Models

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1 The Prior

1.1 Theory

Question 1.1

Choosing a Gaussian likelihood encodes the assumption that the observations of the variates are going to behave like most probabilistic natural processes and are going to contain some inherent noise. The central limit theorem states that in most cases, when independent random variables are sampled the result is a Gaussian distribution. In other words, most probabilistic processes in nature tend to be noisy, and that noise tends to follow a Gaussian distribution. Hence this is generally a good first assumption to make about unknown data.

Question 1.2

Choosing a spherical covariance matrix means that we are assuming that the distribution is equally likely to deviate from the mean in all directions. Additionally, we assume that all dimensions of y are independent, and therefore do not covary with one another. Again, this is a good place to start.

Choosing a non-spherical covariance would imply that we know something in advance about the relationship between the different dimensions of y, which is not true in this case.

Question 2

If we did not assume independence of the data, the covariance matrix would not be in terms of the identity matrix. We would have non-zero values in the offset diagonals which correspond to the correlations between different variables.

1.1.1 Linear Regression

Question 3

The specific form of the likelihood can be written as

$$p(\mathbf{Y}|\mathbf{X}, \mathbf{W}, \beta) = \prod_{i=0}^{N} \mathcal{N}(y_i|\mathbf{W}^T\phi(x_i), \beta^{-1}). \quad (1)$$

Question 4

A distribution is conjugate to another if they both take the same algebraic form, meaning that they are in the same probability distribution family. For example, Gaussians are conjugate to each other, and the conjugate to a Bernoulli distribution is a Beta distribution. Conjugates are used as a convenience to avoid calculating the denominator in Baye's rule (the evidence) which can often be an integral. If the prior and likelihood are conjugate, then their product will be proportional to the posterior.

Question 5

The distance function of a Gaussian distribution represents the dissimilarity of a given value of a random variable (in this case a parameter choice $\mathbf{W}$) from the expected value (the mean). The further away from the mean the parameter choice is, the less likely we think it will be true.

In the 2 dimensional case, it is easy to think about this geometrically as the distance between two points on a Euclidean plane. For a spherical covariance matrix, the distance is going to be the squared Euclidean distance from the mean $||x - \mu||$. This is because the variables are independent and we have picked the distribution such that it has unit variance. If those two conditions were not true, the Gaussian would not be spherical and the distribution would be deformed. The

spherical covariance case can be seen as a special case where the distance function is Euclidean. In general the distance between two points in a distribution is called the Mahalanobis distance.

Question 6

We have data generated from a linear model, with added Gaussian noise using the following mapping.

$$y_i = \mathbf{W}x_i + \epsilon$$

The added noise is in the form of a gaussian distribution.

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

The likelihood has been specified using,

$$p(\mathbf{Y}|\mathbf{W}, \mathbf{X}) = \mathcal{N}(\mathbf{WX}, \sigma^2 I)$$

and we have specified a prior distribution.

$$p(\mathbf{W}) = \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$$

To avoid calculating the evidence, we use a posterior distribution that is conjugate to the likelihood. Gaussian distributions are conjugate to themselves, so we use a gaussian for the posterior. The posterior distribution is proportional to the likelihood times the prior.

$$p(\mathbf{W}|\mathbf{Y}, \mathbf{X}) \propto p(\mathbf{Y}|\mathbf{W}, \mathbf{X})p(\mathbf{W})$$

By writing the exponent of the likelihood times the prior, we can split the exponent into three pieces.

$$= \underbrace{\frac{1}{2\sigma^2}\mathbf{Y}^T\mathbf{Y}}_{\text{A}} + \underbrace{\frac{1}{\sigma^2}\mathbf{Y}^T(\mathbf{XW})}_{\text{B}} - \underbrace{\frac{1}{2\sigma^2}(\mathbf{XW})^T(\mathbf{XW}) - \frac{1}{2}\mathbf{W}^T\Sigma^{-1}\mathbf{W}}_{\text{C}} \tag{2}$$

- A is the constant. As it does not contain $\mathbf{W}$, it is used to find the posterior covariance;
- B is linear, and we can use it to find the mean;
- C is quadratic in $\mathbf{W}$.

