

Machine Learning - Notes

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Contents

1	Introduction	2
1.1	Motivation	2
1.2	Probability Theory	2
1.3	Conjugate Priors	5
2	Distributions	5
3	Regression	6
3.1	Linear Regression	6
3.2	Dual Linear Regression	9
3.3	Gaussian Processes	11
0	Appendix	13
0.1	Definitions	13
0.2	Proofs	13

General

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Course Subreddit - <https://www.reddit.com/r/coms30007/>

1 Introduction

1.1 Motivation

Definition 1.1 - *Deductive Reasoning*

A method of reasoning in which the premises are viewed as supplying all the evidence for the truth of the conclusion.

Definition 1.2 - *Inductive Reasoning*

A method of reasoning in which the premises are viewed as supplying some evidence for the truth of the conclusion, rather than all the evidence. This allows for the conclusion of the *Inductive Reasoning* to be false.

Remark 1.1 - *Free-Lunch Theorem*

There are infinite number of hypotheses that perfectly explain the data. Adding a data point removes an infinite number of possibilities, but still leaves infinite possibilities.

Remark 1.2 - *The Task of Machine Learning*

When proposing to use machine learning on a task, one should consider the following questions:

- i) How can we formulate beliefs and assumptions mathematically?
- ii) How can we connect our assumptions with data?
- iii) How can we update our beliefs?

Remark 1.3 - *Useful Models are not always True*

Our goal is to understand realisations of a system. If we can then we can equate our model to the system. It is important to note that our model does not need to be perfectly true to be useful.

1.2 Probability Theory

Definition 1.3 - *Stochastic/Random Variable*

A variable whose value depends on outcomes of random phenomena.
e.g. $x \sim \mathcal{N}(0, 1)$.

Definition 1.4 - *Probability Measure, \mathbb{P}*

A function with signature $\mathbb{P} : \mathcal{F} \rightarrow [0, 1]$, where \mathcal{F} is a sample space of rv X , and fulfils $\int_{-\infty}^{\infty} \mathbb{P}(x) dx = 1$.

Definition 1.5 - *Joint Probability Distribution*

A *Probability Measure* for multiple variables, $\mathbb{P} : X \times Y \rightarrow [0, 1]$.

Let n_{ij} be the number of outcomes where $X = x_i$ and $Y = y_j$ then

$$\mathbb{P}(X = x_i, Y = y_j) = \frac{n_{ij}}{\sum_{i,j} n_{ij}}$$

Definition 1.6 - *Marginal Probability Distribution*

A *Probability Measure* for one variable when the sample space is over multiple variables.

Let n_{ij} be the number of outcomes where $X = x_i$ and $Y = y_j$ then

$$\mathbb{P}(X = x_i) = \frac{\sum_j n_{ij}}{\sum_{i,j} n_{ij}}$$

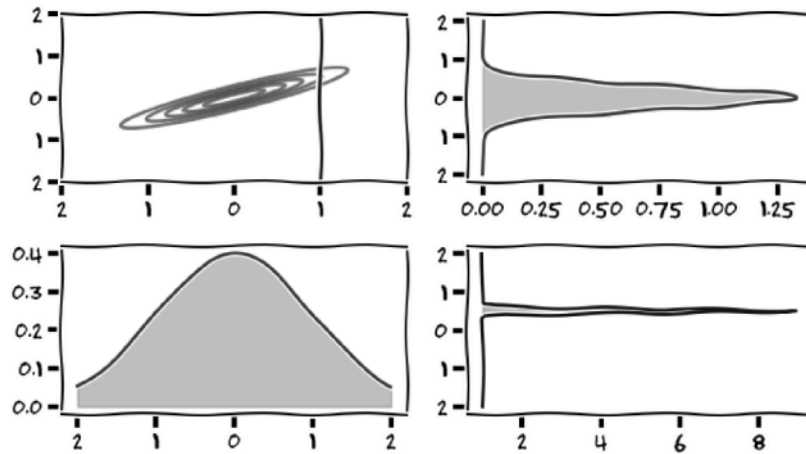
Definition 1.7 - Conditional Probability Distribution

A *Probability Measure* for a variable, given another variable has a defined value. Let n_{ij} be the number of outcomes where $X = x_i$ and $Y = y_j$ then

$$\mathbb{P}(Y = y_j | X = x_i) = \frac{n_{ij}}{\sum_j n_{ij}}$$

Example 1.1 - Joint, Marginal & Conditional Probability

The below image shows two marginals distributions in the bottom-left, X , & top-right, Y , their joint distribution in the top-left and a conditional in the bottom right $\mathbb{P}(Y|X = 1)$.

**Theorem 1.1 - Product Rule**

For random variables X & Y

$$\mathbb{P}(X = x, Y = y) = \mathbb{P}(Y = y | X = x) \mathbb{P}(X = x)$$

Theorem 1.2 - Sum Rule

For random variables X & Y

$$\mathbb{P}(X = x) = \sum_j \mathbb{P}(X = x, Y = y_j)$$

Theorem 1.3 - Bayes' Theorem

For random variables X & Y

$$\mathbb{P}(X = x | Y = y) = \frac{\mathbb{P}(Y = y | X = x) \mathbb{P}(X = x)}{\mathbb{P}(Y = y)}$$

Definition 1.8 - Elements of Bayes' Theorem

The elements of *Bayes' Theory* can be broken down to explain parts of the model.

$$\underbrace{\mathbb{P}(\theta | Y)}_{\text{Posterior}} = \frac{\overbrace{\mathbb{P}(Y | \theta)}^{\text{Likelihood}} \overbrace{\mathbb{P}(\theta)}^{\text{Prior}}}{\underbrace{\mathbb{P}(Y)}_{\text{Evidence}}}$$

Posterior	Which parameters of the model do I believe produce distributions have generated the data Y
Likelihood	How likely is the data to come from the model specifically indexed by θ
Prior	What distribution do I think parameter θ has
Evidence	How likely do I think data Y is for all models.

N.B. The *Evidence* normalises this function.

Definition 1.9 - Expectation Value, \mathbb{E}

The mean value a random variable will produce from a large number of samples.

