University of BRISTOL

Machine Learning

Linear Regression

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Introduction

So Far

- Lecture 1 What is machine Learning
  - assumptions are the fundation of learning
  - probabilities are the language of assumptions

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  - distributions are the parametrised form of a probability

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- Lecture 1 What is machine Learning
  - assumptions are the fundation of learning
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- Lecture 2 Probabilities
  - what are the rules of probability
  - distributions are the parametrised form of a probability
- Lecture 3 Distributions
  - discrete and continous distributions
  - conjugate distributions

Conjugacy

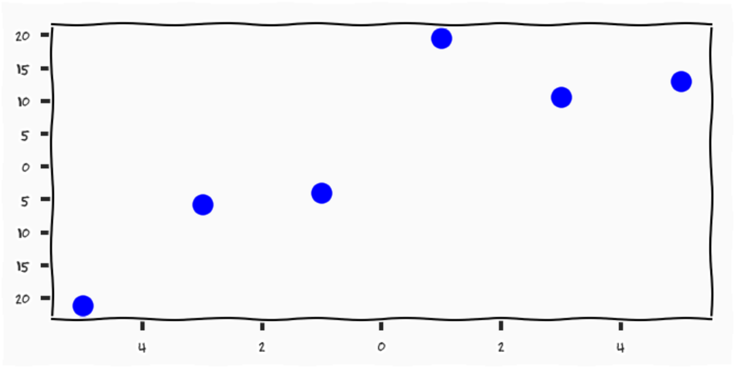
$$p(\theta|y) = P(y|\theta) \cdot p(\theta)\frac{1}{p(y)} \propto P(y|\theta) \cdot p(\theta)$$

$$p(y) = \int p(y|\theta)p(\theta)\mathrm{d}\theta$$

- A conjugate prior to a likelihood is such that the prior and the posterior is in the same functional family
- Knowing the form of the posterior allows us to avoid computing the evidence and just identify parameters

Linear Regression

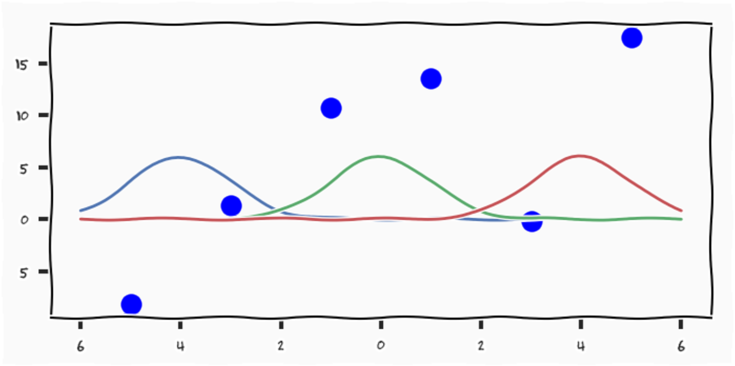
Linear Regression [1] Ch 3.1



- Linear function in both parameters and data

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \dots w_D x_D = \mathbf{w}^{\mathrm{T}} \mathbf{x} + w_0 = \{D = 1\} w_0 + w_1 * x$$

Linear Regression



- Linear function only in parameters

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \{\phi_0(\mathbf{x}) = 1\} = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x})$$

Linear Regression

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x})$$
$$= \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} 1 \\ x \end{bmatrix}$$

- Given observations of data pairs $\mathcal{D} = \{y_i, \mathbf{x}_i\}_{i=1}^{N}$ can we infer what $\mathbf{w}$ should be

Task 1 define a likelihood

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- what output do I consider likely under a given model?

Linear Regression

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Linear Regression

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Linear Regression

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Task 3 update my belief with new observations

- formulate posterior

Task 4 predict using my new belief

- formulate predictive distribution

Linear Regression

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \beta^{-1} I)$$

- We assume that we have been given data pairs $\{t_i, \mathbf{x}_i\}_{i=1}^{N}$ corrupted by addative noise
- We assume that the distribution of the noise follows a Gaussian

Likelihood

$$t = \mathsf{w}^{\mathrm{T}}\phi(\mathsf{x}) + \epsilon$$

Likelihood

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$$t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) = \epsilon$$

Likelihood

$$
\begin{aligned}
t &= \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon \\
t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) &= \epsilon \\
t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) &\sim \mathcal{N}(\epsilon|0, \beta^{-1}I) = \left(\frac{\beta}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)}
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$$
\Rightarrow \mathcal{N}(t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x})|0, \beta^{-1}I) = \left(\frac{\beta}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{1}{2}(t-\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}))\beta(t-\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}))}
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&\Rightarrow \mathcal{N}(t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x})|0, \beta^{-1}I) = \mathcal{N}(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}I)
\end{aligned}
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Likelihood

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$$t - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) \sim \mathcal{N}(\epsilon|0, \beta^{-1}I) = \left(\frac{\beta}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)}$$

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$$\Rightarrow p(t|\mathbf{w}, \mathbf{x}) = \mathcal{N}(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}I)$$