$$C = \frac{1}{2\sigma^2}(\mathbf{XW}) - \frac{1}{2}\mathbf{W}^T\Sigma^{-1}\mathbf{W}$$
$$= -\frac{1}{2}\mathbf{W}^T(\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1})\mathbf{W}$$

Which allows us to define the posterior covariance matrix,

$$S^{-1} = \frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1}$$

and use B to find the mean.

$$B = \frac{1}{\sigma^2}\mathbf{Y}^T(\mathbf{XW}) = \frac{1}{\sigma^2}\mathbf{W}^T\mathbf{X}^T\mathbf{Y}^T$$

We can use the linear term (B) to solve for μ.

$$\mathbf{W}^T S^{-1}\mu = \mathbf{W}^T(\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1})\mu = \frac{1}{\sigma^2}\mathbf{W}^T\mathbf{X}^T\mathbf{Y}$$

$$\mu = \frac{1}{\sigma^2}(\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1})^{-1}\mathbf{X}^T\mathbf{Y}$$

Finally, we can write the posterior distribution for linear regression.

$$p(\mathbf{W}|\mathbf{Y}, \mathbf{X}) = \mathcal{N}(\mathbf{W}|\frac{1}{\sigma^2}(\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1})^{-1}\mathbf{X}^T\mathbf{Y}, (\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \Sigma^{-1})^{-1}) \tag{3}$$

The posterior uses $\frac{1}{\mathbf{Z}}$ as a normalisation constant to ensure that the posterior is a probability distribution.

$$p(\mathbf{W}|\mathbf{Y}, \mathbf{X}) = \frac{1}{\mathbf{Z}}p(\mathbf{Y}|\mathbf{W}, \mathbf{X})p(\mathbf{W})$$

1.1.2 Non-parametric Regression

Question 7

Parametric models make an assumption about the form of the relationship between variates i.e. they specify a finite set of basis functions in advance. For example, we can assume linear basis functions, nonlinear polynomial basis functions of varying degrees, or other types of nonlinear basis function. The "parameters" of these models are the coefficients of the basis functions. Conversely, non-parametric models do not specify explicit basis functions but rather seek to allow an infinite set of functions. Gaussian Processes are a type of non-parametric model that wrap this infinite set of functions in a prior distribution.

Non-parametric models focused on using what we know about the current data to classify new unseen data points. The data can be seen as analogous to the parameters. A good example of this is the K-nearest-neighbour model, which classifies new data points based on its surrounding classes.

Non-parametric models may be more difficult to interpret as they do not have direct parameters to describe the model. It is not always clear how the relationship between variates has been learnt.

Question 8

The GP prior represents a distribution of the space of all possible functions on the 2D plane. By giving the prior a zero mean and uniform variance, we are essentially saying that we think the most likely intersection of a function passing through a vertical line at x will have a y coordinate of 0. Extending out to along the entire x axis, the most likely function will be a flat horizontal line (the x axis itself). However in reality we know that the functions are not likely to be linear - the prior allows for this in that every vertical line through the x axis has a Gaussian likelihood associated with it.

Question 9

Since the prior mean and covariance is the same for all x coordinates, as mentioned above some functions are more likely than others. For example, smoother and

flatter functions are considered more likely by this prior, since the difference between the y coordinates of two adjacent intersection points will be smaller and hence closer to the mean. The covariance $k(\mathbf{X}, \mathbf{X})$ allows us to assume that any two values x_i and x_j covary, therefore f_i and f_j can also be expected to covary.

This means that we think that smooth functions are more likely, however the probability of more rapidly changing functions is non-zero. In fact, all functions have a non-zero probability.

Question 10

The joint distribution of the GP model can be written as

$$p(\mathbf{Y}, \mathbf{X}, f, \theta) = p(\mathbf{Y}|f)p(f|\mathbf{X}, \theta)p(\mathbf{X})p(\theta). \quad (4)$$

The corresponding graphical model is shown in Figure 1.

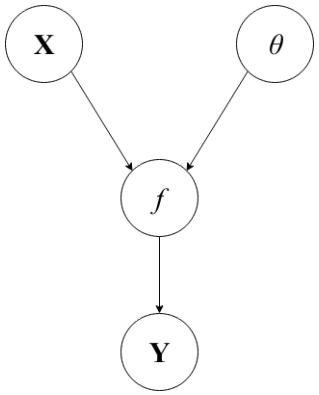


Figure 1: *Graphical model of the joint distribution.*

The assumptions that have been made are:

- $\mathbf{X}$ and θ do not depend on anything;
- f depends on θ and $\mathbf{X}$;
- $\mathbf{Y}$ depends on f, but is is conditionally independent of $\mathbf{X}$ and θ.