Continuous	Discrete
$\mathbb{E}(X) = \int_{-\infty}^{\infty} x\mathbb{P}(X)dx$	$\mathbb{E}(X) = \sum_{-\infty}^{\infty} x\mathbb{P}(X)dx$
$\mathbb{E}(f(X)) = \int_{-\infty}^{\infty} f(x)\mathbb{P}(X)dx$	$\mathbb{E}(f(X)) = \sum_{-\infty}^{\infty} f(x)\mathbb{P}(X)dx$

Definition 1.10 - Variance

Describes the amount of spread in the values a single random variable will produce.

$$\text{var}(X) = \mathbb{E}(x - \mathbb{E}(x))^2 = \mathbb{E}(X^2) - \left(\mathbb{E}(X)\right)^2$$

Definition 1.11 - Covariance

Describes the joint variability between two random variables.

$$\text{cov}(X, Y) = \mathbb{E}\left((X - \mathbb{E}(X))(Y - \mathbb{E}(Y))\right)$$

Definition 1.12 - Marginalisation

The process of summing out the probability of one random variable using its joint probability with another random variable.

$$\begin{array}{ll} \text{Continuous} & \mathbb{P}(X = x) = \int \mathbb{P}(X = x, Y = y)dy \\ \text{Discrete} & \mathbb{P}(X = x) = \sum_i \mathbb{P}(X = x, Y = y_i) \end{array}$$

Definition 1.13 - Likelihood Function

Define $\mathbf{X} \sim f_n(\cdot; \theta^*)$ for some unknown $\theta^* \in \Theta$ and let \mathbf{x} be an observation of \mathbf{X} .

A *Likelihood Function* is any function, $L(\cdot; \mathbf{x}) : \Theta \rightarrow [0, \infty)$, which is proportional to the PMF/PDF of the observed realisation \mathbf{x} .

$$L(\theta; \mathbf{x}) := C f_b(\mathbf{x}; \theta) \quad \forall C > 0$$

N.B. Sometimes this is called the *Observed Likelihood Function* since it is dependent on observed data.

Definition 1.14 - Log-Likelihood Function

Let $\mathbf{X} \sim f_n(\cdot; \theta^*)$ for some unknown $\theta^* \in \Theta$ and \mathbf{x} be an observation of \mathbf{X} .

The *Log-Likelihood Function* is the natural log of a *Likelihood Function*

$$\ell(\theta; \mathbf{x}) := \ln f_n(\mathbf{x}; \theta) + C, \quad C \in \mathbb{R}$$

Definition 1.15 - Maximum Likelihood Estimation

The *Maximum Likelihood Estimate* is an estimate for a parameter of a probability distribution which is the value which maximises the *Likelihood Function* (or the *Likelihood Function*).

$$\hat{\theta} := \operatorname{argmax}_{\theta} L(\theta; \mathbf{x})$$

Definition 1.16 - Central Limit Theorem

The distribution of the sum (or mean) of a large number of independent, identically distributed random variables can be approximated to a normal distribution, regardless of the distributions of the random variables.

1.3 Conjugate Priors

Definition 1.17 - Conjugate Prior

If we have a *Likelihood Function*, $\mathbb{P}(X|\theta)$, with a known distribution (*e.g.* Normal) we can choose our *Prior*, $\mathbb{P}(\theta)$, to be from a distribution which is *Conjugate* to the distribution of the *Likelihood Function*.

These are defined in *tables*

Remark 1.4 - Why use Conjugate Priors?

If we have a *Conjugate Prior* then the *Posterior*, $\mathbb{P}(\theta|X)$, will be in the same distribution family as the *Prior* too. We can then work out the distribution of the *Posterior* by passing the parameters of the *Prior* through pre-derived functions

$$\begin{aligned}\text{Posterior} &\propto \text{Likelihood} \times \text{Prior} \\ \mathbb{P}(\theta|X) &\propto \mathbb{P}(X|\theta) \times \mathbb{P}(\theta)\end{aligned}$$

N.B. - https://en.wikipedia.org/wiki/Conjugate_prior#Table_of_conjugate_distributions

Example 1.2 - Conjugate Priors

Consider a scenario where we are flipping a coin. We may have *Likelihood Function* $\theta^x(1-\theta)^{n-x}$. If we choose our *Prior* to be $\theta^{a-1}(1-\theta)^{b-1}$ which is a *Beta Distribution*. Then (after some maths) we find the *Posterior*

2 Distributions

Definition 2.1 - Bernoulli Distribution

Models an event with a binary outcome (0 or 1) with parameter p st $\mathbb{P}(X = 1) = p$ Let $X \sim \text{Bernoulli}(p)$. Then

$$\begin{aligned}f_X(x) &= \begin{cases} p & , x = 1 \\ 1 - p & , x = 0 \\ 0 & \text{otherwise} \end{cases} \\ F_X(x) &= \begin{cases} 0 & , x < 0 \\ 1 - p & 0 \leq x < 1 \\ 1 & x \geq 1 \end{cases} \\ \mathbb{E}(X) &= p \\ \text{Var}(X) &= p(1 - p)\end{aligned}$$

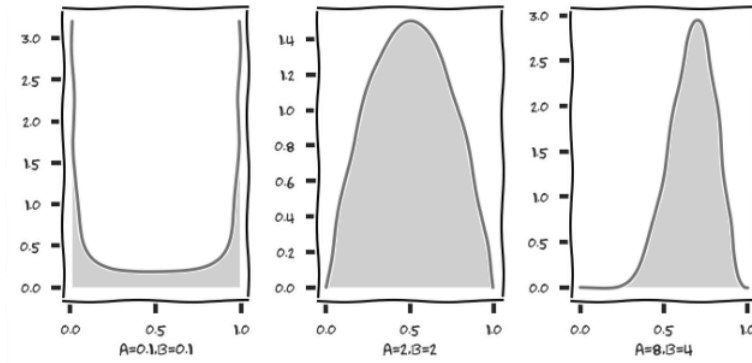
Definition 2.2 - β -Distribution

A β -Distribution is a continuous distribution over interval $[0, 1]$ which is parameterised by two positive *shape parameters*, α & β . A β -Distribution can be used to encode assumptions as a *Prior*.

