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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- Lecture 2 Probabilities
    - what are the rules of probability
    - distributions are the parametrised form of a probability

So Far

- 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

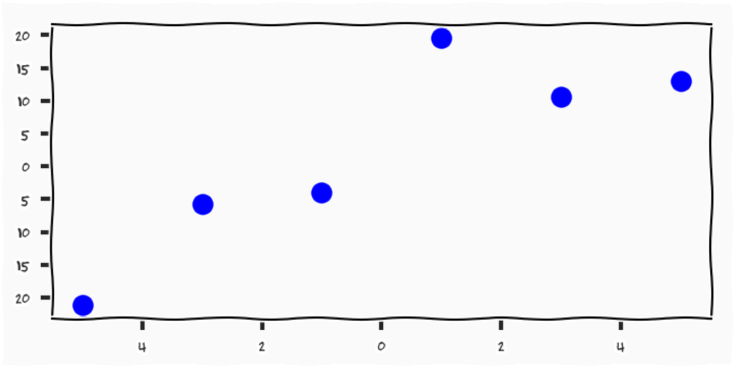
Conjugacy

$$= P(Y|\theta) \cdot p(\theta) \frac{1}{\int p(\mathbf{Y}|\theta) p(\theta) \mathrm{d}\theta} \qquad \propto P(Y|\theta)) \cdot p(\theta)$$

- 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

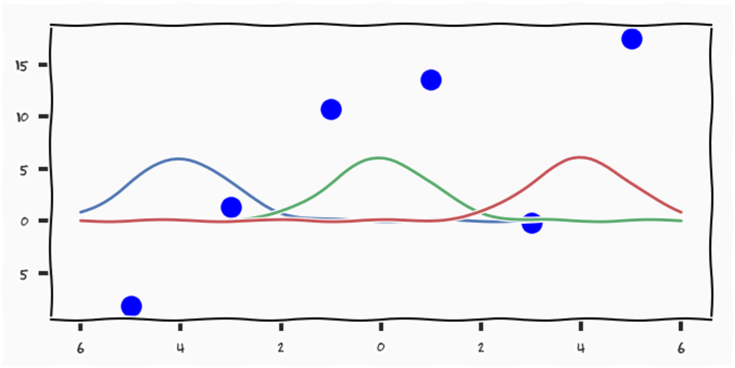
Linear Regression [1] Ch 3.1



- 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

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

- We can choose many types of basis functions $\phi(\mathbf{x})$

Linear Regression

Model

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

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

Linear Regression

Task 1 define a likelihood

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

Task 2 define an assumption of the model

- what types of models do I think are more probable than others
- $\Rightarrow$ what are my beliefs, i.e formulate prior

Task 3 update my belief with new observations

- formulate posterior

Task 4 predict using my new belief

- formulate predictive distribution

Likelihood

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

Likelihood

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

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

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}) &= \mathcal{N}(\epsilon | 0, \beta^{-1} I) = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}(\epsilon - 0)\beta(\epsilon - 0)}
\end{aligned}
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Likelihood

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

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

- By making an assumption of the noise we have reached a conditional distribution over the output given the model, i.e.

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

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

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) \\
&= \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}
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Maximum Likelihood [1] Ch 3.1.1

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&= (\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
\end{aligned}
$$

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

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

Maximum Likelihood

- Take derivative

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- Stationary point

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

Maximum Likelihood

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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

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

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- Solve for parameters **w**

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

- and precision

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

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)

Bayesian Linear Regression [1] Ch 3.3

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

Bayesian Linear Regression [1] Ch 3.3

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

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

Bayesian Linear Regression [1] Ch 3.3

- Likelihood is Gaussian in $\mathbf{w}$
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$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$$

- Posterior

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

Bayesian Linear Regression [1] Ch 3.3

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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

Bayesian Linear Regression [1] Ch 3.3

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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

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

- 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

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- Posterior

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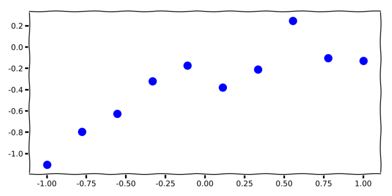
$$\left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1})$$