Question 11

The marginalisation $p(\mathbf{Y}|\mathbf{X}, \theta)$ connects the prior and the data because we now have a way to directly generate $\mathbf{Y}$ values given $\mathbf{X}$ and θ values without knowing the actual form of f.

Because we are uncertain about f, when we marginalise it out, the uncertainty gets pushed onto $\mathbf{Y}$.

The fact that θ is left on the left hand side of the expression after marginalisation means that it is needed, along with $\mathbf{x}$, to calculate $\mathbf{Y}$. This implies that $\mathbf{Y}$ is dependent on theta.

The graphical model of the marginal $p(\mathbf{Y}|\mathbf{X}, \theta)$ is shown in Figure 2 and shows how $\mathbf{Y}$ is now dependent on only $\mathbf{X}$ and θ. The function f (and its uncertainty) has been "baked in" to $\mathbf{Y}$.

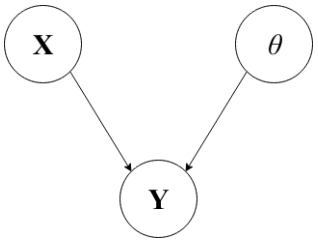


Figure 2: *Graphical model of the marginalised distribution.*

1.2 Practical

1.2.1 Linear Regression

Question 12.1

The prior distribution over $\mathbf{W}$ can be seen in the middle column of the top row of Figure 3. The red cross represents the true value of $\mathbf{W}$. The spherical covariance gives rise to a symmetrical distribution.

The rightmost column of the top row of Figure 3 shows six random samples drawn from the prior which clearly do not have any well defined direction, which is exactly as expected since we have no data to make predictions with.

Question 12.2

The second row of Figure 3 show the result of picking a single data point. The leftmost column plots the likelihood distribution in $\mathbf{W}$-space of the data point. The middle column shows the posterior distribution after the likelihood has been combined with the prior. It can be seen visually that the prior has been squashed along the dimension of the likelihood.

Question 12.3

The rightmost column shows that the sampled functions now all pass through the observed data point, but do not yet agree completely in direction.

Question 12.4

The lower two columns of Figure 3 show the likelihood, posterior and data space samples after adding two and twenty points respectively.

Question 12.5

After a single data point is added, we can see that the posterior distribution begins to squash in one direction to converge onto the parameters $\mathbf{W}$. When we sample from this distribution, there are many lines passing through the point at different gradients, which is because we cannot define two parameters from a single data point. As we begin to reveal more data, the posterior distribution centres onto $\mathbf{W}$ and the sample functions fit more closely to the data points. This is exactly what we want to happen as it shows that we

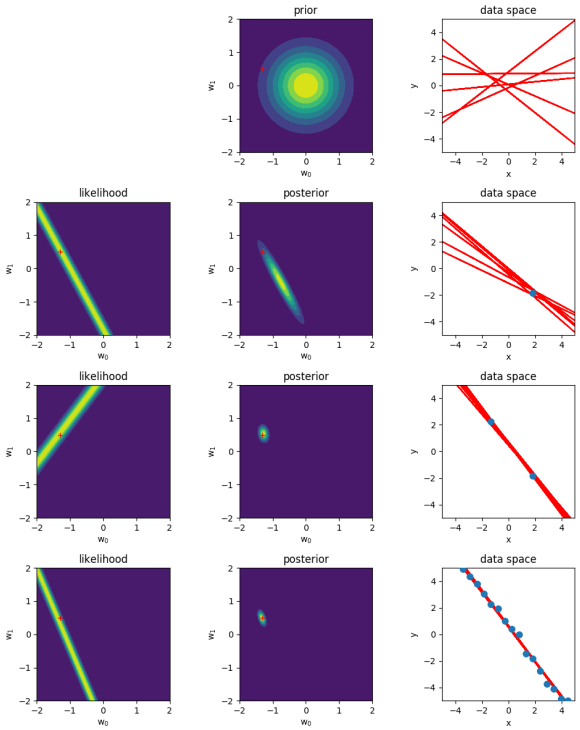


Figure 3: *Implementation of linear regression. The left hand column plots the likelihood. The middle column plots the prior/posterior, and the right hand column shows six random sample functions. Plots are drawn after one, two and twenty data points are revealed.*

have relearned the parameters of the model used to generate the data $\mathbf{X}$.