Likelihood

- Likelihood

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \beta^{-1}\right)$$

- Independence

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n), \beta^{-1}\right)$$

Assume each output to be independent given the input and the parameters

Maximum Likelihood

- If we want we can avoid using our belief and simply pick the model that maximises our likelihood
- In this setting you can think of the likelihood as a quantification of an error
- Find the parameters that minimises the error

Maximum Likelihood

- If we want we can avoid using our belief and simply pick the model that maximises our likelihood
- In this setting you can think of the likelihood as a quantification of an error
- Find the parameters that minimises the error
- *Why is this a scary thing to do?*

Maximum Likelihood [1] Ch 3.1.1

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n), \beta^{-1}\right)$$

Maximum Likelihood [1] Ch 3.1.1

$$
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p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) &= \prod_{n=1}^{N} \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n), \beta^{-1}\right) \\
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Maximum Likelihood [1] Ch 3.1.1

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Maximum Likelihood [1] Ch 3.1.1

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$$= \prod_{n=1}^{N} \frac{1}{(2\pi\beta^{-1})^{\frac{1}{2}}} e^{-\frac{1}{2}\beta(t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n))^2}$$

$$= (\frac{\beta}{2\pi})^{\frac{N}{2}} e^{-\frac{\beta}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n))^2}$$

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \frac{N}{2}(\log(\beta) - \log(2\pi)) - \beta\frac{1}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n))^2$$

Maximum Likelihood

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \frac{N}{2}(\underbrace{\log(\beta)}_{\text{A}} - \underbrace{\log(2\pi)}_{\text{B}}) \underbrace{- \beta\frac{1}{2}\sum_{n=1}^{N}(t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n))^2}_{\text{C}}$$

A noise precision

B constant

C error

Maximum Likelihood

- Take derivative

$$\nabla \log p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \beta \sum_{n=1}^{N} (t_n - \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_n)) \phi(\mathbf{x}_n)^{\mathrm{T}}$$

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- Stationary point

$$0 = \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n)^{\mathrm{T}} - \mathbf{w}^{\mathrm{T}} \left(\sum_{n=1}^{N} \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^{\mathrm{T}} \right)$$

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- Solve for parameters $\mathbf{w}$

$$\mathbf{w}_{\mathrm{ML}} = (\phi(\mathbf{X})^{\mathrm{T}} \phi(\mathbf{X}))^{-1} \phi(\mathbf{X})^{\mathrm{T}} \mathbf{t}$$

Maximum Likelihood

- Take derivative

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- and precision

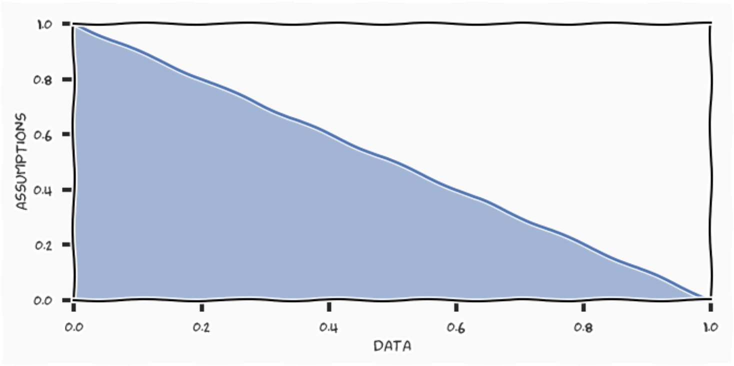
$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{n=1}^{N} (t_n - \mathbf{w}_{\mathrm{ML}}^{\mathrm{T}} \phi(\mathbf{x}_n))^2$$

Maximum Likelihood

$$\mathbf{w}_{\mathsf{ML}} = \underbrace{(\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X}))^{-1}\phi(\mathbf{X})^{\mathrm{T}}}_{\phi(\mathbf{X})^{+}}\mathbf{t}$$

- Moore-Penrose inverse (`np.linalg.pinv` in numpy)

Data



Bayesian Linear Regression [1] Ch 3.3

- Likelihood is Gaussian in $\mathbf{w}$

$$p(t|\mathbf{w}, \mathbf{x}) = \mathcal{N}(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}I)$$

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- Conjugate Prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$$

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$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$$

- Posterior

$$p(w|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N\right)$$

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- $\mathbf{m}_N, \mathbf{S}_N$ is the mean and the co-variance of the posterior after having seen N data-points

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- $\mathbf{m}_N, \mathbf{S}_N$ is the mean and the co-variance of the posterior after having seen N data-points
- Gaussian identities

Posterior

- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{t},\mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N,\mathbf{S}_N)$$

Posterior

- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

- Identification

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

Posterior

- Posterior is Gaussian

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

- Identification

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- Posterior

$$\mathbf{m}_N = \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}\left(S_0^{-1}\mathbf{m}_0 + \beta\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}\right)$$
$$\mathbf{S}_N = \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}$$

Posterior

- Assumption Zero mean isotropic Gaussian

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

Posterior

- Assumption Zero mean isotropic Gaussian

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

- Posterior

$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\beta \left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1} \phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}, \left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1})$$