- 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

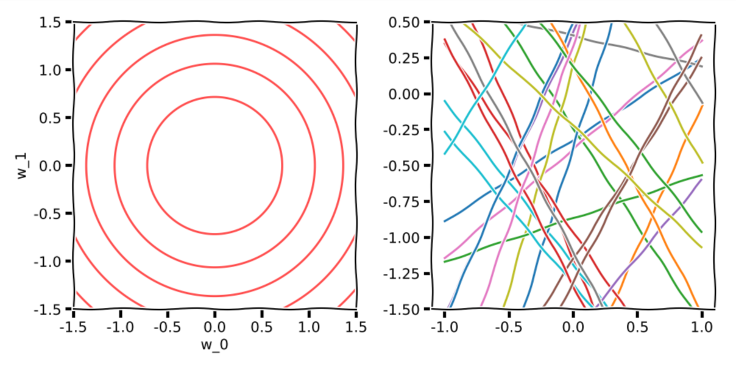
$$f(x, \mathbf{a}) = a_0 + a_1 x,\ \{a_0, a_1\} = \{-0.3, 0.5\}$$

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

- Prior

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

Linear Regression Example



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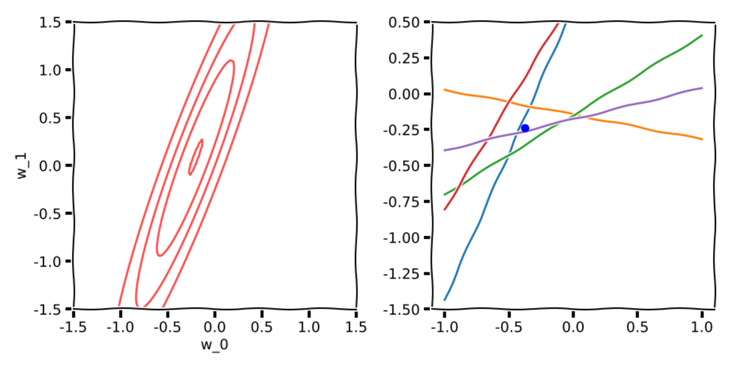

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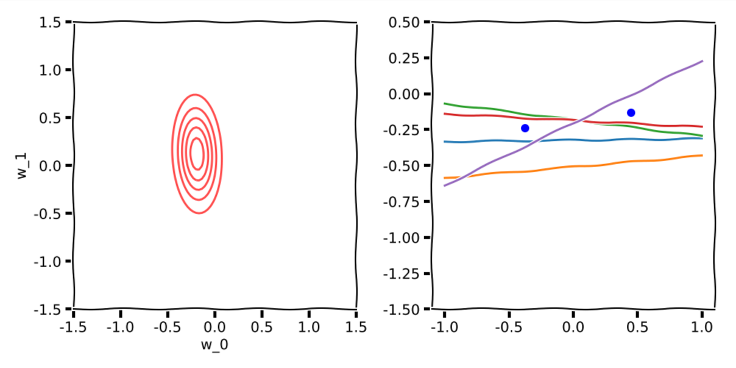

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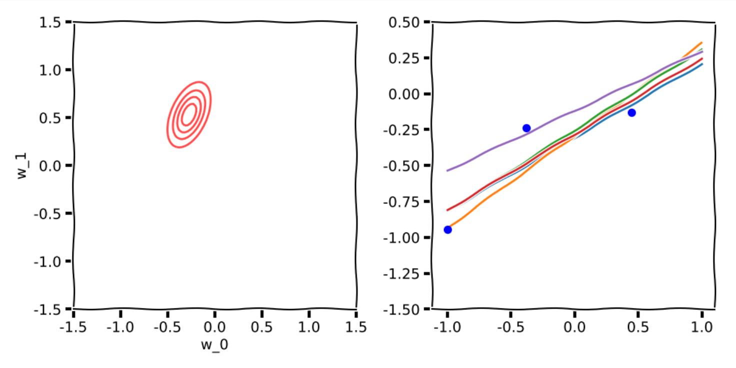

