DD2434 Machine Learning, Advanced Course
Assignment 1

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1 The prior

1.1 Theory

Question 1: *Why is choosing a Gaussian likelihood a sensible thing to do? What does it mean that we have chosen a spherical covariance matrix for the likelihood?*

Since we have no previous knowledge about the uncertainty in the observations, we can assume that the source of this uncertainty is a large number of measurement errors that are independent and identically distributed. According to the Central Limit Therorem, the noise resulting from this sum of errors will be normally distributed. Since the likelihood is for a given f and x_i, it only depends on the noise, and therefore it is sensible to assume that the likelihood is Gaussian.
A spherical covariance matrix for the likelihood means that the components y_j^j of the vector y_i do not covary with each other conditionally given f and x_i, which means they are uncorrelated.

$$\forall i \leq N,\ \forall j,k \leq D\ j \neq k \quad cov(y_i^j, y_i^k | f, x_i) = 0$$

The variance of all the components y_j^j of the vector y_i conditionally given f and x_i is constant and equal.

$$\forall i \leq N \quad var(y_i^j | f, x_i) = \sigma^2$$

Question 2: *If we do not assume that the data points are independent how would the likelihood look then?*

By applying the product rule, we obtain:

$$p\left(Y|f,X\right) = p\left(y_N|f,X\right) \prod_{i=1}^{N-1} p\left(y_i|y_{i+1},\ldots,y_{N-1},y_N,f,X\right)$$

1.1.1 Linear Regression

Question 3: *What is the specific form of the likelihood above, complete the right-hand side of the expression.*

We assume our observations are corrupted by additive noise, that is normally distributed.Therefore, the likelihood has the following form:

$$p\left(Y|W,X\right) = \prod_{i=1}^{N} p\left(y_i|W,x_i\right) \quad \text{where} \quad p\left(y_i|W,x_i\right) = \mathcal{N}(Wx_i, \sigma^2 I)$$

Question 4: *Explain the concept of conjugate distributions. Why is this a motivated choice?*

The likelihood function is a Gaussian with a known variance, so a Gaussian prior would be a conjugate to the likelihood function. This way, the posterior will have the same functional form as the prior, ie a Gaussian, and we will only need to estimate its parameters.

Question 5: *The prior in Eq.8 is a spherical Gaussian. This means that the "preference" is encoded in terms of a L2 distance in the in the space of the parameters. With this view, how would the preference change if the preference was rather encoded using a L1 norm? Compare and discuss the different type of solutions these two priors would encode.*

If the preference was encoded using a L1 norm, that would mean that we would choose a Laplace distribution to model the prior, ie $W \sim \frac{\sqrt{\lambda}}{2} e^{-\sqrt{\lambda}|W|}$.
the Laplace distribution is peaked at the mean while the Gaussian distribution is smooth around the mean, therefore The laplacian prior assigns more weight to regions near the mean than the normal prior. If we have no prior knowledge about this mean and take it to be 0 by symmetry, it expresses the prior belief that the distribution of feature relevances with relation to the target is strongly peaked around zero. If one of the components of W happens to be irrelevant, a Gaussian prior will not set it exactly to zero, but will prune it to some small value. On the other hand, under a Laplacian prior, some of the components of W may be exactly zero.

Question 6: *Derive the posterior over the parameters. I recommend that you do these calculations by hand as it is very good practice. However, in order to pass the assignment you only need to outline the calculation and highlight the important steps. Why does it have the form that it does?*
What is the effect of the constant Z, are we interested in this?