Let $X \sim \beta(\alpha, \beta)$. Then

$$f_X(x) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

Example 2.1 - β -Distribution

**Definition 2.3 - Dirichlet Distribution**

Let $X \sim \text{Dir}(\alpha)$. Then

$$f_X(x) := \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1) \times \dots \times \Gamma(\alpha_N)} \prod_{i=1}^N x_i^{\alpha_i-1}$$

Definition 2.4 - Exponential Distribution Family

The *Exponential Distribution Family* is a set of probability distributions which fit the form.

$$\mathbb{P}(\mathbf{x}|\boldsymbol{\theta}) = h(\mathbf{x})g(\boldsymbol{\theta})e^{\boldsymbol{\theta}^T \mathbf{u}(\mathbf{x})}$$

With conjugate prior

$$\mathbb{P}(\boldsymbol{\theta}|\chi, \nu) = f(\chi, \nu)g(\chi)^\nu e^{\nu \boldsymbol{\theta}^T \chi}$$

Definition 2.5 - Multivariate Normal Distribution

Let $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Then

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$

N.B. Also known as *Gaussian Distribution*.

3 Regression

3.1 Linear Regression

Definition 3.1 - Linear Regression

Linear Regression is the process of taking a set of data points & producing a linear relationship between a dependent variable & one of more explanatory variables.

Let $\mathbf{x} \in \mathbb{R}^n$ be a set of observed values from n explanatory variables & $\mathbf{a} \in \mathbb{R}^n + 1$ be a set of parameters. Then we predict the value of the dependent variable to be

$$y(\mathbf{x}, \mathbf{a}) = a_0 + \sum_{i=0}^n a_{i+1} x_i$$

Remark 3.1 - Limitation of Linear Regression

The formula defined in **Definition 3.1** is a linear function of the coefficients defined by \mathbf{a} and the observed values of \mathbf{x} this limits the relationships we can model between elements of \mathbf{x} . The model can be extended to avoid this using *Basis Functions*.

Definition 3.2 - Linear Regression - Basis Functions

We can extend *Linear Regression* to include *Basis Functions* so that relationships between explanatory variables can be modelled.

Let $\mathbf{x} \in \mathbb{R}^n$ be a set of observed values from explanatory variables, $\mathbf{a} \in \mathbb{R}^m$ be a set of coefficients

(weightings), and $\phi : \mathbb{R}^n \rightarrow \mathbb{R}^{m-1}$ be a set of basis functions. Then we can predict the dependent variable to be

$$y(\mathbf{x}, \mathbf{a}) = a_0 + \sum_{i=1}^m a_i \phi_{i-1}(\mathbf{x})$$

Remark 3.2 - Linear Regression - Basis Function

To simplify the equation used in **Definition 3.2** we can define $\phi : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $\phi_0(\mathbf{x})$. Then

$$y(\mathbf{x}, \mathbf{a}) = \sum_{i=0}^m a_i \phi_i(\mathbf{x}) = \mathbf{a}^T \phi(\mathbf{x})$$

Proposition 3.1 - Noise

We will often introduce the concept of *Noise* into a *Linear Regression* model. Typically we assume noise to be modelled by a zero-mean Normal distribution with precision β , $\varepsilon \sim \text{Normal}(0, \beta^{-1})$, so

$$t := y(\mathbf{x}, \mathbf{a}) = \mathbf{a}^T \phi(\mathbf{x}) + \varepsilon$$

From this we can derive a likelihood

$$\mathbb{P}(t|\mathbf{x}, \mathbf{a}, \beta) \sim \text{Normal}(t|\mu = y(\mathbf{x}, \mathbf{a}), \sigma^2 = \beta^{-1}) = \text{Normal}(t|\mu = \mathbf{a}^T \phi(\mathbf{x}), \sigma^2 = \beta^{-1})$$

If we have a series of sets of observations, $\mathbf{X} \in \mathbb{R}^{m \times n}$, then

$$\mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) \sim \prod_{i=1}^m \text{Normal}(t_i|\mu = \mathbf{a}^T \phi(\mathbf{x}_i), \sigma^2 = \beta^{-1})$$

Definition 3.3 - Maximum Likelihood Estimate

A *Maximum Likelihood Estimate* is estimating the value of a parameter to be the most likely, according to our *Likelihood Function*.

Remark 3.3 - Finding Maximum Likelihood Estimate

Suppose we have a defined *Likelihood Function* $\mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta)$ and we want to find *Maximum Likelihood Estimates* for parameters \mathbf{a} . Then

- i) Define the *Likelihood Function*, $\mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta)$.
- ii) Take the natural log, $\ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta)$.
- iii) Take the derivative wrt \mathbf{a} , $\frac{\partial}{\partial \mathbf{a}} \ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta)$.
- iv) Set the derivative to 0, $\frac{\partial}{\partial \mathbf{a}} \ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) = 0$.
- v) Solve to find the stationary point of \mathbf{a} .
- vi) Check this stationary point is a maximum, if it is then it is a *Maximum Likelihood Estimate*

Example 3.1 - Maximum Likelihood Estimate

Here I shall find the *Maximum Likelihood Estimate* for \mathbf{a}

$$\begin{aligned}
 \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) &\sim \prod_{i=1}^m \text{Normal}(t_i | \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i), \beta^{-1}) \\
 &= \prod_{i=1}^m \frac{1}{\sqrt{2\pi\beta^{-1}}} e^{-\frac{1}{2}\beta(t_i - \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i))^2} \\
 &= \left(\frac{\beta}{2\pi}\right)^{\frac{m}{2}} e^{-\frac{\beta}{2} \sum_{i=1}^m (t_i - \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i))^2} \\
 \implies \ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) &= \frac{m}{2} \left(\underbrace{\ln(\beta)}_{\text{Noise Precision}} - \underbrace{\ln(2\pi)}_{\text{Constant}} \right) - \underbrace{\frac{\beta}{2} \sum_{i=1}^m (t_i - \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i))^2}_{\text{Error}} \\
 \implies \frac{\partial}{\partial \mathbf{a}} \ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) &= \beta \sum_{i=1}^m (\mathbf{t}_i - \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i)) \boldsymbol{\phi}(\mathbf{x}_i)^T \\
 \text{Setting } 0 &= \frac{\partial}{\partial \mathbf{a}} \ln \mathbb{P}(\mathbf{t}|\mathbf{X}, \mathbf{a}, \beta) \\
 \implies 0 &= \beta \sum_{i=1}^m (\mathbf{t}_i - \mathbf{a}^T \boldsymbol{\phi}(\mathbf{x}_i)) \boldsymbol{\phi}(\mathbf{x}_i)^T \\
 &= \left(\sum_{i=1}^m \mathbf{t}_i \boldsymbol{\phi}(\mathbf{x}_i)^T \right) - \mathbf{a}^T \left(\sum_{i=1}^m \boldsymbol{\phi}(\mathbf{x}_i) \boldsymbol{\phi}(\mathbf{x}_i)^T \right) \\
 \implies \mathbf{a}_{MLE} &= (\boldsymbol{\phi}(\mathbf{X})^T \boldsymbol{\phi}(\mathbf{X}))^{-1} \boldsymbol{\phi}(\mathbf{X})^T \mathbf{t}
 \end{aligned}$$