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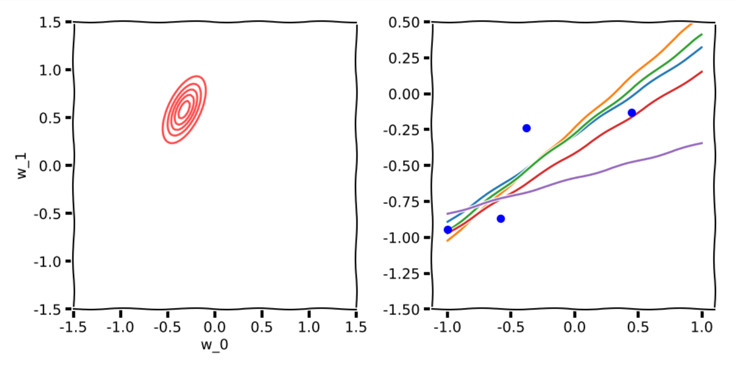

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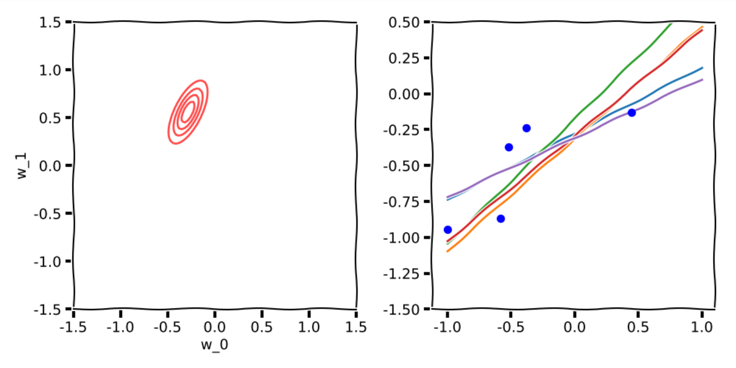

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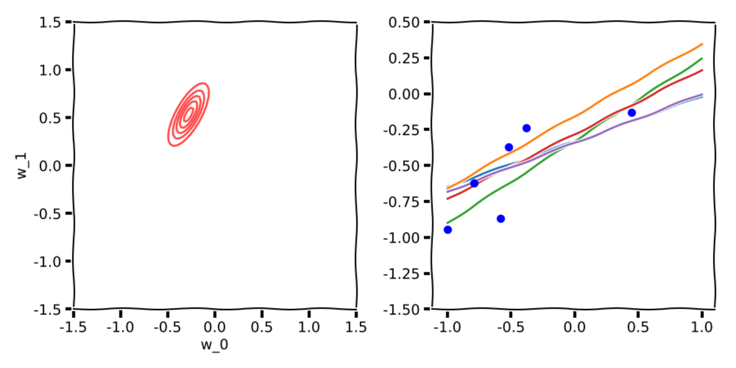

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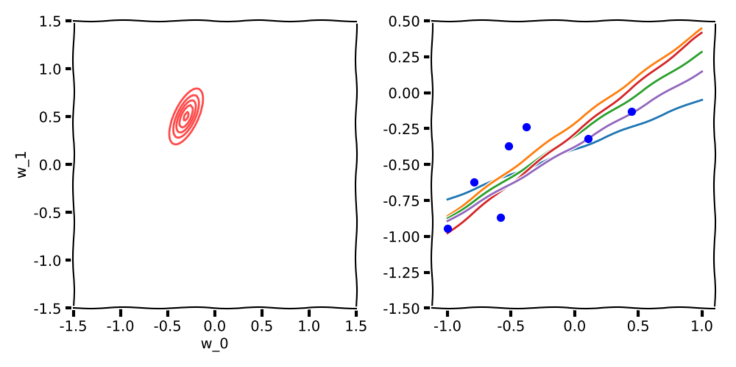

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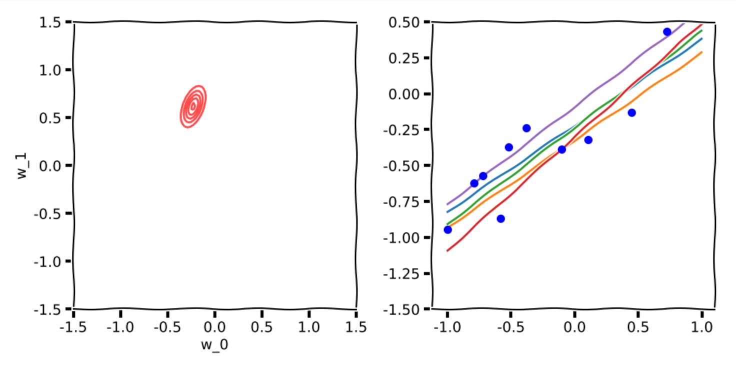