Posterior

- Assumption Zero mean isotropic Gaussian

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

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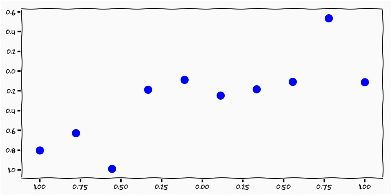
$$\left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1})$$

- ML

$$\mathbf{w}_{\mathrm{ML}} = (\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X}))^{-1}\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}$$

Linear Regression Example [1] Figure 3.7



- Model

$$y(x, \mathbf{w}) = w_0 + w_1 x$$

- Data

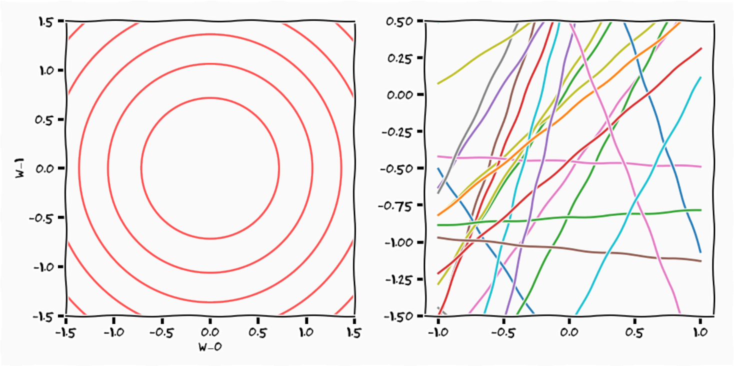
$$f(x, \mathbf{a}) = a_0 + a_1 x, \ \{a_0, a_1\} = \{-0.3, 0.5\}$$

$$t = f(x, \mathbf{a}) + \epsilon, \ \epsilon \sim \mathcal{N}(0, 0.2^2)$$

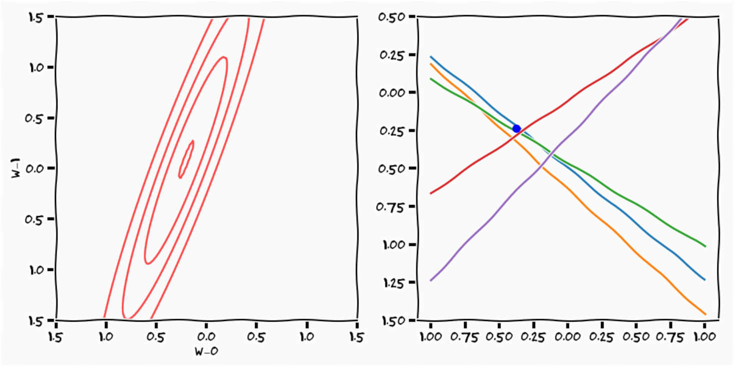
- Prior

$$p(\mathbf{w}) = \mathcal{N}(\boldsymbol{w} | \mathbf{0}, 2.0 \cdot \mathbf{I})$$

Linear Regression Example



Linear Regression Example



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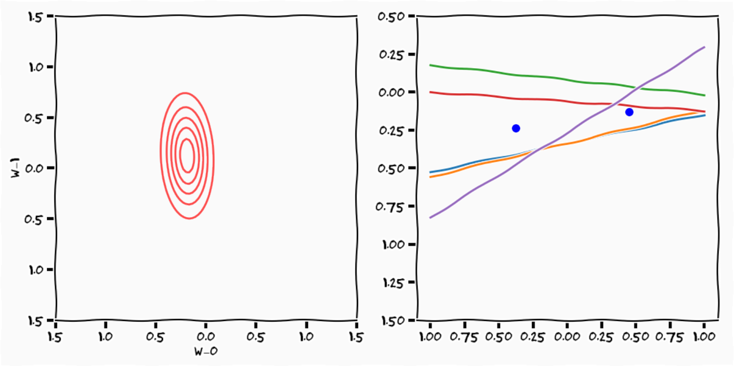