The likelihood of the data has the following form:

$$p\left(Y|W,X\right) = \prod_{i=1}^{N} p\left(y_i|W,x_i\right) \quad \text{where} \quad p\left(y_i|W,x_i\right) = \mathcal{N}(Wx_i, \sigma^2 I)$$

Since the product of Gaussians is a Gaussian, and the covariance matrix for the likelihood of each point y_i is spherical, we can write the likelihood as :

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

We choose a Gaussian prior with a zero mean over the parameter:

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

The pdf of a general normal has the following form:

$$\mathcal{N}(\mu, \Sigma) \propto e^{\frac{-1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

According to Bayes rule, we write the posterior as:

$$p(W|Y,X) \propto p(Y|W,X)p(W) \propto e^{\frac{-1}{2\sigma^2}(y-XW)^T(y-XW)}\ e^{\frac{-1}{2}W^T\Sigma^{-1}W}$$

Gaussians are self-conjugate, so a Gaussian prior and a Gaussian likelihood give a Gaussian posterior, ie $\mathcal{N}(\mu, S)$. We rewrite the exponent as:

$$\frac{-1}{2\sigma^2}(y-XW)^T(y-XW)\frac{-1}{2}W^T\Sigma^{-1}W = \frac{-1}{2\sigma^2}Y^TY+\frac{1}{2\sigma^2}Y^T(XW)-\frac{1}{2\sigma^2}(XW)^T(XW)-\frac{1}{2}W\Sigma^{-1}W$$

The first term (A) is the constant term of the normal, the second term (B) is the mixed term and the two last terms (C) correspond to the terms with a quadratic in parameters.
By rewriting (C), we obtain:

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

We can therefore identify the inverse covariance matrix of the posterior as:

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

By rewriting the term (B) it we obtain:

$$B = \frac{1}{2\sigma^2}W^TX^TY$$

Since the mean appears in the mixed term, we can write using the expression of the covariance matrix that we previously found:

$$\frac{1}{2\sigma^2}W^TX^TY = W^T(\frac{1}{\sigma^2}X^TX + \sigma^{-1})\mu$$

After solving for μ, we obtain:

$$\mu = \frac{1}{\sigma^2}(\frac{1}{\sigma^2}X^TX + \Sigma^{-1})^{-1}X^TY$$

The constant Z is a normalising constant so that the posterior represents a true probability distribution, ie $p(W|Y,X) = \frac{1}{Z}p(Y|W,X)p(W) \leq 1$. Z represents the evidence, which we will use for model selection.

1.1.2 Non-parametric Regression

Question 7: *What is a non-parametric model and what is the difference between non-parametrics and parametrics? In specific discuss these two aspects of non-parametrics: representability and interpretability?*

In a non-parametric model, we do not give the function between the two variates a predefined specific form, but instead define a prior probability distribution over functions directly.
While the validity of parametric models relies on the correctness of the specified model, non-parametric models assumes no specific form of the function, and adapt to the underlying function using the empirical data. Therefore non-parametric models provide a better representability and goodness of fit to the data. However, parametric model have directly interpretable parameters, while non-parametric yield relationship that are difficult to describe, especially if the we map the features to spaces with high or infinite dimensionality. Therefore parametric models give better interpretability.

Question 8: *Explain what this prior does? Why is it a sensible choice? Use images to show your reasoning. Clue: use the marginal distribution to explain the prior*

The Gaussian process allows us to define a prior probability distribution over functions directly. We know 2 points about the mapping f between Y and X:

1. it's a function, ie: $\forall x_i \in \mathbb{R}^q,\ \exists! y_i \in \mathbb{R}^D\ /\ f(x_i) = y_i$
2. $f(x_i) \in \mathbb{R}^D$, which means that we can map an input to any value in our output space.

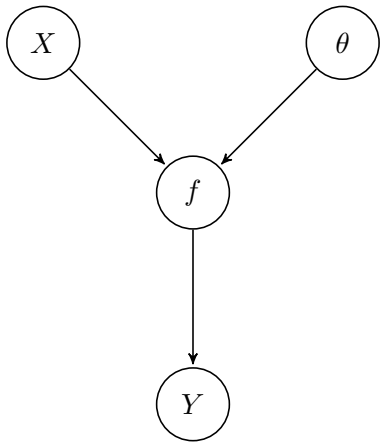
If we choose a Gaussian process, ie $p(f|X, \theta) = \mathcal{N}(0, k(X, X))$, then according to the definition of a Gaussian process, the marginal distribution $p(f)$ is Gaussian, which has the following characteristics:

- A Gaussian is uni-modal, which addresses point 1.
- the pdf of a Gaussian is such that $f(x|\mu, \sigma) > 0$, which addresses point 2.