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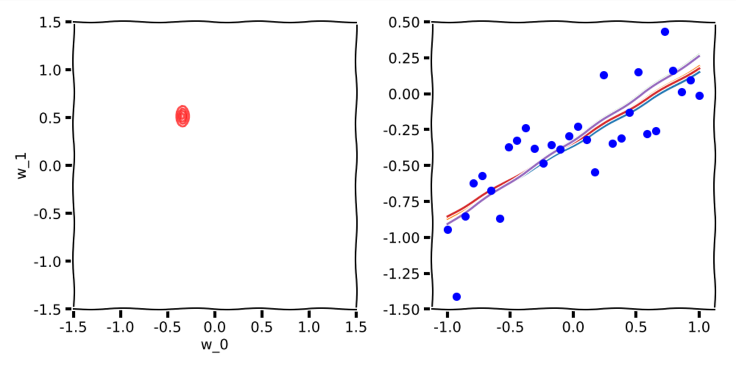

Linear Regression

- Don't underestimate what we just did

Linear Regression

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

Linear Regression

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- We generated knowledge from data!!!

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 generated knowledge from data!!!
- Understand [1] 3.3

Statistics or Machine Learning

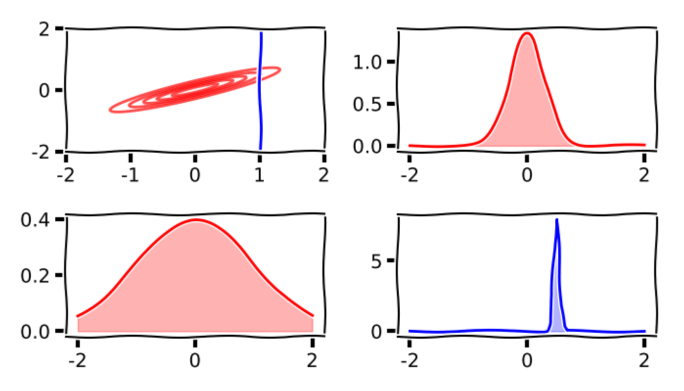
"The difference between statistics and machine learning is that the former cares about parameters while the latter cares about prediction"
– Prof. Neil D. Lawrence

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

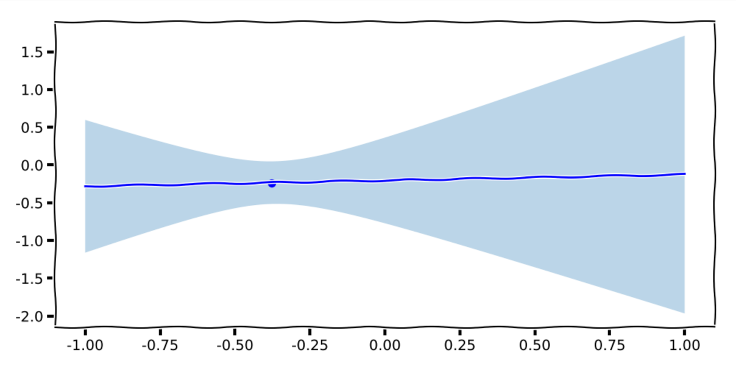
Prediction



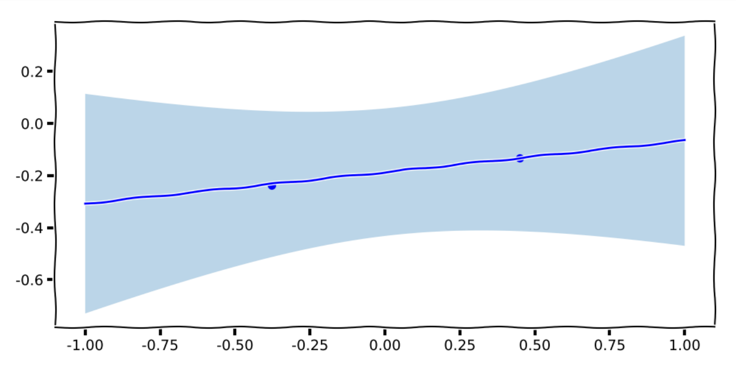
$$p(t_*|\mathbf{t},\mathbf{x}_*,\mathbf{X},\alpha,\beta) = \int p(t_*|\mathbf{x}_*,\mathbf{w},\beta)p(\mathbf{w}|\mathbf{t},\mathbf{X},\alpha,\beta)\mathrm{d}\mathbf{w}$$