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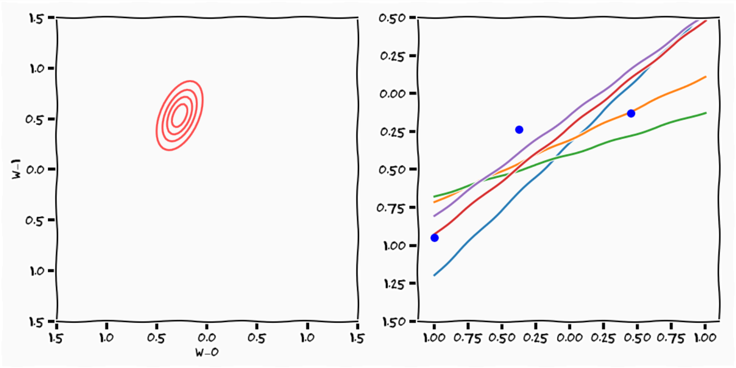
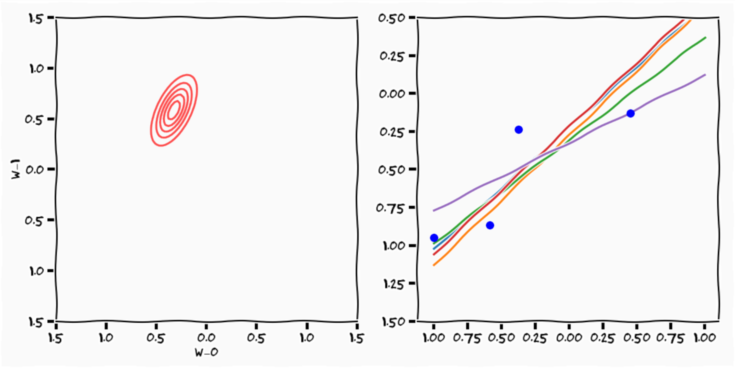
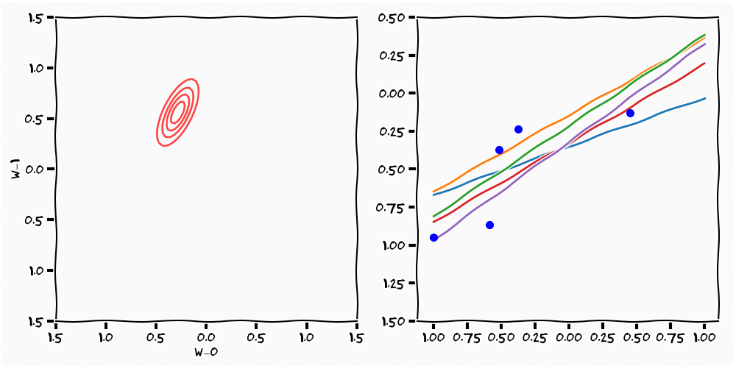


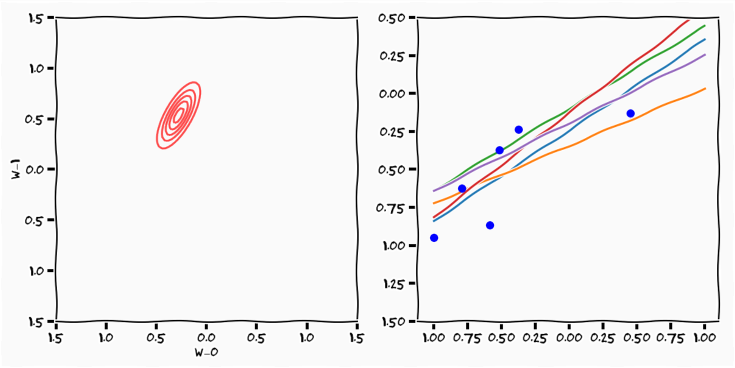
Linear Regression Example



Linear Regression Example



Linear Regression Example



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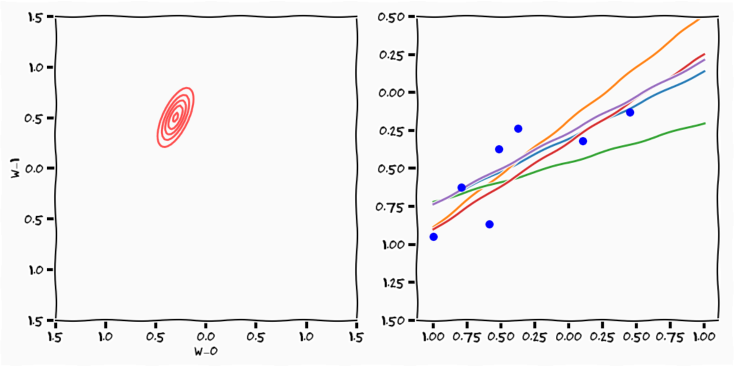
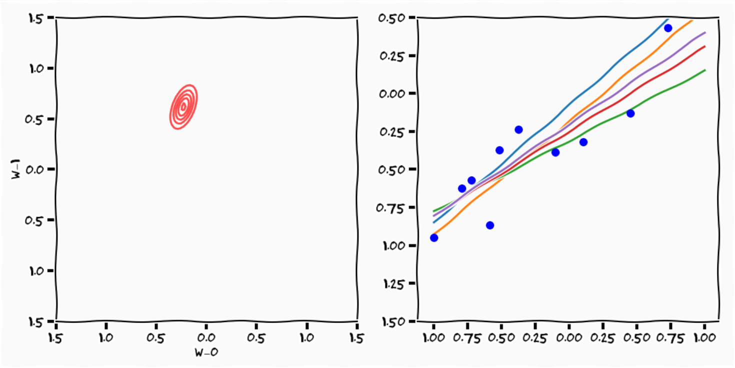


