Bayesian Regression

Bayesian Treatment of Linear Regression

Haiping Lu - COM4509/6509 MLAI2018

Based on slides by Neil D. Lawrence MLAI2015 version

Review - Session 5 (VIS)

- Introduced important ML concepts: **overfitting** and **generalisation** Watch (by ML grand master): Machine Learning A Cappella - Overfitting Thriller! (https://www.youtube.com/watch?v=DQWI1kvmwRg)
- Explained the difference between extrapolation and interpolation, and how to choose validation set respectively
- Examined the bias variance decomposition and trade-off
- Showed how to evaluate prediction models (estimate risk) by **cross validation (CV)**: LOO, k-fold, hold out.

Overview - Session 6

- Another important ML concept: **Bayesian** Watch (by statistician): The Fifth Moment -- I Think I'm A Bayesian (https://www.youtube.com/watch?v=JmSKam4BCvU)

Mauricio A. Álvarez @maalvarezl · Oct 1

With @haipinglu, we started teaching a Module in Machine Learning for > 230 students. We're gonna be teaching at the St George's Church, now part of the Univ. of Sheffield. So, we're now teaching the Bayesian religion (and other non-holy pieces of ML) in an actual Church!

Haiping Lu
@haipinglu

Replying to @maalvarezl

This is how it looks from outside. It will be a unique experience for sure.

- **Bayesian** treatment/approach: placing a probability distribution (*prior* density) over the model parameters for their probabilistic interpretation
- **Bayesian** regression: Bayesian treatment of linear regression (model parameters)
- Key **Bayesian** concepts: prior, posterior, likelihood, marginal likelihood, Bayes' rule, marginalisation

Note by Haiping

- Headings marked as *optional* are background / more challenging info for your interest, which can be safely skipped if you would like to be more focused on the core / essentials and have less interest in the background / more advanced materials.

In [1]:

```
import pods
import mlai
import numpy as np
import matplotlib.pyplot as plt
import teaching_plots as plot
%matplotlib inline

from ipywidgets import *
def display_plots(filebase, directory=None, width=700, height=500, **kwargs):
    """Display a series of plots controlled by sliders. The function relies on Pytho
    def show_figure(filebase, directory, **kwargs):
        """Helper function to load in the relevant plot for display."""
        filename = filebase.format(**kwargs)
        if directory is not None:
            filename = directory + '/' + filename
        display(HTML("<img src='{filename}'>".format(filename=filename)))

    interact(show_figure, filebase=fixed(filebase), directory=fixed(directory), **kw
```

Two Simultaneous Equations

A system of two simultaneous equations with two unknowns.

$$\begin{aligned} y_1 &= mx_1 + c \\ y_2 &= mx_2 + c \end{aligned}$$

$$y_1 - y_2 = m(x_1 - x_2)$$

$$\frac{y_1 - y_2}{x_1 - x_2} = m$$

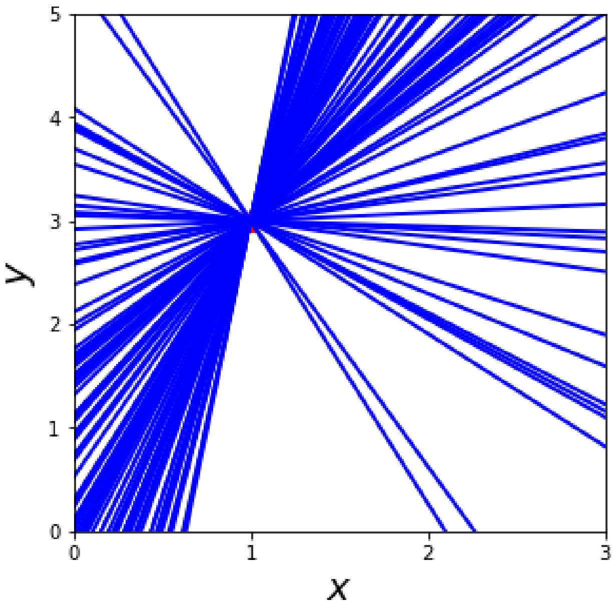
$$\begin{aligned} m &= \frac{y_2 - y_1}{x_2 - x_1} \\ c &= y_1 - mx_1 \end{aligned}$$

Underdetermined System

- What about two unknowns and *one* observation?

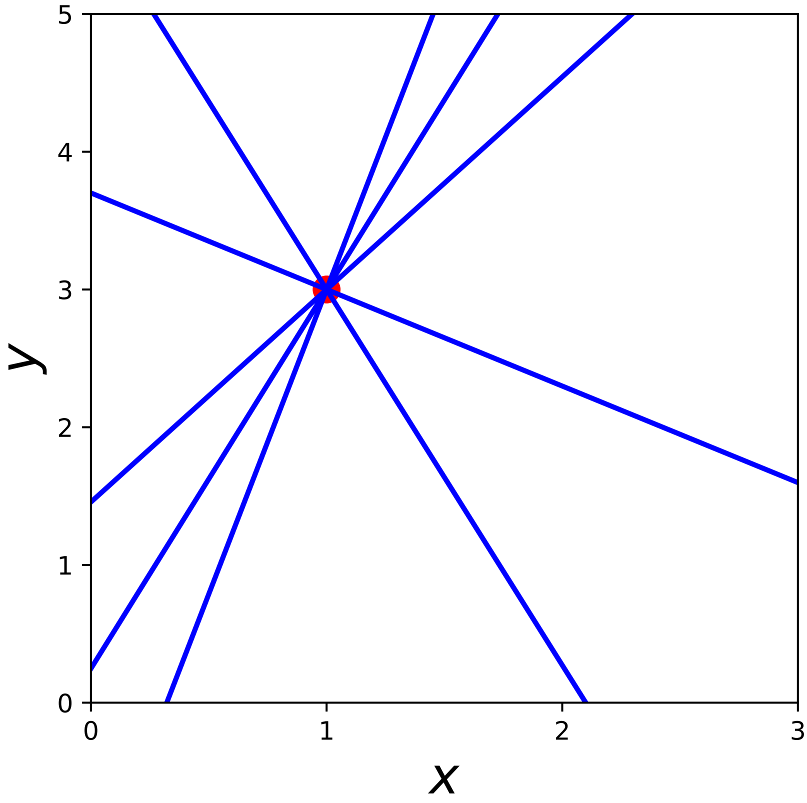
$$y_1 = mx_1 + c$$

```
In [2]: plot.under_determined_system()
```



```
In [3]: display_plots('under_determined_system{samp:0>3}.svg', directory='./diagrams', samp=
```

samp 5



- We can compute m given c.

$$m = \frac{y_1 - c}{x}$$

- Or we can compute m given c.