All instantiations of the function are jointly Gaussian, and covariance allows us to express that for points x_i and x_j that are similar, the corresponding values f_i and f_j will be more strongly correlated than for dissimilar points. The parameter θ defines this similarity, which allows us to control the smoothness of the function, for example.

Question 9: *Formulate the joint likelihood of the full model that you have defined above, $p(Y, X, f, \theta)$. Draw the graphical model to clearly show the assumptions that you have made.*

We know that X and θ are independent. We also know that Y is conditionally independent of X and θ given f (Y depends on X, but all the information in X relevant to determine Y is captured by f and θ). This gives us the following Bayesian network:



The joint likelihood for this model is therefore:

$$p(Y, X, f, \theta) = p(Y|f)p(f|X, \theta)p(X)p(\theta)$$

Question 10: *Explain the marginalisation in Eq.12. Explain how this connects the prior and the data? How does the uncertainty filter through this? What does it imply that θ is left on the left-hand side of the expression after marginalisation?*

$$p(Y|X, \theta) = \int p(Y|f)p(f|X, \theta)df$$

- We average the likelihood of the data points over all possible functions given by the prior over function realisations.

- We merge the uncertainty in the observations given by $p(Y|f)$ with the uncertainty in the relationship between X and Y given by $p(f|X, \theta)$.
- Since we average over all functions of the Gaussian process, θ is constant in this integral, therefore the result is a function of θ.

1.2 Practical

1.2.1 Linear Regression

Question 11: *Describe the plots, and the behavior when adding more data? Is this a desirable behavior?*

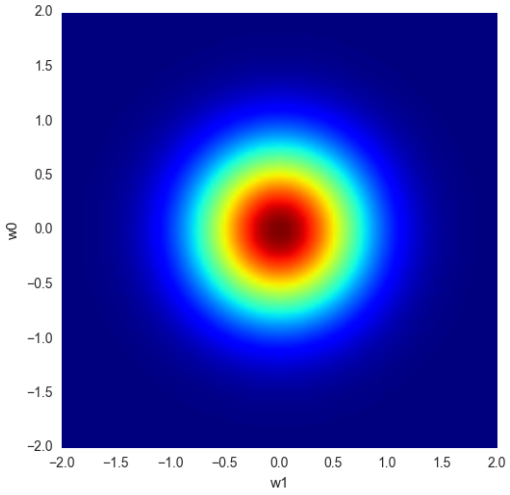
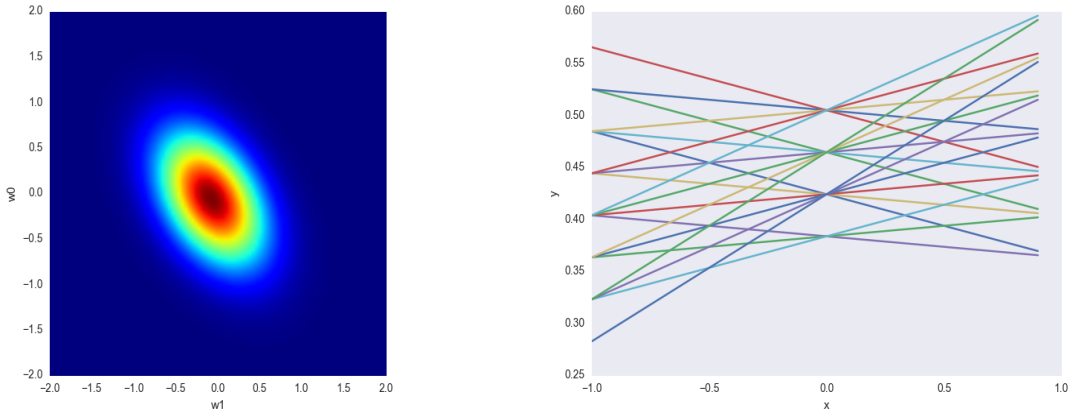