Linear Regression Example



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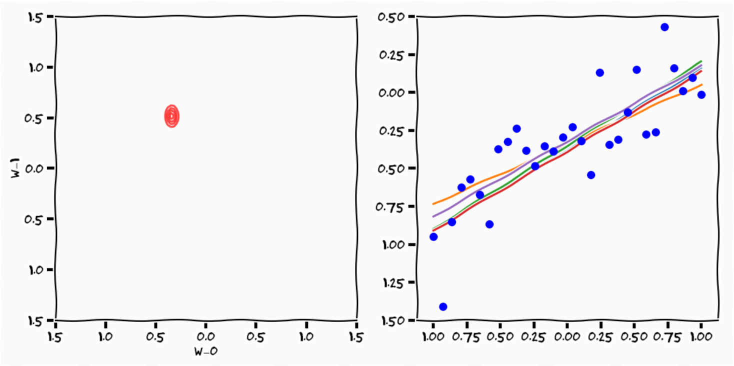

Linear Regression

- Don't underestimate what we just did

- Don't underestimate what we just did
- We saw data, which we knew where it came from

Linear Regression

- Don't underestimate what we just did
- We saw data, which we knew where it came from
- We made an assumption

Linear Regression

- Don't underestimate what we just did
- We saw data, which we knew where it came from
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- We recovered the system

Linear Regression

- Don't underestimate what we just did
- We saw data, which we knew where it came from
- We made an assumption
- We recovered the system
- We updated our knowledge from data!!!

- Don't underestimate what we just did
- We saw data, which we knew where it came from
- We made an assumption
- We recovered the system
- We updated our knowledge from data!!!
- Understand [1] 3.3

Statistics or Machine Learning

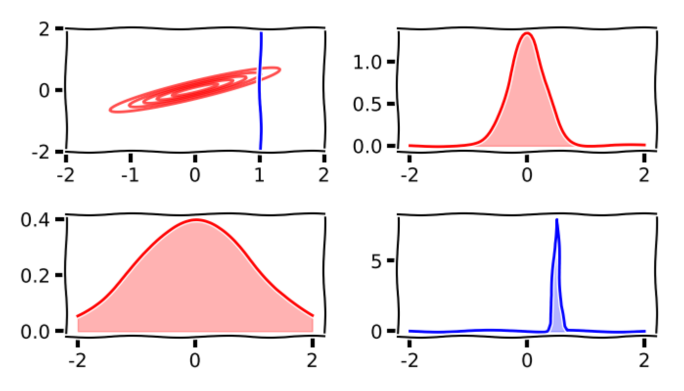
"The difference between statistics and machine learning is that the former cares about parameters while the latter cares about prediction"
– Prof. Neil D. Lawrence

Prediction

$$p(t_*|\mathbf{t}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta)p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta)\mathrm{d}\mathbf{w}$$

- we do not really care about w we care about new prediction t_* at location $\mathbf{x}_*$
- look at the marginal distribution, i.e. when we average out the weight
- integrate a Gaussian over a Gaussian $\Rightarrow$ Gaussian identities

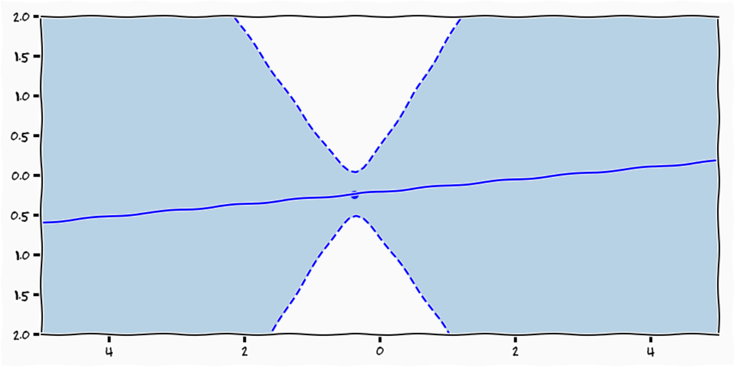
Prediction



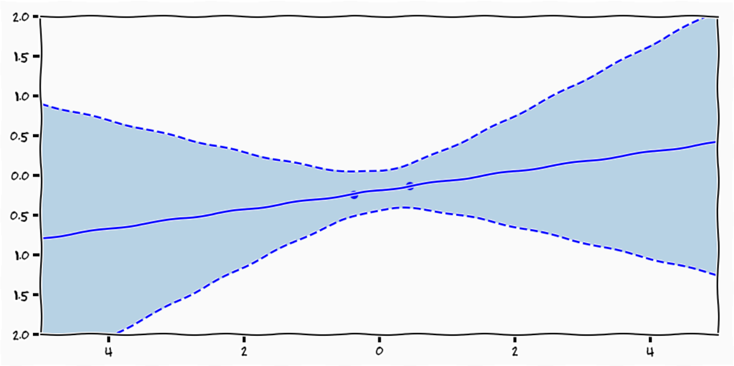
$$p(t_*|\mathbf{t}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta) \mathrm{d}\mathbf{w}$$

$$\mathcal{N}(t_*|\mathbf{m}_N^{\mathrm{T}} \phi(\mathbf{x}_*), \frac{1}{\beta} + \phi(\mathbf{x}_*)^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}_*))$$