Assume

$$c \sim \mathcal{N}(0, 4),$$

Overdetermined System

- With two unknowns and two observations:

$$\begin{aligned} y_1 &= mx_1 + c \\ y_2 &= mx_2 + c \end{aligned}$$

- Additional observation leads to *overdetermined* system.

$$y_3 = mx_3 + c$$

- This problem is solved through a noise model $\epsilon \sim \mathcal{N}(0, \sigma^2)$

$$\begin{aligned} y_1 &= mx_1 + c + \epsilon_1 \\ y_2 &= mx_2 + c + \epsilon_2 \\ y_3 &= mx_3 + c + \epsilon_3 \end{aligned}$$

Noise Models

- Motivation: Simple linear models are not modeling entire system.
- Noise model gives *mismatch* between model and data.
- Gaussian model is justified by appeal to central limit theorem.
- Other models also possible (Student-t for heavy tails).
- Maximum likelihood with Gaussian noise leads to *least squares*.

Different Types of Uncertainty (*optional*)

- The first type of uncertainty we are assuming is *aleatoric* uncertainty.
- The second type of uncertainty we are assuming is *epistemic* uncertainty.

Aleatoric Uncertainty (*optional*)

- This is uncertainty we couldn't know even if we wanted to. e.g. the result of a football match before it's played.
- Where a sheet of paper might land on the floor.

Epistemic Uncertainty (*optional*)

- This is uncertainty we could in principal know the answer too. We just haven't observed enough yet, e.g. the result of a football match *after* it's played.
- What colour socks your lecturer is wearing.

Reading

- @Bishop:book06 Section 1.2.3 (pg 21–24).
- @Bishop:book06 Section 1.2.6 (start from just past eq 1.64 pg 30-32).
- @Rogers:book11 use an example of a coin toss for introducing Bayesian inference Chapter 3, Sections 3.1-3.4 (pg 95-117). Although you also need the beta density which we haven't yet discussed. This is also the example that @Laplace:memoire74 used.

- Bayesian Inference
  - @Rogers:book11 use an example of a coin toss for introducing Bayesian inference Chapter 3, Sections 3.1-3.4 (pg 95-117). Although you also need the beta density which we haven't yet discussed. This is also the example that @Laplace:memoire74 used.
  - @Bishop:book06 Section 1.2.3 (pg 21–24).
  - @Bishop:book06 Section 1.2.6 (start from just past eq 1.64 pg 30-32).

Bayesian Inference in the Univariate Case

Prior Distribution

- Bayesian inference requires a prior on the parameters.
- The prior represents your belief *before* you see the data of the likely value of the parameters.
- For linear regression, consider a Gaussian prior on the intercept:

$$c \sim \mathcal{N}(0, \alpha_1)$$

Posterior Distribution

- Posterior distribution is found by combining the prior with the likelihood.
- Posterior distribution is your belief *after* you see the data of the likely value of the parameters.
- The posterior is found through **Bayes' Rule**