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

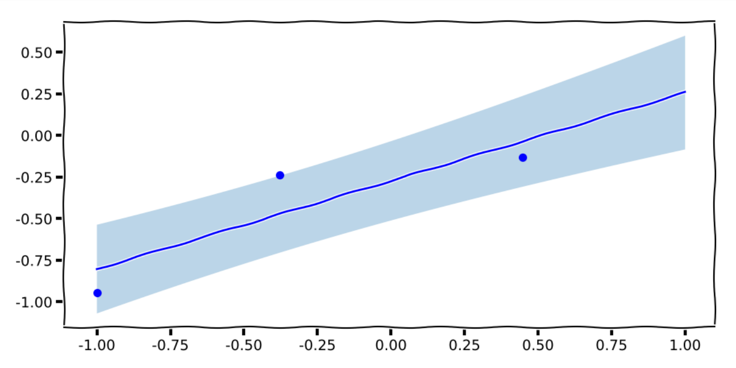
Predictive Posterior



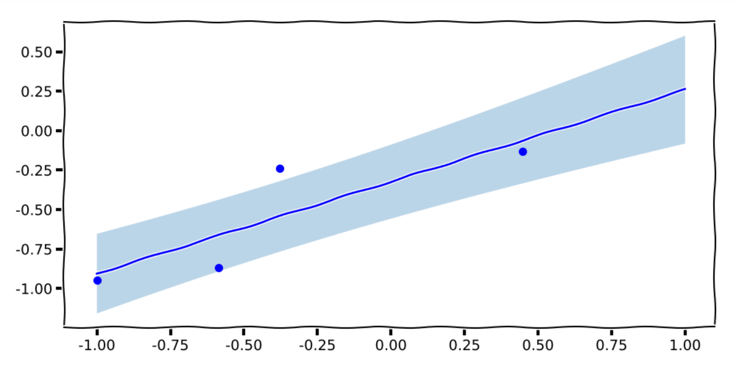
Predictive Posterior



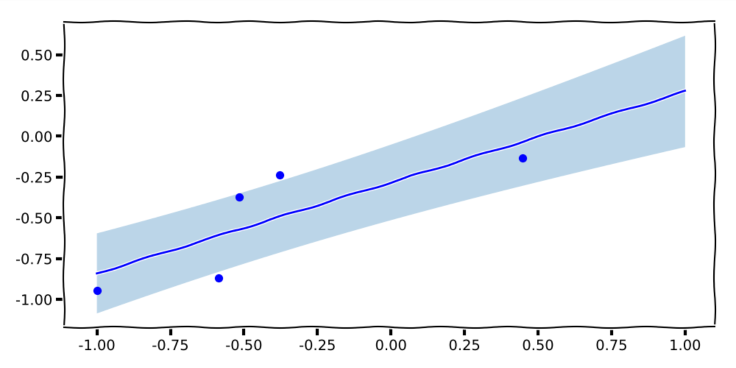
Predictive Posterior



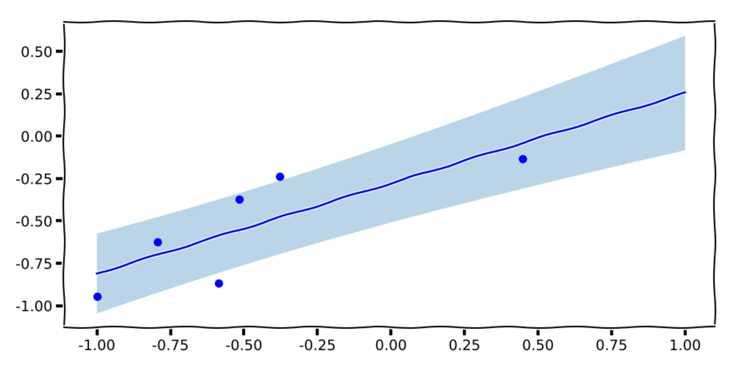
Predictive Posterior



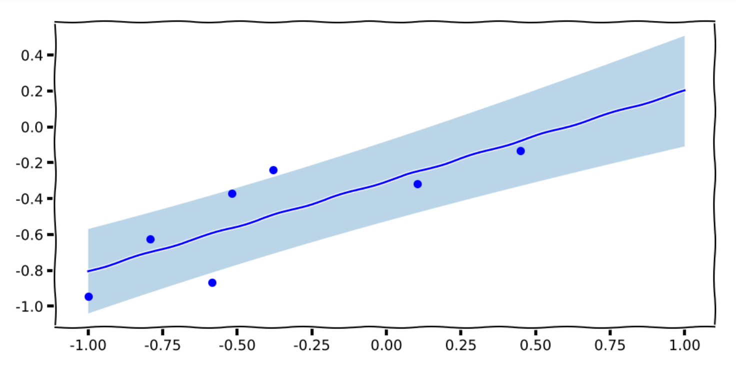
Predictive Posterior



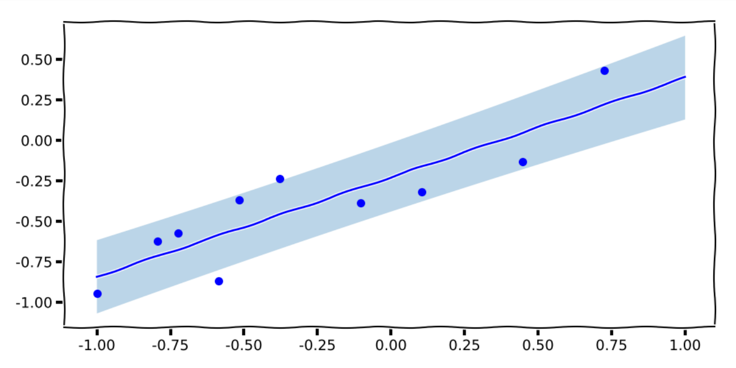
Predictive Posterior



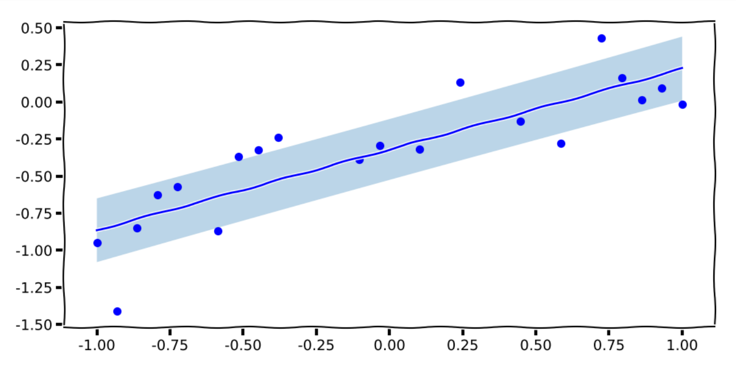
Predictive Posterior