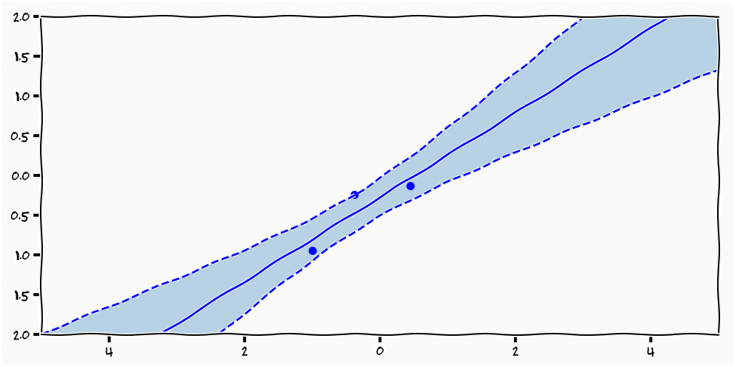
Predictive Posterior



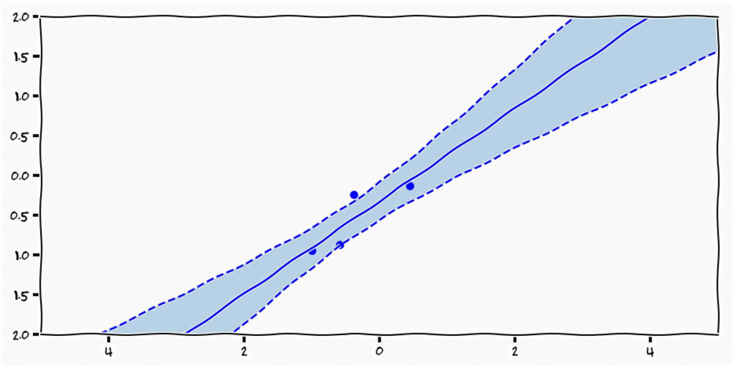
Predictive Posterior



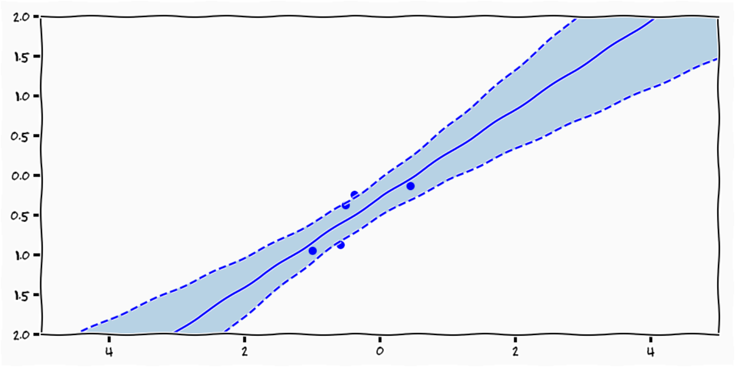
Predictive Posterior



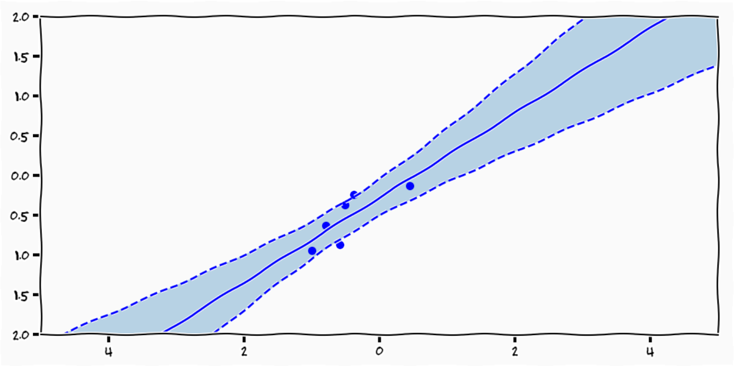
Predictive Posterior



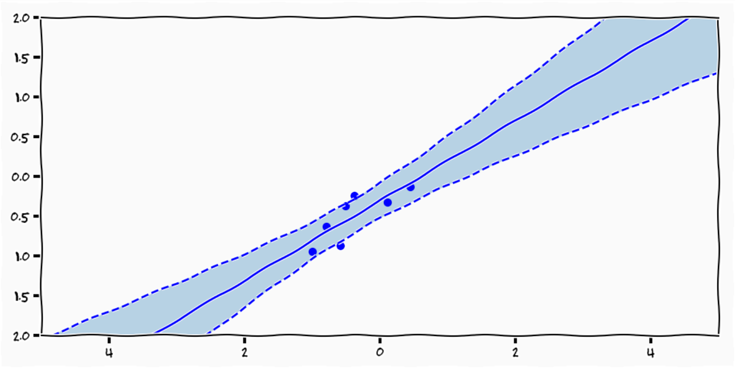
Predictive Posterior



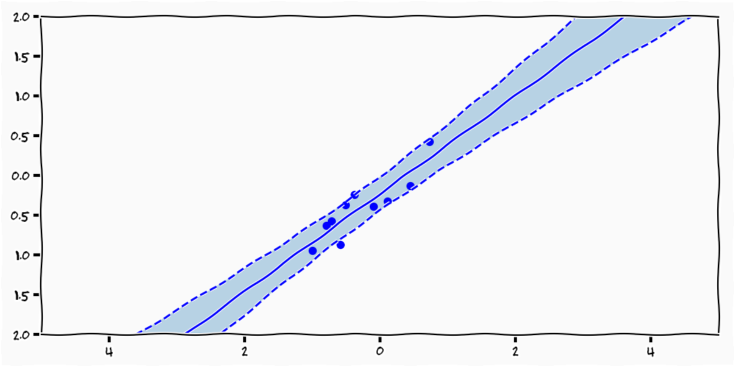
Predictive Posterior



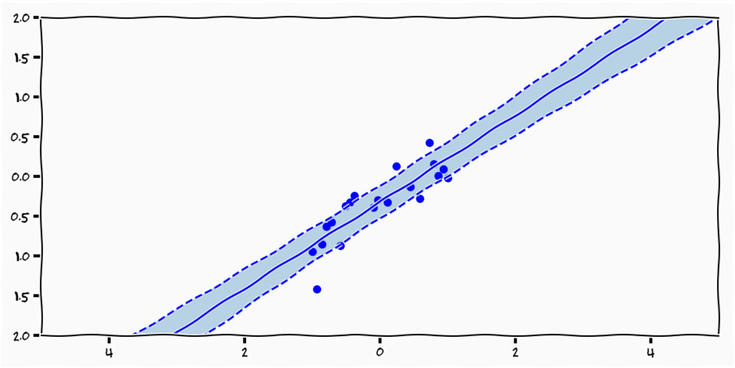
Predictive Posterior



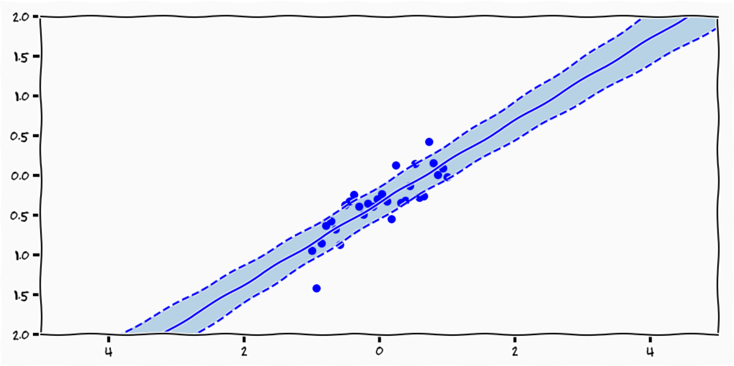
Predictive Posterior



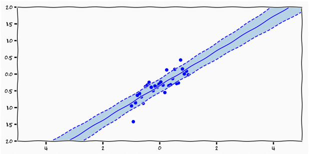
Predictive Posterior

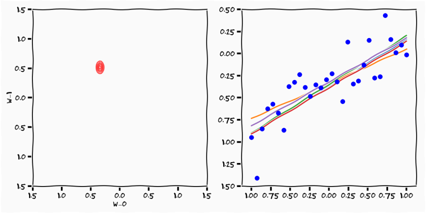


Predictive Posterior

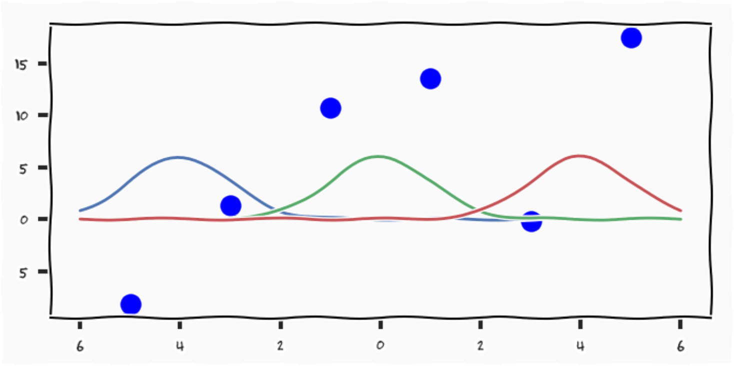


Signal and Noise





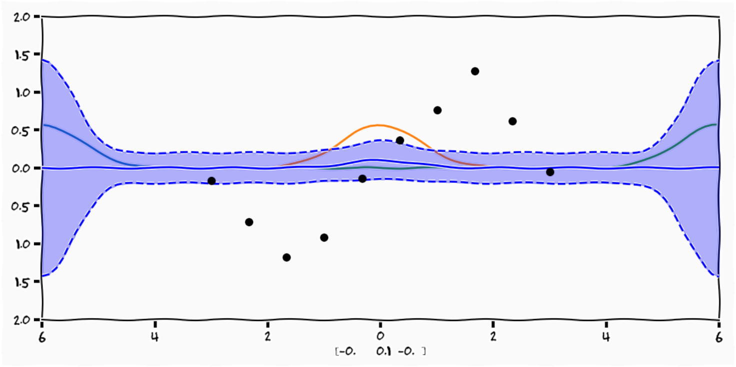
Linear Regression

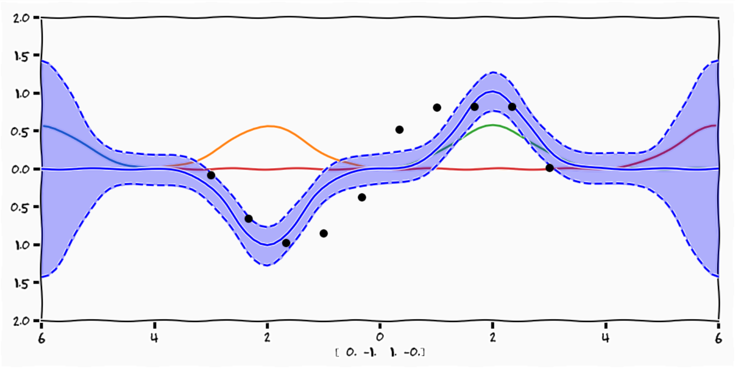


- Linear function only in parameters