Figure 1: Prior Distribution over W

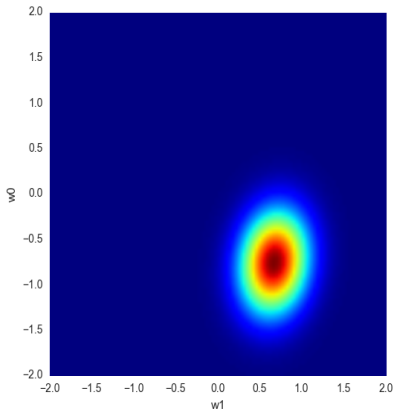


(a) Posterior Distribution over W

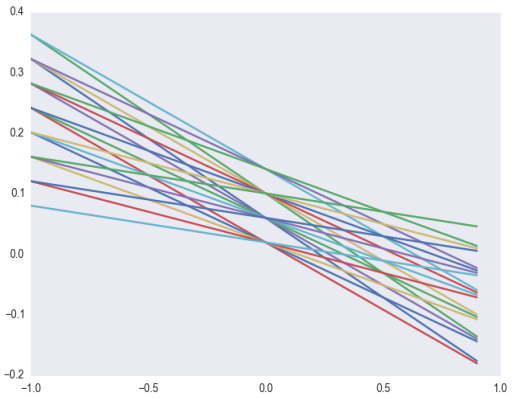
(b) Samples from the posterior

Figure 2: After 1 observation

After observing a single data point (figure 2), the posterior becomes constrained by the corresponding likelihood. When we sample from the posterior and draw it in the data space, there are many possible solutions with different slopes/intercepts, which makes sense since we cannot infer two parameters from

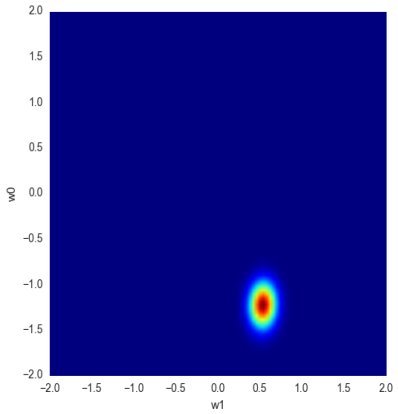


(a) Posterior Distribution over W

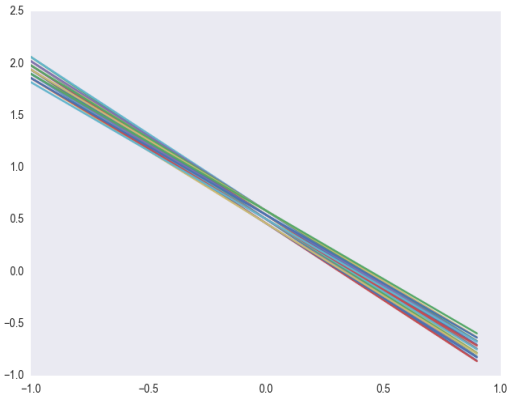


(b) Samples from the posterior

Figure 3: After 2 observations



(a) Posterior Distribution over W



(b) Samples from the posterior

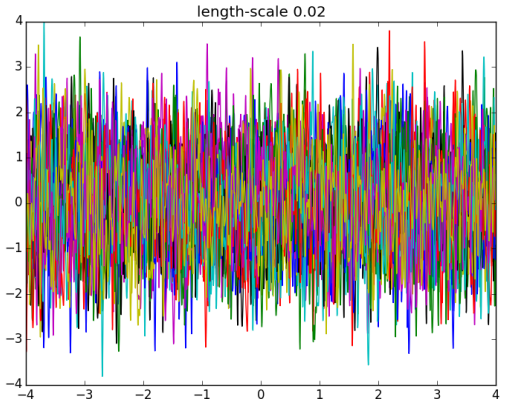
Figure 4: After 25 observations

one observation. After we see two data points (figure 3), the posterior becomes narrower, and the samples from the posterior have similar slopes and intercepts than before. After 25 observations (figure 4), we can see that the posterior is centered on the true value, $w0 = -1.3$ and $w1 = 0.5$. Since the data was generated from this model, this is the desirable behavior because the estimate converges to the true value.