$$p(c|y) = \frac{p(y|c)p(c)}{p(y)}$$

$p(c)$: prior

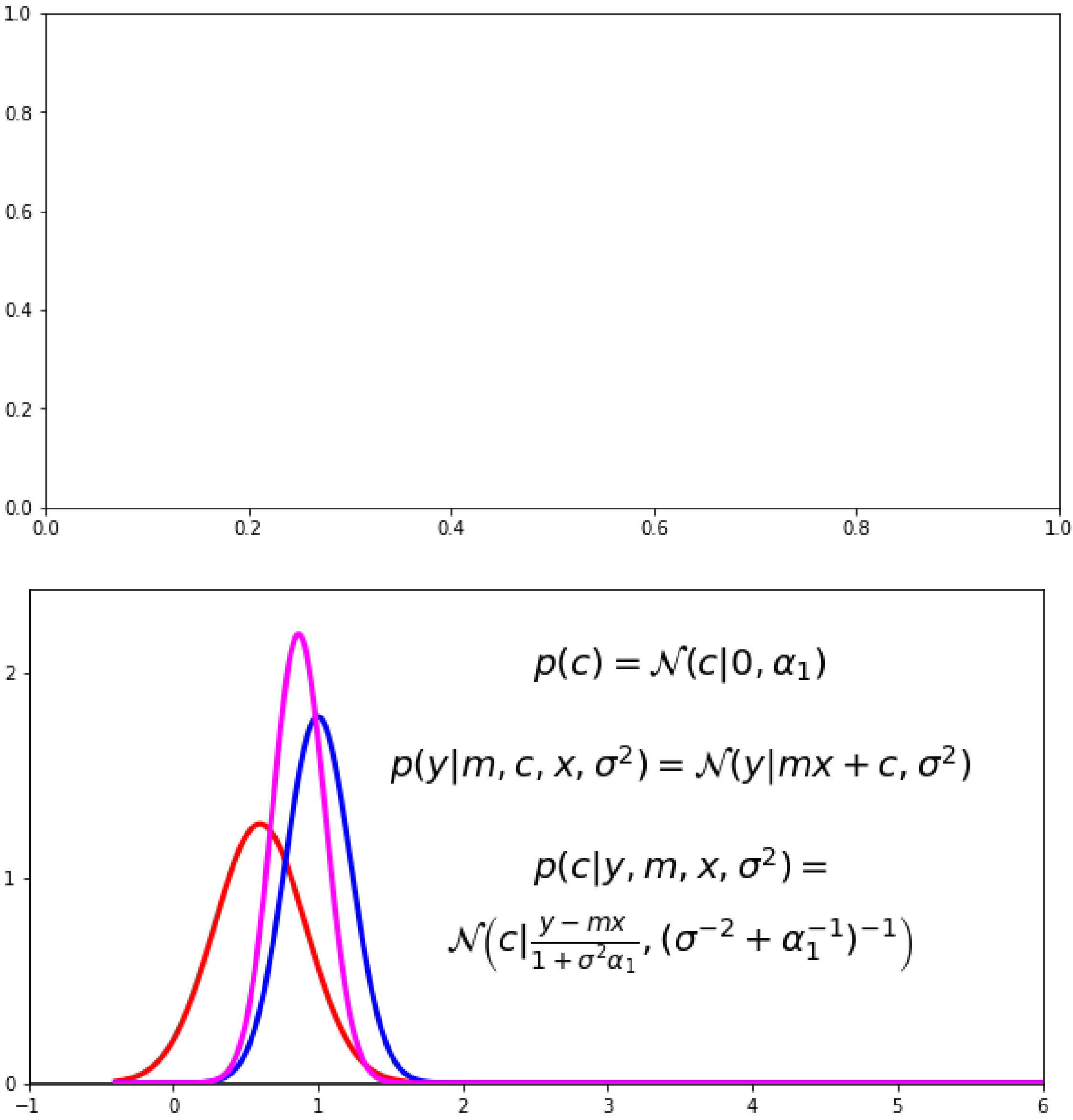
$p(y|c)$: likelihood

$p(y)$: marginal likelihood

$p(c|y)$: posterior

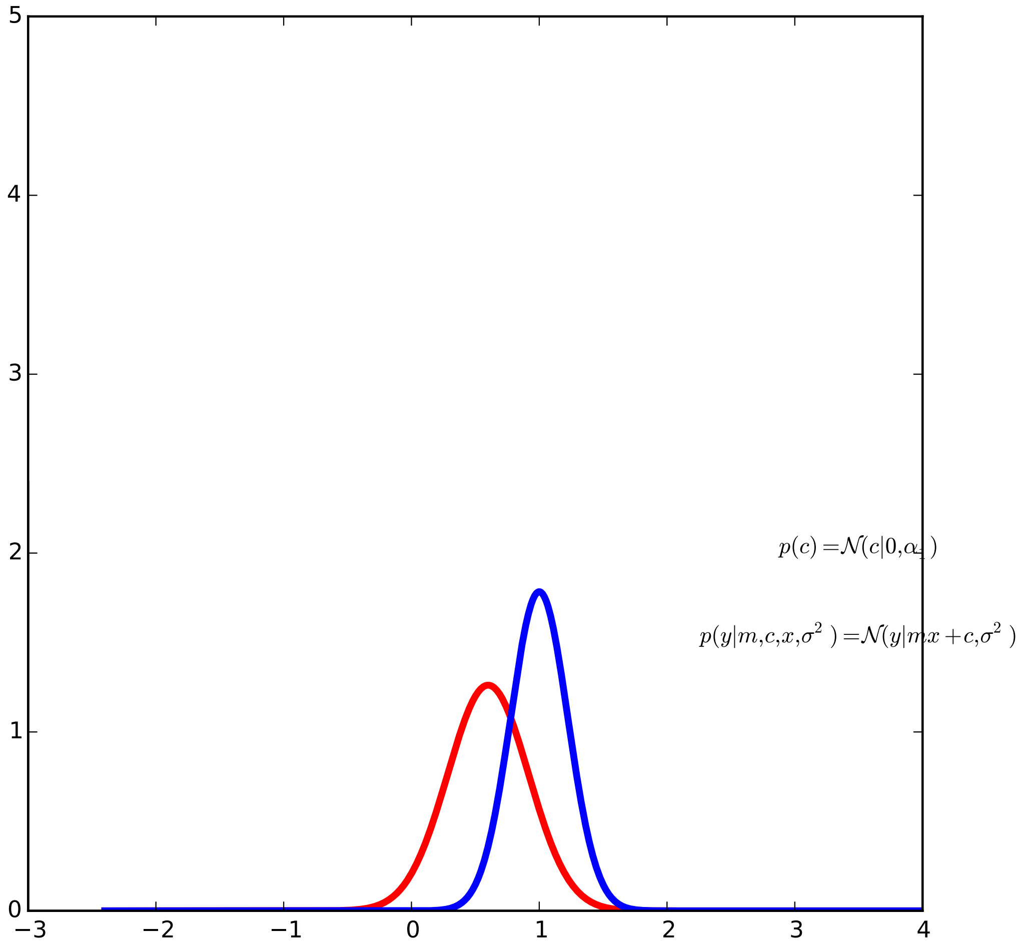
Bayes Update

```
In [4]: plot.bayes_update()
```



```
In [5]: display_plots('dem_gaussian{stage:0>2}.svg', './diagrams', stage=(1, 3))
```

stage 2



Stages to Derivation of the Posterior

- Multiply likelihood by prior
    - They are "exponentiated quadratics", the answer is always also an exponentiated quadratic because
$$\exp(a^2)\exp(b^2) = \exp(a^2 + b^2)$$
- Complete the square to get the resulting density in the form of a Gaussian.
- Recognise the mean and (co)variance of the Gaussian. This is the estimate of the posterior.

Main Trick

$$p(c) = \frac{1}{\sqrt{2\pi\alpha_1}}\exp\left(-\frac{1}{2\alpha_1}c^2\right)$$

$$p(\mathbf{y}|\mathbf{x}, c, m, \sigma^2) = \frac{1}{\left(2\pi\sigma^2\right)^{\frac{n}{2}}}\exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - mx_i - c)^2\right)$$

$$p(c|\mathbf{y}, \mathbf{x}, m, \sigma^2) = \frac{p(\mathbf{y}|\mathbf{x}, c, m, \sigma^2)p(c)}{p(\mathbf{y}|\mathbf{x}, m, \sigma^2)}$$

$$p(c|\mathbf{y}, \mathbf{x}, m, \sigma^2) = \frac{p(\mathbf{y}|\mathbf{x}, c, m, \sigma^2)p(c)}{\int p(\mathbf{y}|\mathbf{x}, c, m, \sigma^2)p(c)\text{d}c}$$

$$p(c|\mathbf{y}, \mathbf{x}, m, \sigma^2) \propto p(\mathbf{y}|\mathbf{x}, c, m, \sigma^2)p(c)$$

$$\begin{aligned}\log p(c|\mathbf{y}, \mathbf{x}, m, \sigma^2) &= -\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - c - mx_i)^2 - \frac{1}{2\alpha_1}c^2 + \text{const}\\ &= -\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - mx_i)^2 - \left(\frac{n}{2\sigma^2} + \frac{1}{2\alpha_1}\right)c^2\\ &+ c\frac{\sum_{i=1}^{n}(y_i - mx_i)}{\sigma^2},\end{aligned}$$

complete the square of the quadratic form to obtain

$$\log p(c|\mathbf{y}, \mathbf{x}, m, \sigma^2) = -\frac{1}{2\tau^2}(c - \mu)^2 + \text{const},$$