Theorem 3.1 - Variance of Posterior

Let α be the parameter of the prior, β be the parameter for the likelihood and \mathbf{X} be the observed values from the predictor variables.

$$\begin{aligned}
 s_n &= (I\alpha + \beta \mathbf{X}^T \mathbf{X})^{-1} \\
 &= \left(I\alpha + \beta \begin{pmatrix} \sum_{i=1}^n 1 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix} \right)^{-1} \\
 &= \begin{pmatrix} \beta n + \alpha & \beta \sum_{i=1}^n x_i \\ \beta \sum_{i=1}^n x_i & \alpha + \beta \sum_{i=1}^n x_i^2 \end{pmatrix}^{-1} \\
 &= \frac{1}{(\beta n + \alpha) \left(\alpha + \beta \sum_{i=1}^n x_i^2 \right) - \left(\beta \sum_{i=1}^n x_i \right)^2} \begin{pmatrix} \alpha + \beta \sum_{i=1}^n x_i^2 & -\beta \sum_{i=1}^n x_i \\ -\beta \sum_{i=1}^n x_i & \beta n + \alpha \end{pmatrix} \\
 &\quad \text{Assume data is centred so } \sum_{i=1}^n x_i = 0 \\
 &= \frac{1}{(\beta n + \alpha) \left(\alpha + \beta \sum_{i=1}^n x_i^2 \right)} \begin{pmatrix} \alpha + \beta \sum_{i=1}^n x_i^2 & 0 \\ 0 & \beta n + \alpha \end{pmatrix} \\
 &= \begin{pmatrix} \frac{1}{\beta n + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_{i=1}^n x_i^2} \end{pmatrix}
 \end{aligned}$$

Theorem 3.2 - Mean of Posterior Let α be the parameter of the prior, β be the parameter for the likelihood, \mathbf{X} be the observed values from the predictor variables and \mathbf{t} be the observed

values for the dependent variable.

$$\begin{aligned}
 m_n &= (\alpha I + \beta \mathbf{X}^T \mathbf{X})^{-1} \beta \mathbf{X}^T \mathbf{t} \\
 &= s_n \beta \mathbf{X}^T \mathbf{t} \\
 &= \beta s_n \begin{pmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{pmatrix} \begin{pmatrix} t_1 \\ \vdots \\ t_n \end{pmatrix} \\
 &= \beta s_n \begin{pmatrix} \sum_{i=1}^n t_i \\ \sum_{i=1}^n t_i x_i \end{pmatrix} \\
 &\quad \text{Assume data is centred so } \sum_{i=1}^n x_i = 0 \\
 &= \beta \begin{pmatrix} \frac{1}{\beta n + \alpha} & 0 \\ 0 & \frac{1}{\alpha + \beta \sum_{i=1}^n x_i^2} \end{pmatrix} \begin{pmatrix} \sum_{i=1}^n t_i \\ \sum_{i=1}^n t_i x_i \end{pmatrix} \\
 &= \begin{pmatrix} \frac{\beta \sum_{i=1}^n t_i}{\beta n + \alpha} \\ \frac{\beta \sum_{i=1}^n t_i x_i}{\alpha + \beta \sum_{i=1}^n x_i^2} \end{pmatrix}
 \end{aligned}$$

Proposition 3.2 - Prediction

Suppose we are given as inputs to the model: \mathbf{X} observations from the predictor variables, \mathbf{t} observations from the dependent variable; α , parameter for the prior; and β , parameter for the likelihood.

If we now want to predict the value \hat{t} at position $\hat{\mathbf{x}}$ we want to solve

$$\mathbb{P}(\hat{t}|\hat{\mathbf{x}}, \mathbf{t}, \mathbf{X}, \alpha, \beta) = \int \mathbb{P}(\hat{t}|\hat{\mathbf{x}}, \mathbf{a}, \beta) \mathbb{P}(\mathbf{a}|\mathbf{t}, \mathbf{X}, \alpha, \beta) d\mathbf{a}$$

where \mathbf{a} is the coefficient for weighting each parameter.

3.2 Dual Linear Regression

Definition 3.4 - Kernel

A *Kernel* is a function that defines an inner-product in some space.

Let \mathbf{x} be a vector in the original space & $\phi(\cdot)$ map from the original space to the kernel space.

Then the *Kernel Function* is defined as

$$k(\mathbf{x}_i, \mathbf{x}_j) := \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

Remark 3.4 - Usefulness of Kernels

It is generally easier to define the inner-product of a space than to define a space & kernels allow us to never have to realise a space. This allows us to work with infinite dimensional spaces.

N.B. The space defined by the *Kernel* is called the *Induced Space*.

Definition 3.5 - Kernel Regression

Kernel Regression is the act of performing a linear regression in an *Induced Space*.

Let \mathbf{X} & \mathbf{t} be training data, λ be a parameter for noise, $\hat{\mathbf{x}}$ be an unseen data point which we wish to predict a value \hat{y} for. Then

$$\hat{y}(\hat{\mathbf{x}}) = k(\hat{\mathbf{x}}, \mathbf{x})(k(\mathbf{X}, \mathbf{X}) + \lambda I)^{-1} \mathbf{t}$$

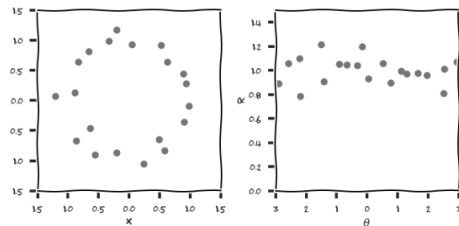
Remark 3.5 - Usefulness of Kernel Regression

Note that the problem is linear in the *Induced Space* but not in the original space, thus allowing us to learn non-linear functions using lines.