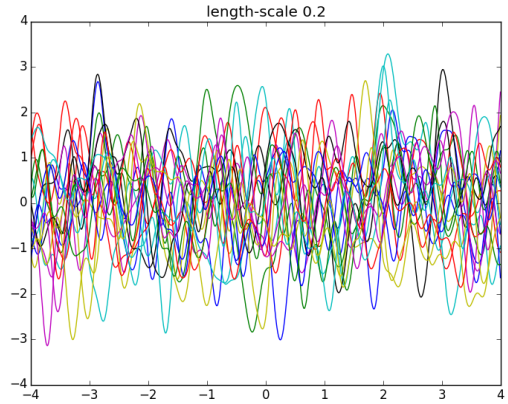
1.2.2 Non-parametric Regression

Question 12: *Create a $\mathcal{GP}$-prior with a squared exponential co-variance function, sample from this prior and visualise the samles and show samples using different length-scale for the squared exponential. Explain the behavior of altering the length-scale of the covariance function.*

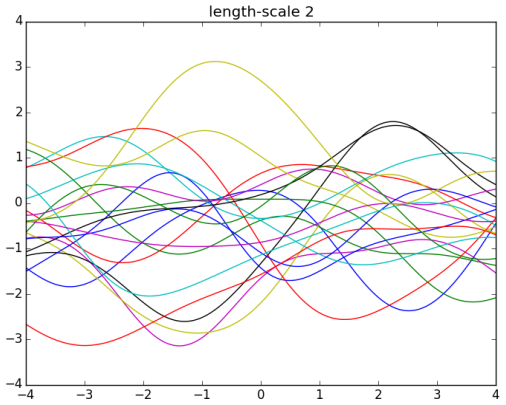
As we can observe in figure 5, the larger the length scale the smoother the samples become. The squared exponential covariance of a $\mathcal{GP}$ has the following form : $k(x_i, x_j) = \sigma_f^2 e - \frac{(x_i - x_j)^T (x_i - x_j)}{l^2}$.
For a constant squared euclidean distance between two points x_i and x_j, the larger l, the larger $k(x_i, x_j)$ is, which means that the instantiations f_i and f_j will be more strongly correlated. For a very small value of the length-scale ($l^2 \ll (x_i - x_j)^T (x_i - x_j)$), we can see that that the instantiations are uncorrelated



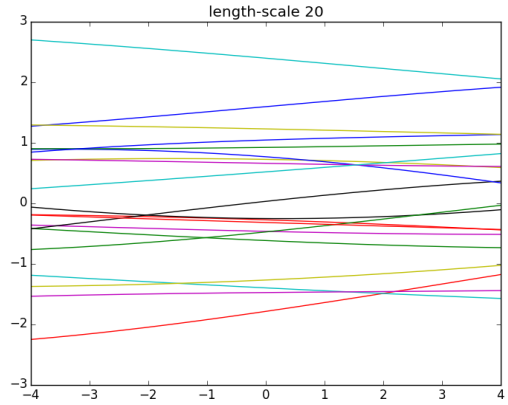
(a) Length-scale = 0.02



(b) Length-scale = 0.2



(c) Length-scale = 2



(d) Length-scale = 20

Figure 5: Samples from the $\mathcal{GP}$ with different length-scales

even for very points that are very close (figure 5a). For a very large value, $l^2 \gg (x_i - x_j)^T(x_i - x_j)$, and all the points are equally strongly correlated (figure 5d).