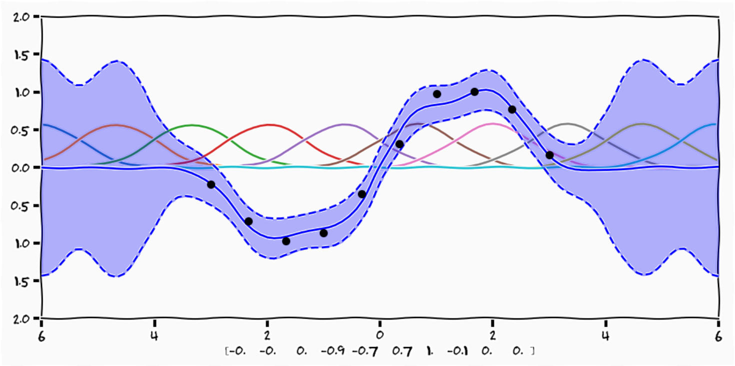
$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \{\phi_0(\mathbf{x}) = 1\} = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

Non-Linear Basis Functions

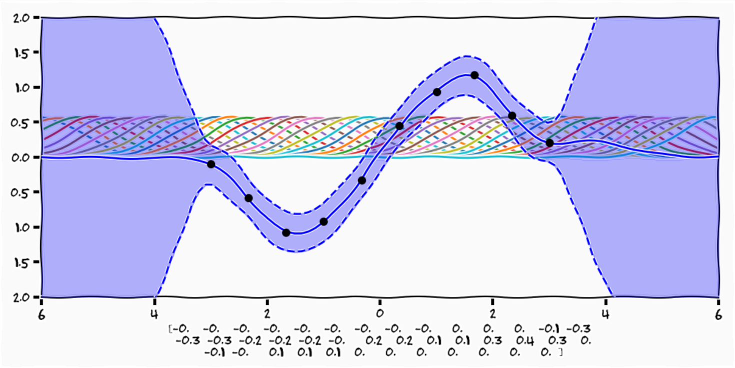


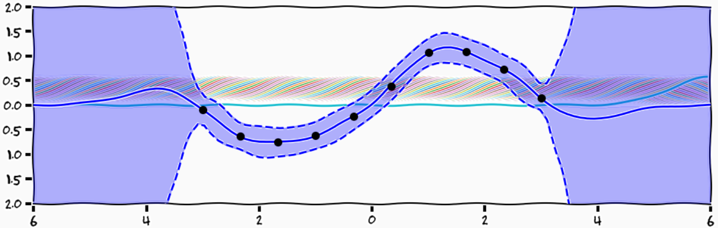

2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
6
4
2
0
2
4
6
[0. -1. 1. -0.]

Non-Linear Basis Functions



Non-Linear Basis Functions






```
[ 0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.   0.
  0.   0.   0.   0.   0.   0.   0.   0.  -0.  -0.  -0.  -0.1 -0.1 -0.1
 -0.1 -0.1 -0.1 -0.1 -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.1 -0.1
 -0.1 -0.1 -0.1 -0.1 -0.  -0.  -0.  -0.   0.   0.   0.   0.  -0.  -0.
 -0.  -0.  -0.  -0.  -0.   0.   0.   0.1  0.1  0.1  0.1  0.1  0.1  0.1
  0.1  0.1  0.1  0.1  0.1  0.   0.   0.   0.   0.   0.   0.1  0.1  0.1
  0.1  0.1  0.1  0.   0.   0.   0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.
 -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.
 -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0.  -0. ]
```

Summary

So Far

Lecture 1 What is machine Learning

- assumptions are the fundation of learning
- probabilities are the language of assumptions

Lecture 2 Probabilities

- what are the rules of probability
- distributions are the parametrised form of a probability

Lecture 3 Distributions

- discrete and continous distributions
- conjugate distributions

Today Models

- how to apply our assumptions to data
- how to learn for real

References

Christopher M. Bishop.
***Pattern Recognition and Machine Learning (Information Science and Statistics)*.**
Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006.