Remark 3.6 - Changing Basis

Some data is clearly non-linear & it may be helpful to transform it into another basis where linear regression is possible.

e.g. If the data appears as to fit a circle in a cartesian basis, it can be translated into polar co-ordinates which should be linear.

**Proposition 3.3 - Changing Basis**

Let \mathbf{a} be weightings for observed parameters and \mathbf{x} be a set of observed parameters.

Suppose we want to change the basis of \mathbf{x} , if we have a function $\phi : \mathcal{X} \rightarrow \mathcal{Z}$ which can do this then we predict y as

$$t = \mathbf{a}^T \phi(\mathbf{x}) = \mathbf{a}^T \mathbf{z}$$

Definition 3.6 - Dual Linear Regression

Standard *Linear Regression* is defined as a linear combination of columns. *Dual Linear Regression* is a linear combination of the inner product of a new data point with each of the training data, this allows it to consider combinations of data points.

Remark 3.7 - Intuition of Dual Regression

Dual Regression can be considered as describing an unseen data points as a combination of seen ones. *i.e.* Has the shape of a rhino, fur of a tiger, ...

Proposition 3.4 - Dual Linear Regression Steps

To perform a *Dual Linear Regression* perform the following

- i) Formulate Posterior, $\mathbb{P}(\theta|\mathbf{X})$;
- ii) Find stationary point of posterior;
- iii) Re-write the coefficients \mathbf{a} in terms of the data;
- iv) Perform Kernel regression.

Remark 3.8 - Useful Kernels

Not all functions can be used as *Kernels*. Some that can, and can be useful,

- i) Kernelised Euclidean Distance $\|\phi(\mathbf{x}_i) - \phi(\mathbf{x}_j)\|^2 = k(\mathbf{x}_i, \mathbf{x}_i) - 2k(\mathbf{x}_i, \mathbf{x}_j) + k(\mathbf{x}_j, \mathbf{x}_j)$
- ii) Exponentiated Quadratic $k(\mathbf{x}_i, \mathbf{x}_j) = \sigma^2 e^{-\frac{1}{2\ell^2}(\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j)}$.

Remark 3.9 - Limitations of Linear/Dual Regression

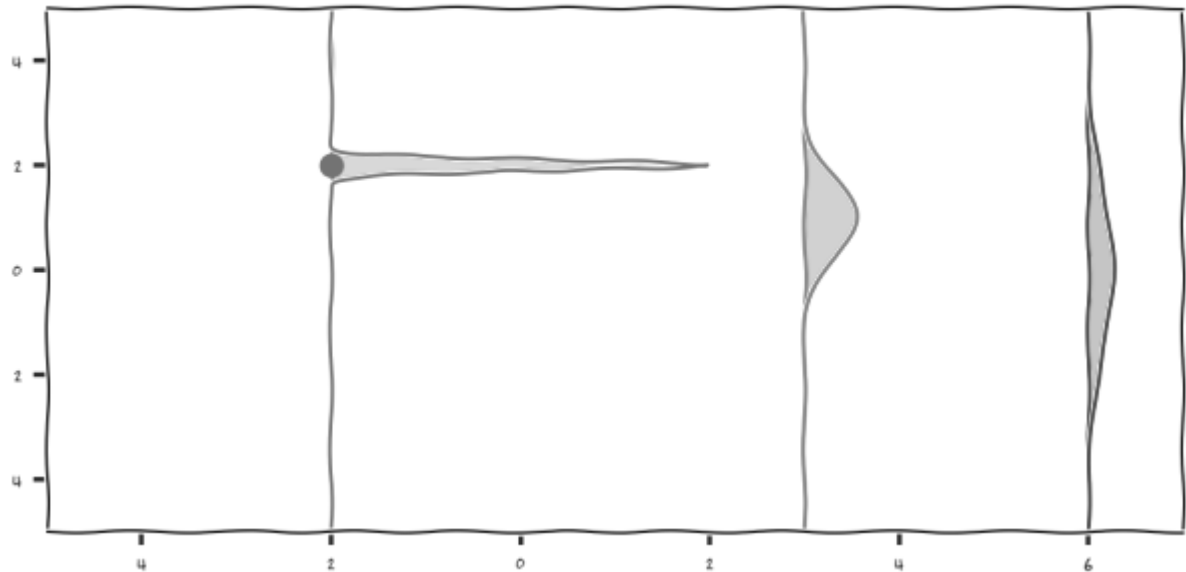
- i) No uncertainty in our observed outputs;
- ii) No uncertainty in our mapping;
- iii) We have to make assumptions over the space of functions

3.3 Gaussian Processes

Remark 3.10 - Motivation

Here we want to introduce uncertainty into our observed outputs & mappings. This means that instead of outputting a discrete value we return a probability distribution. Now we can consider a few more features for our observations, such as how much does observing a value at \mathbf{x}_0 tell us about an observation at \mathbf{x}_1 .

N.B. In the image before we have an observation for $x = -2$ and three marginals for $x = -2, 3, 6$ which our observation has a decreasing affect on, as distance increases.