Question 13: *"The posterior and the prior are the same object if we do not have any observed data." Explain the statement, why is this?*

The predictive posterior is given by:

$$\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k(X,X) & k(X,x_*) \\ k(x_*,X) & k(x_*,x_*) \end{bmatrix} \right)$$

If we do not have any observed data, the predictive posterior becomes:

$$f_* \sim \mathcal{N}(0, k(x_*, x_*))$$

which is a sample from the $\mathcal{GP}$ prior.

Question 14:

1. *Compute the predictive posterior distribution of the model*
2. *Sample from this posterior with points both close to the data and far away from the observed data.*
3. *Plot the data, the predictive mean and the predictive variance of the posterior from the data.*

Explain the behavior of the samples and compare the samples of the posterior with the ones from the prior. Is this behavior desirable? What would happen if you would add a diagonal co-variance matrix to the squared exponential?

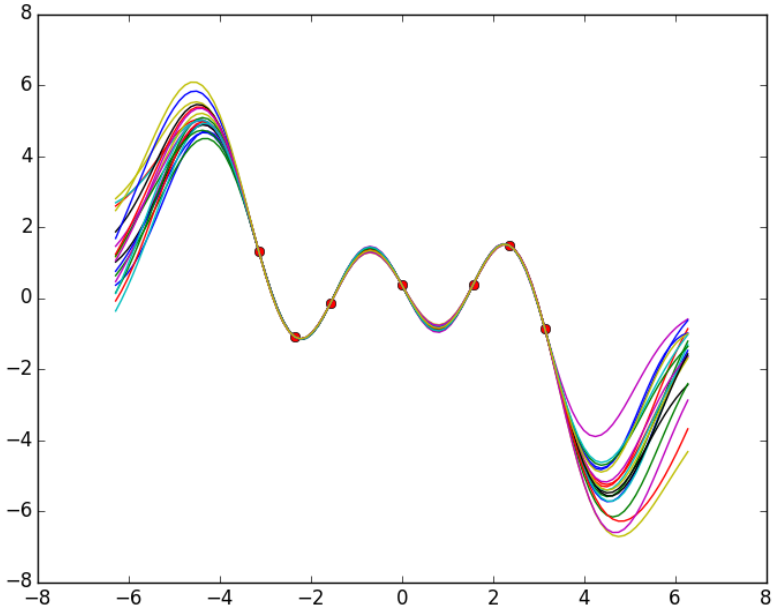
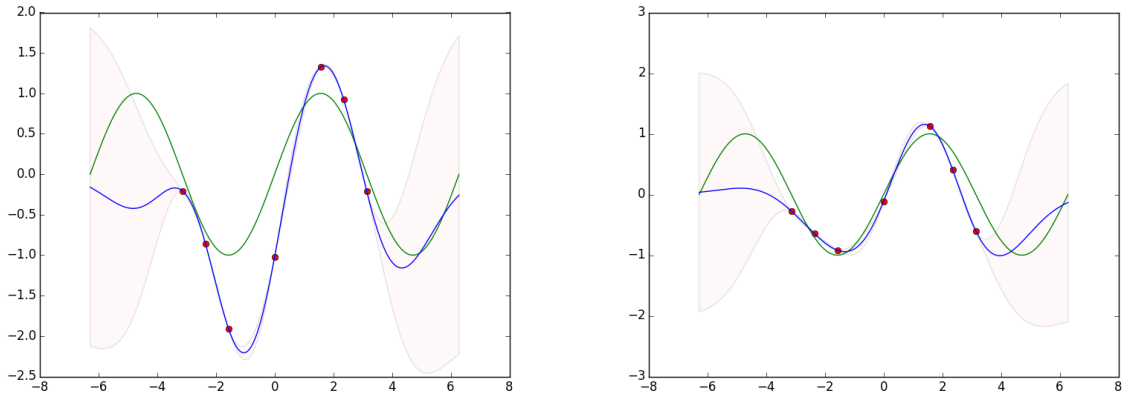


Figure 6: Samples from the posterior over $[-2\pi, 2\pi]$, length-scale = 2



(a) $\epsilon \sim \mathcal{N}(0, 0.5)$ (b) $\epsilon \sim \mathcal{N}(0, 0.05)$

Figure 7: Gaussian process regression over $[-2\pi, 2\pi]$, length-scale = 2

We apply non-parametric regression using a Gaussian process prior with an exponential kernel, to a data-set of 7 observations yi such as $yi = sin(x_i) + \epsilon$, where ϵ is independent Gaussian noise and $x_i \in [-\pi, ..., \pi]$.