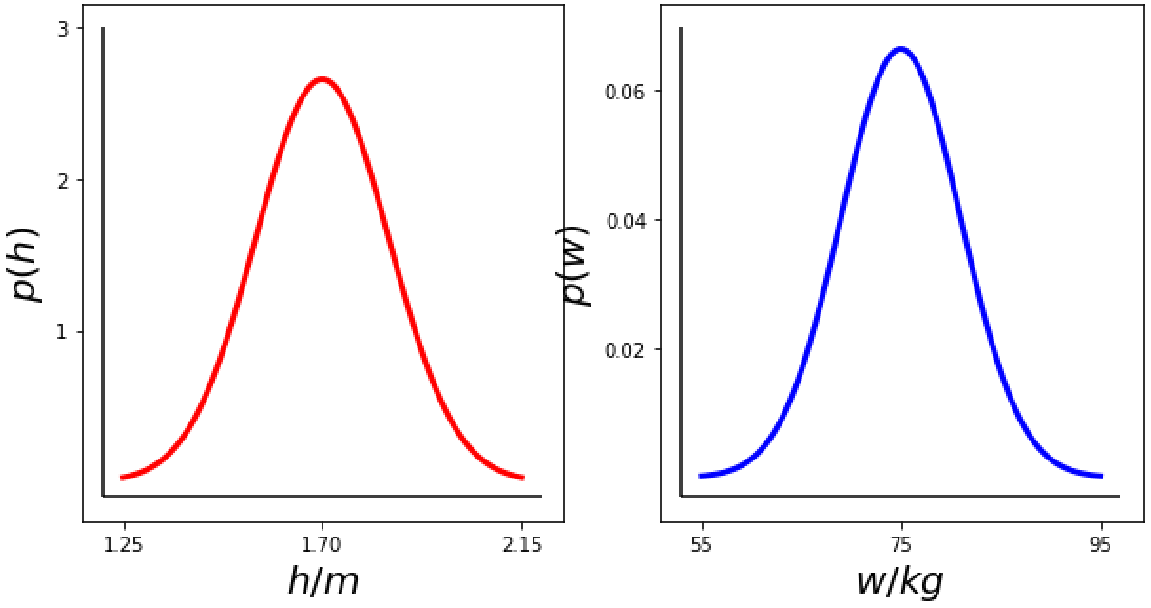
where $\tau^2 = \left(n\sigma^{-2} + \alpha_1^{-1}\right)^{-1}$ and $\mu = \frac{\tau^2}{\sigma^2}\sum_{i=1}^{n}(y_i - mx_i)$.

The Joint Density - Two-Dimensional Gaussian

Height and Weight Models (2D Gaussian)

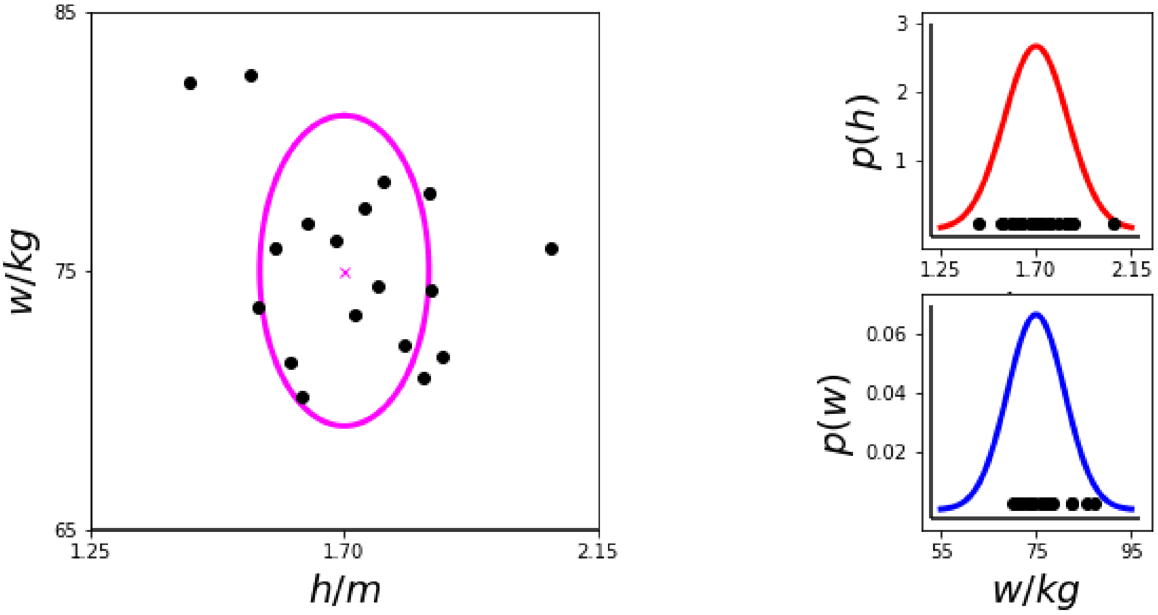
In [6]:

```
plot.height_weight()
```



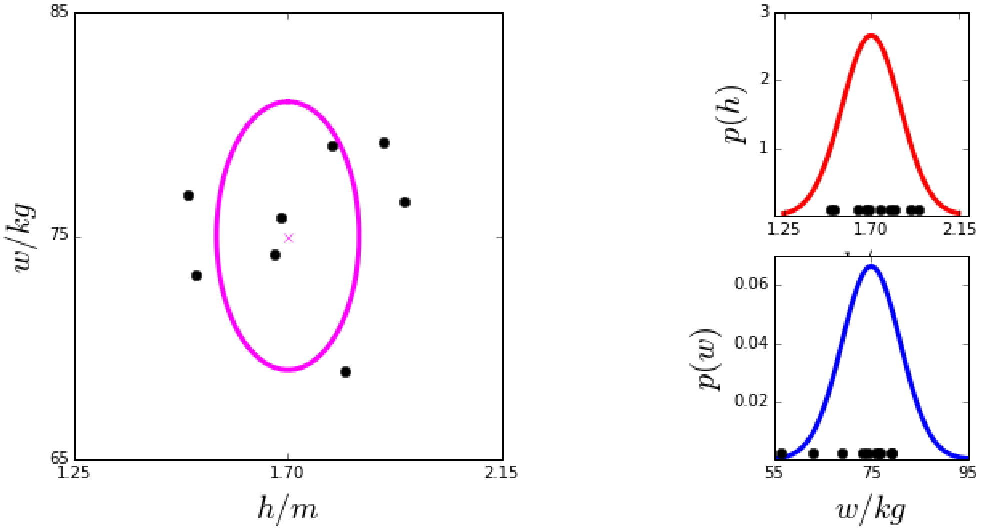
Sampling Two Independent Dimensional Variables