Definition 3.7 - Gaussian Process

A *Gaussian Process* is a generalisation of random variables into an infinite number of *Gaussian Distributions*. The specific process is defined by a mean function $\mu(\cdot)$ and a co-variance function $k(\cdot)$.

$$\mathbb{P}(f_1, f_2, \dots | \mathbf{x}, \boldsymbol{\theta}) \sim \mathcal{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x})) = \text{Normal} \left(\begin{pmatrix} \mu(x_1) \\ \mu(x_2) \\ \vdots \end{pmatrix}, \begin{pmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots \\ k(x_2, x_1) & k(x_2, x_2) & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \right)$$

Remark 3.11 - Covariance Function

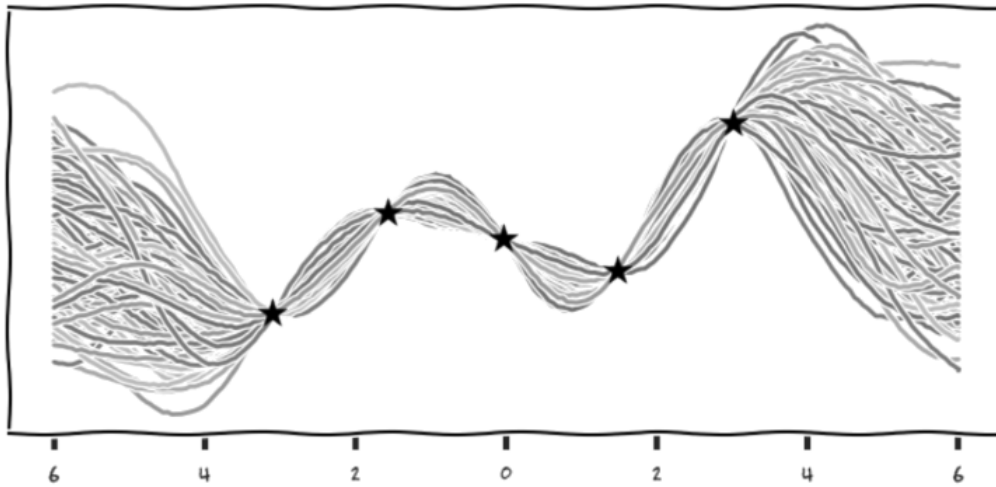
The *Covariance Function* of a *Gaussian Process* defines how much an observation at \mathbf{x}_0 affects our prediction for \mathbf{x}_1 . The greater the covariance values (Not on the main diagonal) the more an observation tells us. We can define the *Covariance Functions* to vary with distance & other factors.

$$\text{Very little effect} = \begin{pmatrix} 1 & .1 \\ .1 & 1 \end{pmatrix}. \quad \text{A lot of effect} = \begin{pmatrix} 1 & .9 \\ .9 & 1 \end{pmatrix}$$

Remark 3.12 - Sampling from a Gaussian Process

When we take a sample from a *Gaussian Process* we are given a function which fits the distributions defined the *Gaussian Process*.

Example 3.2 - Sampling from a Gaussian Process



Proposition 3.5 - Gaussian Process - Posterior, No Noise

Let \mathbf{f}, \mathbf{X} be training data, f^*, \mathbf{x}^* be training data and k be the co-variance function. We have

$$\begin{pmatrix} \mathbf{f} \\ f^* \end{pmatrix} \sim \text{Normal} \left(\begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}, \begin{pmatrix} k(\mathbf{X}, \mathbf{X}) & k(\mathbf{X}, \mathbf{x}^*) \\ k(\mathbf{x}^*, \mathbf{X}) & k(\mathbf{x}^*, \mathbf{x}^*) \end{pmatrix} \right)$$

$$\mathbb{P}(f^* | \mathbf{x}^*, \mathbf{X}, \mathbf{f}) \sim \text{Normal} \left(k(\mathbf{x}^*, \mathbf{X})^T k(\mathbf{x}^*, \mathbf{X})^{-1} \mathbf{f}, k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{X})^T k(\mathbf{X}, \mathbf{X})^{-1} k(\mathbf{X}, \mathbf{x}^*) \right)$$

Proposition 3.6 - Gaussian Process - Posterior, Noise

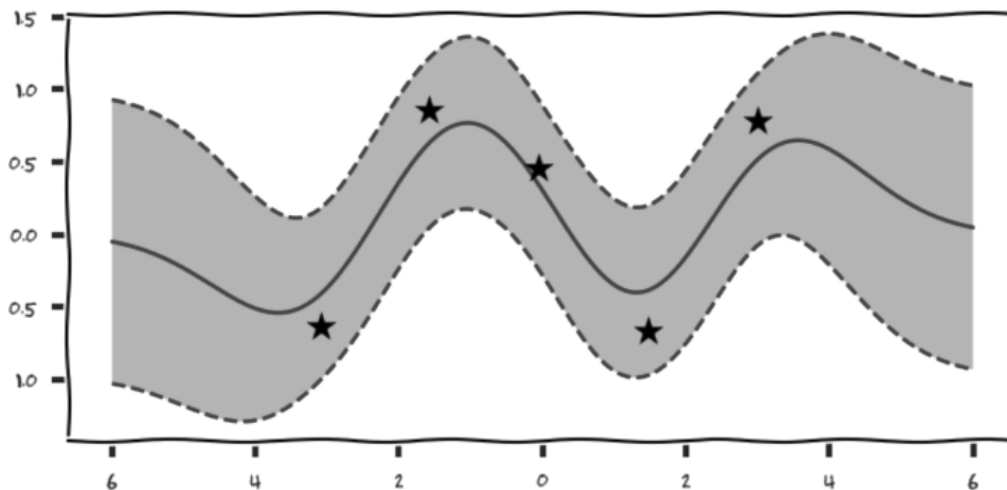
Let \mathbf{f}, \mathbf{X} be training data, f^*, \mathbf{x}^* be training data and k be the co-variance function.

Define $\mathbf{y}_i = f_i + \varepsilon$ where $\varepsilon \sim \text{Normal}(0, \sigma^2 I)$ We have

$$\begin{pmatrix} \mathbf{y} \\ f^* \end{pmatrix} \sim \text{Normal} \left(\begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}, \begin{pmatrix} k(\mathbf{X}, \mathbf{X}) + \sigma^2 I & k(\mathbf{X}, \mathbf{x}^*) \\ k(\mathbf{x}^*, \mathbf{X}) & k(\mathbf{x}^*, \mathbf{x}^*) \end{pmatrix} \right)$$

$$\mathbb{P}(f^* | \mathbf{x}^*, \mathbf{x}, \mathbf{y}, \sigma^2) \sim \text{Normal} \left(k(\mathbf{x}^*, \mathbf{x})^T (k(\mathbf{x}, \mathbf{x}) + \sigma^2 I)^{-1} \mathbf{y}, k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{x})^T (k(\mathbf{x}, \mathbf{x}) + \sigma^2 I)^{-1} k(\mathbf{x}, \mathbf{x}^*) \right)$$

Example 3.3 - Noisy Gaussian Process



0 Appendix

0.1 Definitions

Definition 0.1 - Memory-Based Methods

Memory-Based Methods for classification store the entire training set in order to make predictions for future data points. *e.g.* Nearest-Neighbours.