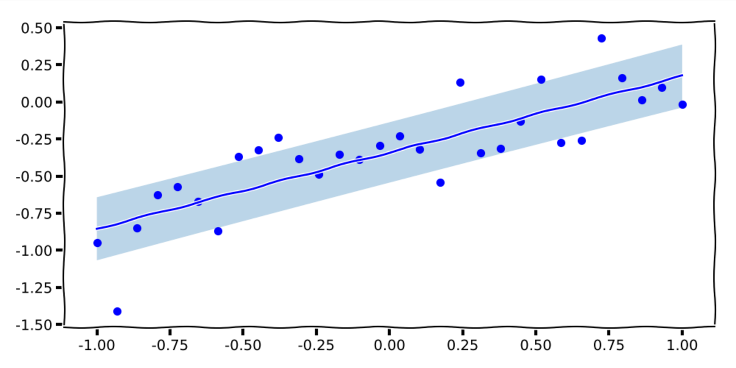
Predictive Posterior



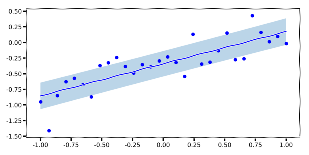
Predictive Posterior

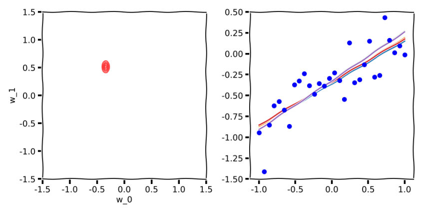


Predictive Posterior

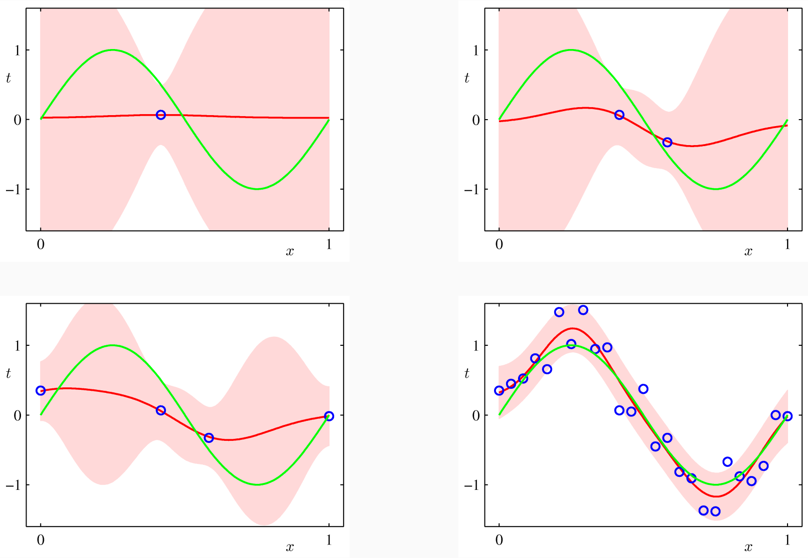


Signal and Noise





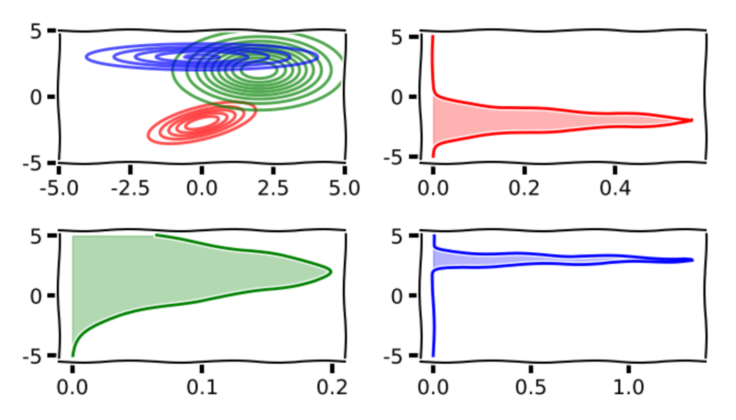
Predictive Posterior [1] Figure 3.8



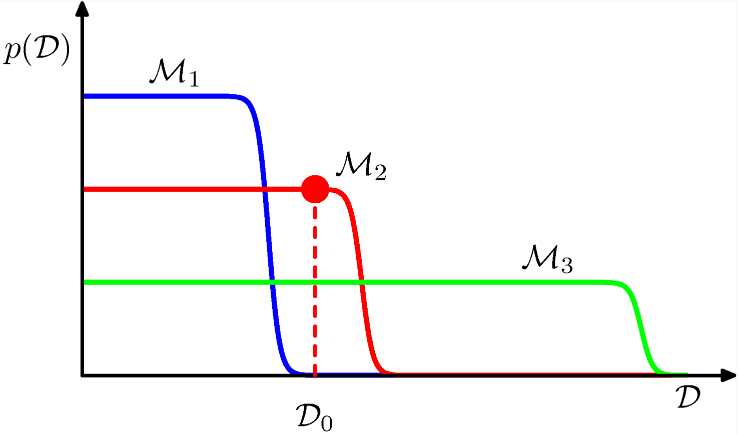
Which Parametrisation

- Should I use a line, polynomial, quadratic basis function?
- Likelihood won't help me
- How do we proceed?

Marginal Distribution



Marginal Likelihood [1] Figure 3.13



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

Next week

- Linear models can only take us that far
    - Monday - Non-linear models
- Fixed model complexity
    - Tuesday - Non-parametric models

Question 1-6 12

References

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Pattern Recognition and Machine Learning (Information Science and Statistics).
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