Question 12.6

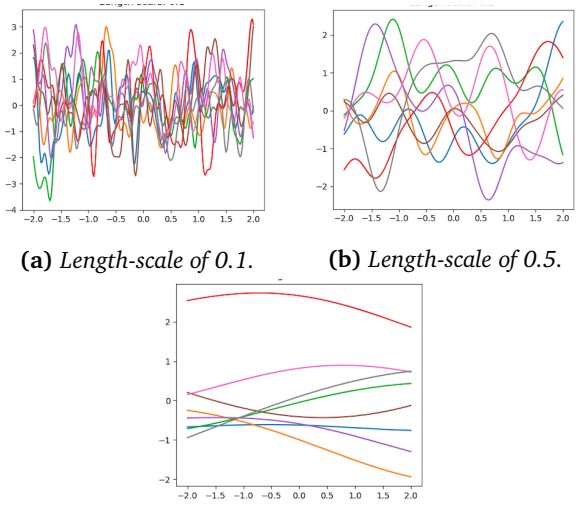
The posterior converges on the position of $\mathbf{W}$ because after a new data point is added, we update the parameters using the newly calculated mean and covariance. As we see more data, we become more and more confident about the true value of $\mathbf{W}$.

1.2.2 Non-parametric Regression

Question 13

Figure 4 shows three examples of samples taken from a GP prior with a squared exponential covariance function that has a single hyper-parameter l which encodes the length scale of the sample functions. The three values of l are 0.1, 0.5 and 5 respectively.

Increasing the length-scale of the covariance function allows us to constrain the smoothness of the sample functions. A smaller length-scale creates functions with more rapid changes than those with a larger length-scale. This is because a higher length-scale means that, for two random variables x_i and x_j where the covariance is $k(x_i, x_j)$, their instantiations as f_i and f_j are similar.



(a) *Length-scale of 0.1.* **(b)** *Length-scale of 0.5.*

(c) *Length-scale of 5*

Figure 4: *Squared exponential with varying length scales.*

Choosing a larger length-scale encodes the assumption that smoother function with lower frequency is preferable to high frequency, more oscillatory functions. In other words, we prefer functions that change less rapidly.

1.2.3 Question 14

The predictive posterior distribution is a Gaussian given by

$$p(\mathbf{Y}_{N+1}|\mathbf{Y}) = \mathcal{N}(\mathbf{M}_{N+1}, \mathbf{C}_{N+1}) \tag{5}$$

where

$$\mathbf{M}_{N+1} = \mathbf{k}^{\mathbf{T}}\mathbf{C}_N^{-1}\mathbf{Y} \tag{6}$$

$$\mathbf{C}_{N+1} = c - \mathbf{k}^{\mathbf{T}}\mathbf{C}_N^{-1}\mathbf{k} \tag{7}$$

and $\mathbf{C_N}$ is the previous covariance matrix, $\mathbf{k}$ has elements $k(\mathbf{x}_n, \mathbf{x}_{N+1}$ (i.e. the kernel function invoked with all the previous data points and the new data point) and c is a scalar that equals $k(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}$ (i.e. the kernel function over just the new data point).

Need to describe the plots. What happens if we use a diagonal covariance matrix to the squared exponential.

2 Posterior

Question 15

We use our beliefs to find a starting point for the problem and to make assumptions about the data, or any other characteristics of the problem. Assumptions are what we assume to be true about something. If we had all the data we required for a problem, there would be no need to assume anything. This gives us a way to reason when we have very little information.