N.B. These generally require a distance measure to be defined.

0.2 Proofs

Proof 0.1 - Deriving Gaussian Marginal Distribution

NOTE - This is dense as fuck & uses quite a bit of bullshit.

$$\text{Let } \mathbf{X} \sim \mathcal{N} \left(\begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \begin{pmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{pmatrix}^{-1} \right).$$

$\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$ can be considered as two parts of the mean vector $\boldsymbol{\mu}$.

Let \mathbf{x} be a realisation of \mathbf{X} where $\mathbf{x} := (\mathbf{x}_1, \mathbf{x}_2)$ with \mathbf{x}_1 & \mathbf{x}_2 representing the same partition as $\boldsymbol{\mu}_1$ & $\boldsymbol{\mu}_2$ respectively.

Define $D := \dim(\mathbf{x})$, $D_1 := \dim(\mathbf{x}_1)$ & $D_2 := \dim(\mathbf{x}_2)$.

Here we want to get from $\mathbb{P}(\mathbf{x}_1, \mathbf{x}_2)$ to $\mathbb{P}(\mathbf{x}_1)$.

Consider the exponent of the joint distribution

$$E = -\frac{1}{2}(\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Lambda_{11} (\mathbf{x}_1 - \boldsymbol{\mu}_1) - \frac{1}{2}(\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Lambda_{12} (\mathbf{x}_2 - \boldsymbol{\mu}_2) - \frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T \Lambda_{21} (\mathbf{x}_1 - \boldsymbol{\mu}_1) - \frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T \Lambda_{22} (\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

To produce the marginal for x_1 we want to isolate the terms involving x_2 so they are easy to remove.

$$\begin{aligned} E &= -\frac{1}{2} \left[(\mathbf{x}_2^T \Lambda_{22} \mathbf{x}_2 - 2\mathbf{x}_2^T \Lambda_{22} (\boldsymbol{\mu}_2 - \Lambda_{22}^{-1} \Lambda_{21} (\mathbf{x}_1 - \boldsymbol{\mu}_1))) \right. \\ &\quad - 2\mathbf{x}_1^T \Lambda_{12} \boldsymbol{\mu}_2 + 2\boldsymbol{\mu}_1^T \Lambda_{12} \boldsymbol{\mu}_2 + \boldsymbol{\mu}_2^T \Lambda_{22} \boldsymbol{\mu}_2 + \mathbf{x}_1^T \Lambda_{11} \mathbf{x}_1 \\ &\quad \left. - 2\mathbf{x}_1^T \Lambda_{11} \boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T \Lambda_{11} \boldsymbol{\mu}_1 \right] \\ &= \underbrace{-\frac{1}{2} (\mathbf{x}_2 - (\boldsymbol{\mu}_2 - \Lambda_{22}^{-1} \Lambda_{21} (\mathbf{x}_1 - \boldsymbol{\mu}_1)))^T \Lambda_{22} (\mathbf{x}_2 - (\boldsymbol{\mu}_2 - \Lambda_{22}^{-1} \Lambda_{21} (\mathbf{x}_1 - \boldsymbol{\mu}_1)))}_{E_1} \\ &\quad + \underbrace{\frac{1}{2} (\mathbf{x}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \mathbf{x}_1 - 2\mathbf{x}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \boldsymbol{\mu}_1)}_A \\ &\quad - \underbrace{\frac{1}{2} (\mathbf{x}_1^T \Lambda_{11} \mathbf{x}_1 - 2\mathbf{x}_1^T \Lambda_{11} \boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T \Lambda_{11} \boldsymbol{\mu}_1)}_B \end{aligned}$$

Note that A & B do not contain any x_2 terms.

Since the co-variance matrix is symmetric we have $\Lambda_{12} = \Lambda_{21}^T$ we have

$$\mathbf{x}_1^T \Lambda_{12} \boldsymbol{\mu}_2 = \mathbf{x}_1^T \Lambda_{21}^T \boldsymbol{\mu}_2 = (\Lambda_{21} \mathbf{x}_1)^T \boldsymbol{\mu}_2 = \boldsymbol{\mu}_2^T \Lambda_{21} \mathbf{x}_1$$

We shall not rewrite A & B as quadratic expressions

$$\begin{aligned}
A &= \frac{1}{2} (\mathbf{x}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \mathbf{x}_1 - 2 \mathbf{x}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T \Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} \boldsymbol{\mu}_1) \\
&= \frac{1}{2} (\mathbf{x}_1 - \boldsymbol{\mu}_1)^T (\Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21}) (\mathbf{x}_1 - \boldsymbol{\mu}_1) \\
B &= \frac{1}{2} (\mathbf{x}_1^T \Lambda_{11} \mathbf{x}_1 - 2 \mathbf{x}_1^T \Lambda_{11} \boldsymbol{\mu}_1 + \boldsymbol{\mu}_1^T \Lambda_{11} \boldsymbol{\mu}_1) \\
&= \frac{1}{2} (\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Lambda_{11} (\mathbf{x}_1 - \boldsymbol{\mu}_1) \\
\Rightarrow A - B &= \frac{1}{2} (\mathbf{x}_1 - \boldsymbol{\mu}_1)^T (\Lambda_{12} \Lambda_{22}^{-1} \Lambda_{21} - \Lambda_{11}) (\mathbf{x}_1 - \boldsymbol{\mu}_1) \\
\text{Let } E_2 &:= A - B
\end{aligned}$$

Now the exponent has been organised we can consider the whole gaussian expression.

$$\begin{aligned}
\mathbb{P}(\mathbf{x}_1, \mathbf{x}_2) &= \frac{e^{E_1} e^{E_2}}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} \\
\mathbb{P}(\mathbf{x}_1) &= \int \mathbb{P}(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_2 \\
&= \int \frac{e^{E_1} e^{E_2}}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} d\mathbf{x}_2 \\
&= \frac{e^{E_1}}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} \int e^{E_2} d\mathbf{x}_2 \quad \text{Since } E_2 \text{ is independent of } \mathbf{x}_2
\end{aligned}$$

Now we consider $\int e^{E_1} d\mathbf{x}_2$.