In [7]:
```
plot.independent_height_weight()
```



In [8]:
```
display_plots('independent_height_weight{fig:0>3}.png', './diagrams', fig=(0, 79))
```

fig 39



Independence Assumption

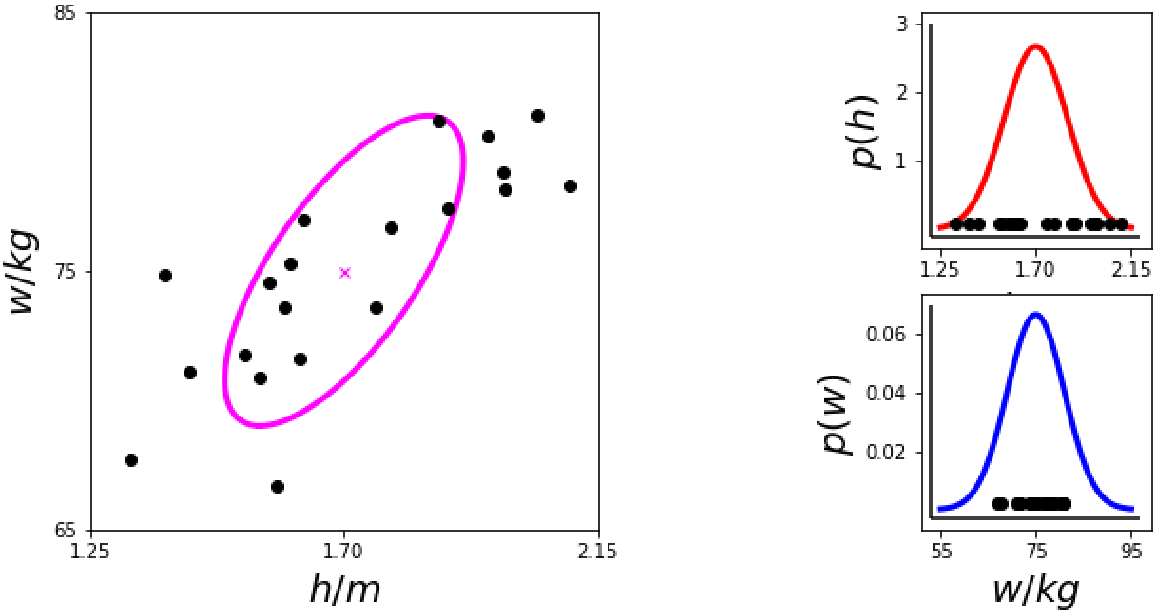
- This assumes height and weight are independent.

$$p(h, w) = p(h)p(w)$$

- In reality they are dependent (body mass index) $= \frac{w}{h^2}$.

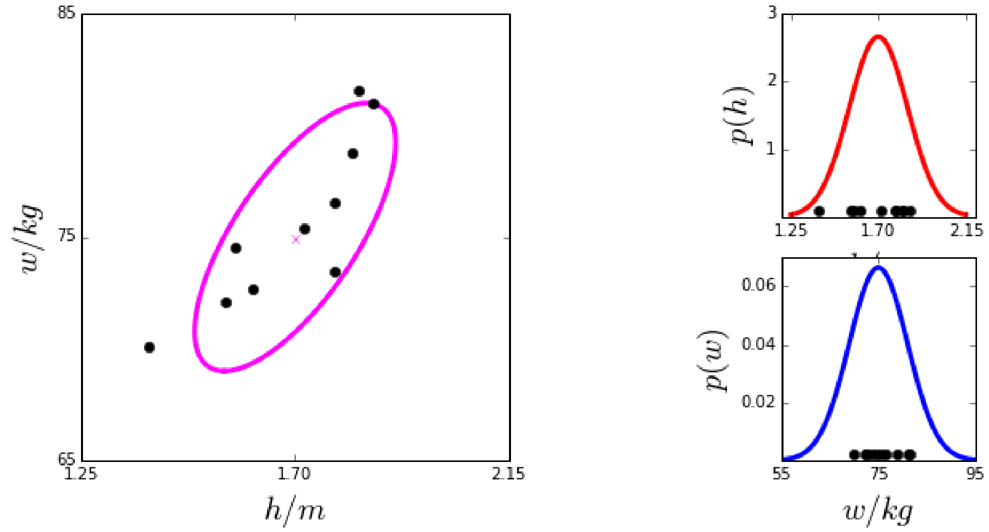
Sampling Two Dependent Dimensional Variables

```
In [9]: plot.correlated_height_weight()
```



```
In [10]: display_plots('correlated_height_weight{fig:0>3}.png', './diagrams', fig=(0, 79))
```

fig 39



Independent Gaussians (2D)

$$p(w,h) = p(w)p(h)$$

$$p(w,h) = \frac{1}{\sqrt{2\pi\sigma_1^2}\sqrt{2\pi\sigma_2^2}}\exp\left(-\frac{1}{2}\left(\frac{(w-\mu_1)^2}{\sigma_1^2}+\frac{(h-\mu_2)^2}{\sigma_2^2}\right)\right)$$

Independent Gaussians (rewritten in vector form)

$$p(w,h) = \frac{1}{\sqrt{2\pi\sigma_1^2 2\pi\sigma_2^2}} \exp\left(-\frac{1}{2}\left(\begin{bmatrix} w \\ h \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right)^\top \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}^{-1} \left(\begin{bmatrix} w \\ h \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right)\right)$$

Independent Gaussians (rewritten in vector/matrix notation)

$$p(\mathbf{y}) = \frac{1}{|2\pi\mathbf{D}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \mathbf{D}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right)$$

From Independent (uncorrelated) Gaussian to Correlated Gaussian

Read: Correlation and dependence (https://en.wikipedia.org/wiki/Correlation_and_dependence): Uncorrelatedness is equivalent to independence for jointly normal variables.

Form correlated from original by rotating the data space using rotation matrix (https://en.wikipedia.org/wiki/Rotation_matrix) $\mathbf{R}$.

$$p(\mathbf{y}) = \frac{1}{|2\pi\mathbf{D}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \mathbf{D}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right)$$

Multiply the data by a rotation matrix $\mathbf{R}$

$$p(\mathbf{y}) = \frac{1}{|2\pi\mathbf{D}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{R}^\top\mathbf{y}-\mathbf{R}^\top\boldsymbol{\mu})^\top \mathbf{D}^{-1}(\mathbf{R}^\top\mathbf{y}-\mathbf{R}^\top\boldsymbol{\mu})\right)$$

Collect $\mathbf{R}$ to the left and right of $\mathbf{D}$

$$p(\mathbf{y}) = \frac{1}{|2\pi\mathbf{D}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \mathbf{R}\mathbf{D}^{-1}\mathbf{R}^\top(\mathbf{y}-\boldsymbol{\mu})\right)$$

Let

$$\mathbf{C}^{-1} = \mathbf{R}\mathbf{D}^{-1}\mathbf{R}^\top$$

Rewritten in typical Guassian form

$$p(\mathbf{y}) = \frac{1}{|2\pi\mathbf{C}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\top \mathbf{C}^{-1}(\mathbf{y}-\boldsymbol{\mu})\right)$$

This gives a **covariance matrix** for correlated variables (the general case):

$$\mathbf{C} = \mathbf{R}\mathbf{D}\mathbf{R}^\top$$

Note $|\mathbf{C}| = |\mathbf{D}|$, see Determinant of Matrix Product (https://proofwiki.org/wiki/Determinant_of_Matrix_Product)

Practical multivariate data are correlated. Thus, we can rotate the axis to make the new, transformed data uncorrelated. This is exactly what Principal Component Analysis is doing, which is the topic of the next Session. In the assigment, you will deal with correlated Gaussians. And we need to determine the mean $\boldsymbol{\mu}$ and the covariance $\mathbf{C}$, instead of the mean and variance in the univariate case.