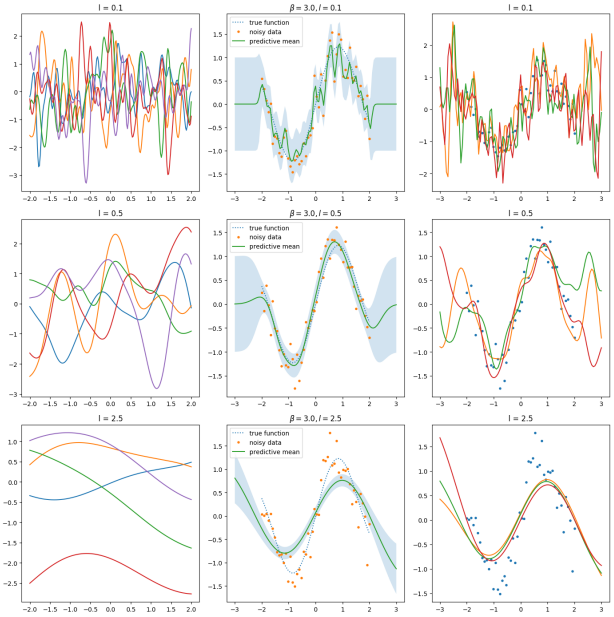


Figure 5: *Implementation of non-parametric regression with changing length-scales.*

A preference is an assumption that we want to use because it is easier to do so. For example using a gaussian likelihood so that the posterior is also gaussian.

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We use beliefs and assumptions to formulate a prior. Believe that the smooth lines are more likely. Prefer straight or flat lines.

Question 16

Since the covariance matrix is spherical, we have assumed that the latent input variables are independent and that they are centred around the origin.

Question 17

One way to obtain the marginal distribution $p(\mathbf{Y}|\mathbf{W})$ would be to write out the exponents of the likelihood and the prior and do a lot of algebra to work out the actual integral. But there is a simpler way.

Firstly, we know that $\mathbf{Y} = \mathbf{WX} + \epsilon$ and we know that $\mathbf{X}$ is Gaussian since we put a prior over it. We know that we can do any linear transformation to a Gaussian and it is still a Gaussian because Gaussians are closed under linear transformation. So we know that $p(\mathbf{Y}|\mathbf{W})$ is going to be a gaussian. All we need to do is work out the mean and the covariance of the distribution we are looking for.

We know that the mean is the expectation of $\mathbf{Y}$, so we can therefore write

$$\mathbb{E}[\mathbf{Y}] = \mathbb{E}[\mathbf{WX} + \epsilon]. \tag{8}$$

We know the expected value of $\mathbf{X}$ since we picked a prior over $\mathbf{X}$ and gave it a zero mean, so ti will be zero. We can also ignore ϵ in the expectation since it is just a noise parameter. Therefore we can deduce that the mean μ is just going to be zero.

Now to work out the covariance, we know that it is going to be the expected value of $\mathbf{Y}$ multiplied by its transpose, which we can write similarly to (8) as

$$\mathbb{E}[\mathbf{YY^T}] = \mathbb{E}[(\mathbf{WX} + \epsilon)(\mathbf{WX} + \epsilon)^\mathbf{T}] \tag{9}$$

$$= \mathbb{E}[\mathbf{WXX^TW^T}] + \mathbb{E}[\epsilon\epsilon^\mathbf{T}] \tag{10}$$

The expectation of the noise parameter ϵ we have already defined as being $\sigma^2\mathbf{I}$. Since our prior over $\mathbf{X}$ was zero-mean, we know that $\mathbf{XX^T}$ is going to be the identity matrix, therefore can simply write the covariance as

$$\mathbb{E}[\mathbf{Y}] = \mathbf{WW^T} + \sigma^\mathbf{2}\mathbf{I} \tag{11}$$

which gives us the resulting marginal distribution

$$p(\mathbf{Y}|\mathbf{W}) = \mathcal{N}(0, \mathbf{WW^T} + \sigma^\mathbf{2}\mathbf{I}) \tag{12}$$

and we are done.

Question 18.1

A maximum-a-posteriori (MAP) estimation is equal to the mode of the posterior. It finds the parameters that maximise the posterior distribution. Because it takes the posterior into account, it is a more computationally expensive operation.

The maximum likelihood (ML) can be seen as a type of MAP estimation, which assumes a uniform prior distribution of the parameters. In doing so, it finds the parameters that maximise the likelihood.

Type-II Maximum likelihood finds the parameters that maximise the marginal likelihood.