Since we know a gaussian must intergrate to 1 over the whole domain we deduce that

$$\begin{aligned}
\int \frac{1}{(2\pi)^{\frac{D_2}{2}} |\Lambda_{22}^{-1}|^{\frac{1}{2}}} e^{E_1} d\mathbf{x}_2 &= 1 \\
\Rightarrow \int e^{E_1} d\mathbf{x}_2 &= (2\pi)^{\frac{D_2}{2}} |\Lambda_{22}^{-1}|^{\frac{1}{2}}
\end{aligned}$$

N.B. Λ_{22}^{-1} is the variance of \mathbf{x}_2 .

Using the result of this intergal we have

$$\begin{aligned}
\mathbb{P}(\mathbf{x}_1) &= (2\pi)^{\frac{D_2}{2}} |\Lambda_{22}^{-1}|^{\frac{1}{2}} \frac{1}{(2\pi)^{\frac{D}{2}} |\Sigma|^{\frac{1}{2}}} e^{E_1} \\
&= \frac{e^{E_1}}{(2\pi)^{\frac{D-D_2}{2}} |\Lambda_{22}^{-1}|^{-\frac{1}{2}} |\Sigma|^{\frac{1}{2}}}
\end{aligned}$$

The Schur complement of Λ_{22} is $\Lambda_{22}^{-1} = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}$.

Thus

$$\begin{aligned}
|\Lambda_{22}^{-1}|^{-\frac{1}{2}} |\Sigma|^{\frac{1}{2}} &= |\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}|^{-\frac{1}{2}} |\Sigma_{11}|^{\frac{1}{2}} |\Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12}|^{\frac{1}{2}} \\
&= |\Sigma_{11}|^{\frac{1}{2}}
\end{aligned}$$

Now we have a full expression

$$\begin{aligned}
\mathbb{P}(\mathbf{x}_1) &= \frac{e^{E_1}}{(2\pi)^{\frac{D-D_2}{2}} |\Lambda_{22}^{-1}|^{-\frac{1}{2}} |\Sigma|^{\frac{1}{2}}} \\
&= \frac{1}{(2\pi)^{\frac{D_1}{2}} |\Sigma_{11}|^{\frac{1}{2}}} e^{-\frac{1}{2} (\mathbf{x}_1 - \boldsymbol{\mu}_1)^T \Sigma_{11}^{-1} (\mathbf{x}_1 - \boldsymbol{\mu}_1)}
\end{aligned}$$

■

Proof 0.2 - Deriving Gaussian Conditional Distribution

Let $\mathbf{X} \sim \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}\right)$.

$\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$ can be considered as two parts of the mean vector $\boldsymbol{\mu}$.

Let \mathbf{x} be a realisation of \mathbf{X} where $\mathbf{x} := (\mathbf{x}_1, \mathbf{x}_2)$ with \mathbf{x}_1 & \mathbf{x}_2 representing the same partition as $\boldsymbol{\mu}_1$ & $\boldsymbol{\mu}_2$ respectively.

Define $D := \dim(\mathbf{x})$.

We want to find the distribution of $\mathbb{P}(\mathbf{x}_1|\mathbf{x}_2)$.

From the product rule we know that $\mathbb{P}(\mathbf{x}_1, \mathbf{x}_2) = \mathbb{P}(\mathbf{x}_1|\mathbf{x}_2)\mathbb{P}(\mathbf{x}_2)$ and we already know the joint & marginal distributions for a gaussian.

We have that

$$\mathbb{P}(\mathbf{x}_1, \mathbf{x}_2) \propto e^{-\frac{1}{2} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix}^T \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix}}$$

We now want to factor the marginal distribution out of this expression.

$$\mathbb{P}(\mathbf{x}_2) \propto e^{-\frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T \Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)}$$

Lets look at the exponent of the joint distribution.

N.B. About to use a lot of Schur Complements

$$\begin{aligned} E &= -\frac{1}{2} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix}^T \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix} \\ &= -\frac{1}{2} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix}^T \begin{pmatrix} I & 0 \\ \Sigma_{22}^{-1}\Sigma_{21} & I \end{pmatrix}^T \begin{pmatrix} (\Sigma/\Sigma_{22})^{-1} & 0 \\ 0 & \Sigma_{22}^{-1} \end{pmatrix} \begin{pmatrix} I & -\Sigma_{12}\Sigma_{22}^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix} \\ &= -\frac{1}{2} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix}^T \begin{pmatrix} (\Sigma/\Sigma_{22})^{-1} & -(\Sigma/\Sigma_{22})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{21}\Sigma_{22}^{-1}(\Sigma/\Sigma_{22})^{-1} & \Sigma_{22}^{-1} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{x}_1 - \boldsymbol{\mu}_1 \\ \mathbf{x}_2 - \boldsymbol{\mu}_2 \end{pmatrix} \\ &= -\frac{1}{2} \left[\mathbf{x}_1 - (\boldsymbol{\mu}_1 + \Sigma_{21}\Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)) \right]^T (\Sigma/\Sigma_{22})^{-1} \left[\mathbf{x}_1 - (\boldsymbol{\mu}_1 + \Sigma_{21}\Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)) \right] \\ &\quad - \underbrace{\frac{1}{2}(\mathbf{x}_2 - \boldsymbol{\mu}_2)^T \Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)}_{E_2} \end{aligned}$$

Note that E_2 is exactly the exponent for the marginal distribution of \mathbf{x}_2 and thus what we want to factory out in order to get to the conditional distribution.

$$\mathbb{P}(\mathbf{x}_1|\mathbf{x}_2) \propto e^{-\frac{1}{2} \left[\mathbf{x}_1 - \underbrace{(\boldsymbol{\mu}_1 + \Sigma_{21}\Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2))}_{\text{mean}} \right]^T \underbrace{(\Sigma/\Sigma_{22})^{-1}}_{\text{covariance}} \left[\mathbf{x}_1 - (\boldsymbol{\mu}_1 + \Sigma_{21}\Sigma_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)) \right]}$$

■