Reading

- Section 2.3 of @Bishop:book06 up to top of pg 85 (multivariate Gaussians).
- Section 3.3 of @Bishop:book06 up to 159 (pg 152–159).

Revisit Olympics Data

- Use Bayesian approach on olympics data with polynomials.
- Choose a prior $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \alpha \mathbf{I})$ with $\alpha = 1$.
- Choose noise variance $\sigma^2 = 0.01$

Sampling the Prior

- Always useful to perform a 'sanity check' and sample from the prior before observing the data.
- Since $\mathbf{y} = \mathbf{\Phi}\mathbf{w} + \epsilon$ just need to sample

$$w \sim \mathcal{N}(0, \alpha)$$
$$\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2)$$

with $\alpha = 1$ and $\sigma^2 = 0.01$.

In [11]:

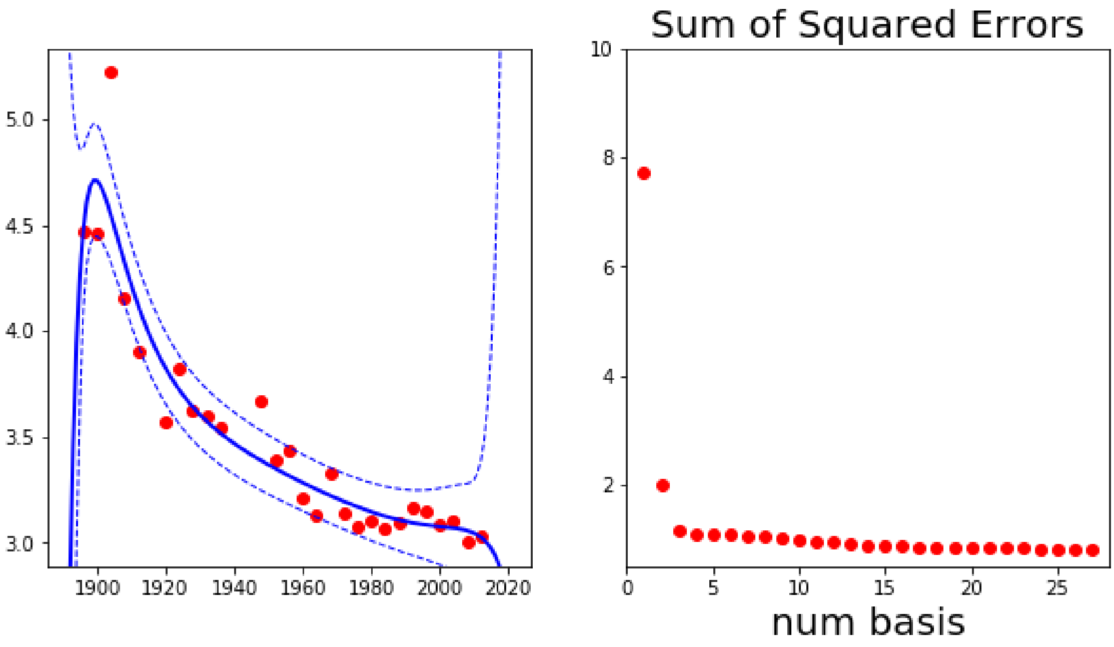
```
basis = mlai.polynomial
data = pods.datasets.olympic_marathon_men()
x = data['X']
y = data['Y']
num_data = x.shape[0]

data_limits = [1892, 2020]

max_basis = y.shape[0]
```

In [12]:

```
plot.rmse_fit(x, y, param_name='num_basis', param_range=(1, max_basis+1),
              model=mlai.BLM, basis=basis, alpha=1, sigma2=0.04, data_limits=data_li
              xlim=data_limits, objective_ylim=[0.5,10])
```

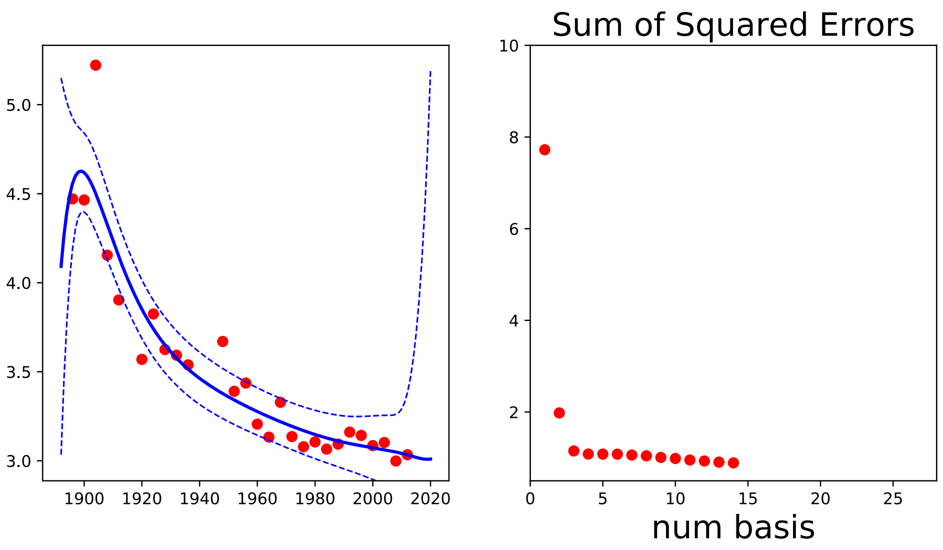


Olympic Data with Bayesian Polynomials

In [13]:

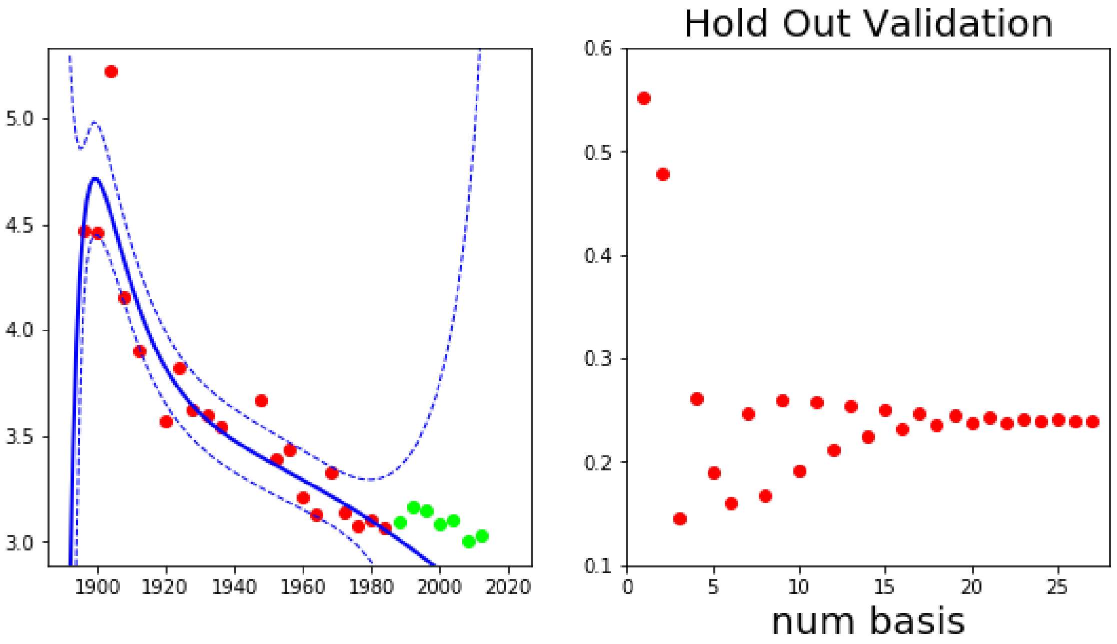
```
display_plots('olympic_BLM_polynomial_num_basis{num_basis:0>3}.svg',
                                directory='./diagrams', num_basis=(1, max_basis))
```

num_basis 14



In [14]:

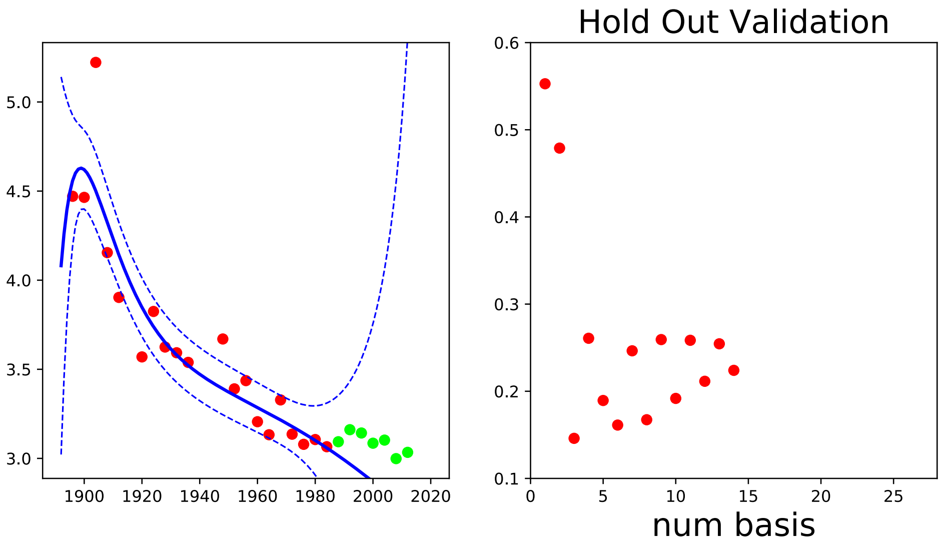
```
plot.holdout_fit(x, y, param_name='num_basis', param_range=(1, max_basis+1),
                model=mlai.BLM, basis=basis, alpha=1, sigma2=0.04, data_limits=data_li
                xlim=data_limits, objective_ylim=[0.1,0.6], permute=False)
```



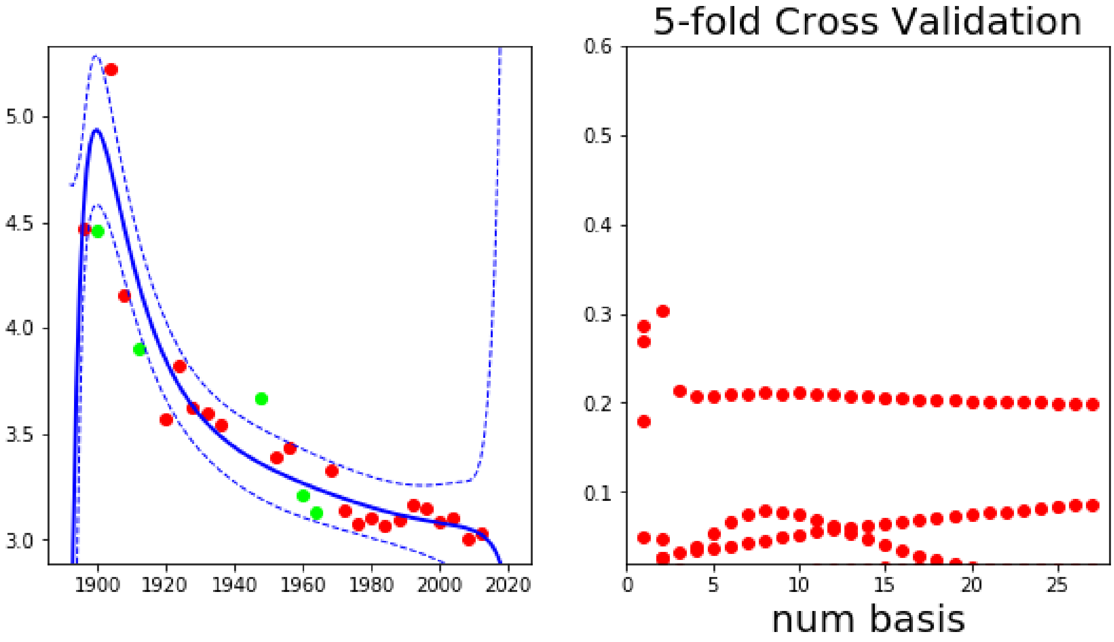
Hold Out Validation

In [15]:
```
display_plots('olympic_val_BLM_polynomial_num_basis{num_basis:0>3}.svg',
                                  directory='./diagrams', num_basis=(1, 27))
```

num_basis 14



In [16]:
```
num_parts=5
plot.cv_fit(x, y, param_name='num_basis', param_range=(1, max_basis+1),
                 model=mlai.BLM, basis=basis, alpha=1, sigma2=0.04, data_limits=data_li
                 xlim=data_limits, objective_ylim=[0.02,0.6], num_parts=num_parts)
```