Question 18.2

With only one data point, ML will be less accurate than MAP since it does not take the prior into account. However as more data is seen, the two will begin to converge on one another.

Question 18.3

The denominator of the posterior distribution has no bearing on the result as it will always be positive, and depends on the parameters $\mathbf{W}$.

Question 19

The objective function can be written as:

$$\mathcal{L}(\mathbf{W}) = -log(p(\mathbf{Y}|\mathbf{W}, \boldsymbol{\mu}, \boldsymbol{\sigma}^2)) \\ = -\frac{ND}{2}log(2\pi) - \frac{N}{2}log|\mathbf{C}| - tr((\mathbf{YC})^{-1}\mathbf{Y}^{\mathbf{T}}) \tag{13}$$

where $\mathbf{C} = \mathbf{W}\mathbf{W}^{\mathbf{T}} + \boldsymbol{\sigma}^{\mathbf{2}}\mathbf{I}$. The gradients of the objective function with respect to the parameters can be written as:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = tr(\mathbf{C}^{-1}(\mathbf{W}\mathbf{J}_{\mathbf{ij}} + \mathbf{J}_{\mathbf{ji}}\mathbf{W}^{\mathbf{T}})) \\ + tr(\mathbf{Y}^{\mathbf{T}}\mathbf{Y}(-\mathbf{C}^{-1}(\mathbf{W}\mathbf{J}_{\mathbf{ij}} + \mathbf{J}_{\mathbf{ji}}\mathbf{W}^{\mathbf{T}})\mathbf{C}^{-1}) \tag{14}$$

where $\mathbf{W}\mathbf{J}_{\mathbf{ij}} + \mathbf{J}_{\mathbf{ji}}\mathbf{W}^{\mathbf{T}} = \frac{\partial \mathbf{C}}{\partial \mathbf{W}_{\mathbf{ij}}}$.

Question 20

$\mathbf{Y}$ is dependent on both $\mathbf{X}$ and θ, which both contain a level of uncertainty. By marginalising out f, the uncertainty will be filtered down into the marginal distribution of $\mathbf{Y}$.

Marginalising out f is easier than $\mathbf{X}$, as f is only a dependency of $\mathbf{Y}$, whereas $\mathbf{X}$ is a dependency of both f and $\mathbf{Y}$. Because $\mathbf{X}$ is a dependency of f and $\mathbf{Y}$, we would have to deal with both f and $\mathbf{Y}$ when marginalising it out.

Question 21

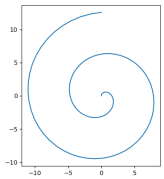
We first mapped the input variables $\mathbf{x}$ non-linearly to a 2D space and plotted the result. This gives a uniform spiral shape as seen in Figure 4a. We then mapped this linearly to a 10D space. Given the objective function and gradients from above, we then minimised the log likelihood to "learn" the linear mapping parameters W. Using the new parameters, we performed the reverse of the linear mapping back to 2D space and obtained another (slightly different) spiral which can be seen in Figure 6b.

We expected the recovered shape to be more similar to the original shape. We suspect there may be an error in the minimisation process (probably somewhere in computing the gradients).

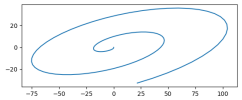
Since we have only learned the parameters for the linear part of the mapping, it does not immediately appear possible to recover the original latent variables themselves.

Question 22

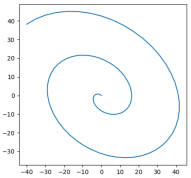
Choosing any randomly initialised W matrix and performing the reverse mapping also results in a spiral shape, as can be seen in Figure 6c. However, the shape is slightly different, the dimensions are different.



(a) *Original 2D subspace.*



(b) *Subspace learnt via Type-II ML.*



(c) *Random subspace.*

Figure 6: *Subspaces representing a 2D non-linear mapping from a 1D input vector.*

3 The Evidence

Question 23

Question 24

Question 25

4 Final Thoughts

Question 30

I feel that the purpose of this assignment was to introduce the basics of machine learning using a statistical, low level approach. In doing this, we have been forced to learn the theory behind algorithms before we are able to implement them.

The main learning point of this assignment has been the methodology of machine learning, which involves defining a prior and likelihood with the goal of finding a posterior distribution.