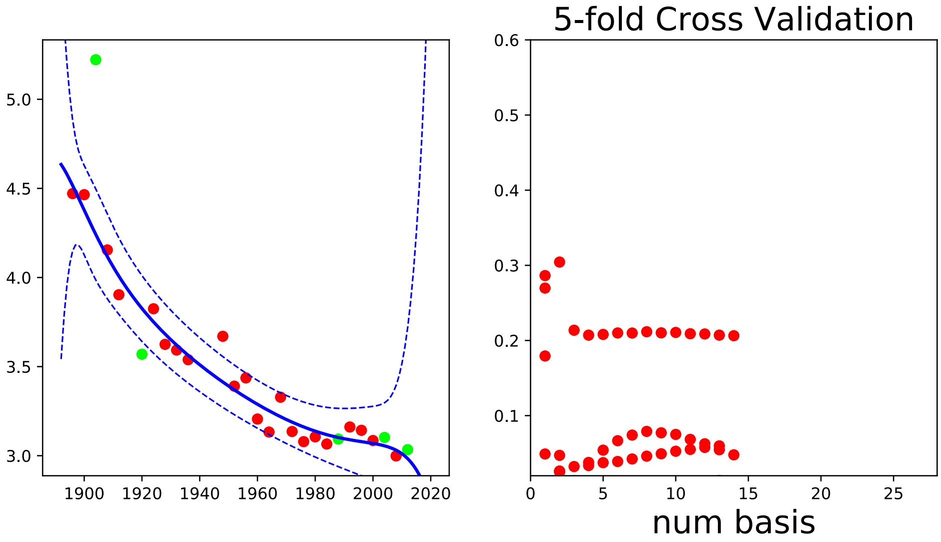


5-fold Cross Validation

In [17]:
```
display_plots('olympic_5cv{part:0>2}_BLM_polynomial_num_basis{num_basis:0>3}.svg',
                            directory='./diagrams', part=(0, 5), num_basis=(1, max_b
```

part 2

num_basis 14



Model Fit: Bayesian vs Maximum Likelihood

- Marginal likelihood doesn’t always increase as model order increases.
- Presented Bayesian model has 2 parameters, regardless of how many basis functions (and here we didn’t even fit them).
- Maximum likelihood model over fits through increasing number of parameters.
- Revisit maximum likelihood solution with validation set.

Regularized Mean

- Validation fit here based on mean solution for $\mathbf{w}$ only.
- For Bayesian solution
$$\boldsymbol{\mu}_w = \left[\sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi} + \alpha^{-1}\mathbf{I}\right]^{-1}\sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y}$$
maximum likelihood solution
$$\mathbf{w}^* = \left[\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\right]^{-1}\boldsymbol{\Phi}^\top\mathbf{y}$$
- Two are equivalent when $\alpha \rightarrow \infty$.
- Equivalent to a prior for $\mathbf{w}$ with infinite variance.
- In other cases $\alpha\mathbf{I}$ *regularizes* the system (keeps parameters smaller).

Sampling the Posterior

- Now check samples by extracting $\mathbf{w}$ from the *posterior*.
- Now for $\mathbf{y} = \boldsymbol{\Phi}\mathbf{w} + \epsilon$ need
$$w \sim \mathcal{N}(\boldsymbol{\mu}_w, \mathbf{C}_w)$$
with $\mathbf{C}_w = \left[\sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi} + \alpha^{-1}\mathbf{I}\right]^{-1}$ and $\boldsymbol{\mu}_w = \mathbf{C}_w\sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y}$
$$\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I})$$
with $\alpha = 1$ and $\sigma^2 = 0.01$.

Marginal Likelihood

- The marginal likelihood can also be computed, it has the form:
$$p(\mathbf{y}|\mathbf{X}, \sigma^2, \alpha) = \frac{1}{(2\pi)^{\frac{n}{2}}|\mathbf{K}|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}\mathbf{y}^\top\mathbf{K}^{-1}\mathbf{y}\right)$$
where $\mathbf{K} = \alpha\mathbf{\Phi}\mathbf{\Phi}^\top + \sigma^2\mathbf{I}$.
- So it is a zero mean n-dimensional Gaussian with covariance matrix $\mathbf{K}$.
- Marginalisation: remove the effect of a random variable from a joint distribution over multiple random variables, resulting in the marginal distribution. For discrete distributions, this means summing over the variable,
$$p(x) = \sum_y p(x, y)$$
For continuous distributions (PDFs), this means integrating,
$$p(x) = \int_y p(x, y)dy$$

Computing the Expected Output

- Given the posterior for the parameters, how can we compute the expected output at a given location?
- Output of model at location $\mathbf{x}_i$ is given by
$$f(\mathbf{x}_i; \mathbf{w}) = \boldsymbol{\phi}_i^\top\mathbf{w}$$
- We want the expected output under the posterior density, $p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \sigma^2, \alpha)$.
- Mean of mapping function will be given by
$$\begin{aligned}\left\langle f(\mathbf{x}_i; \mathbf{w})\right\rangle_{p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \sigma^2, \alpha)} &= \boldsymbol{\phi}_i^\top\left\langle\mathbf{w}\right\rangle_{p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \sigma^2, \alpha)} \\ &= \boldsymbol{\phi}_i^\top\boldsymbol{\mu}_w\end{aligned}$$

Variance of Expected Output

- Variance of model at location $\mathbf{x}_i$ is given by
$$\begin{aligned}\text{var}(f(\mathbf{x}_i; \mathbf{w})) &= \left\langle(f(\mathbf{x}_i; \mathbf{w}))^2\right\rangle - \left\langle f(\mathbf{x}_i; \mathbf{w})\right\rangle^2 \\ &= \boldsymbol{\phi}_i^\top\left\langle\mathbf{w}\mathbf{w}^\top\right\rangle\boldsymbol{\phi}_i - \boldsymbol{\phi}_i^\top\left\langle\mathbf{w}\right\rangle\left\langle\mathbf{w}\right\rangle^\top\boldsymbol{\phi}_i \\ &= \boldsymbol{\phi}_i^\top\mathbf{C}_i\boldsymbol{\phi}_i\end{aligned}$$
where all these expectations are taken under the posterior density, $p(\mathbf{w}|\mathbf{y}, \mathbf{X}, \sigma^2, \alpha)$.

Reading

- Section 3.7–3.8 of @Rogers:book11 (pg 122–133).
- Section 3.4 of @Bishop:book06 (pg 161–165).