In figure 7, the green curve shows the the function sin and the red points show the observations. The blue curve shows the the mean of the Gaussian process predictive distribution, and the shaded region corresponds to plus and minus **2** standard deviations. We observe how the uncertainty increases in the regions that are far from the data points. To the left and to the right, the predictive mean converges towards 0, the mean of the prior, and the standard deviation converges towards 1 ($2\sigma = 2$ in figure 7), which is the value of the parameter σ_f used in the covariance function of the prior.

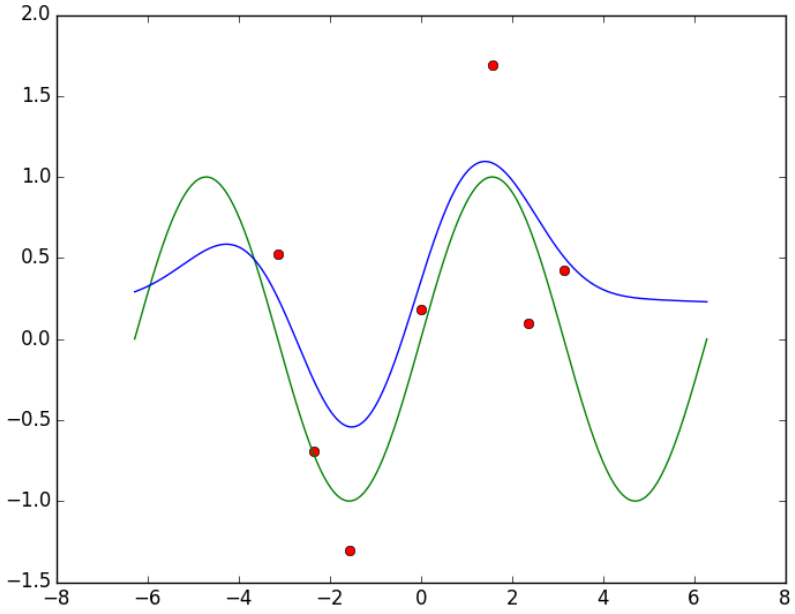


Figure 8: Gaussian process regression with $p(f|X, \theta) \sim k(X*, X) + \sigma^2 I$

After adding a diagonal covariance matrix to the squared exponential in figure 8, we observe that the conditional distribution doesn't pass exactly through the data points as it did in figure 7. It is equivalent to adding independent Gaussian noise to each of the values of y_n obtained by evaluating the function at input values x_n with $p(f|X, \theta) \sim k(X*, X)$, a squared exponential covariance function.

2 The Posterior $p(X|Y)$

2.1 Theory

Question 15: *Elaborate on this, why can one view a prior as encoding a preference?*

Since there is a simple relationship between W and X in the linear model, specifying a prior over X allows us to encode our preference of the form or the properties that the variable X should have, and that automatically constraints the variable W.

Question 16: *What type of "preference" does this prior encode?*

The prior $p(x) = \mathcal{N}(0, I)$ encodes our preference for latent variables x with independent dimensions:

$$\forall i \leq N,\ \forall j, k \leq D\ j \neq k \quad cov(x_i^j, x_i^k | f, x_i) = 0$$

Since there is a simple relationship between W and X in the linear model, specifying a prior over X allows us to encode our preference of the form or the properties that the variable X should have, and that automatically constraints the variable W.

Question 17: *Perform the marginalisation in Eq. 23 and write down the expression. As pre- viously, I do recommend that you do this by hand but to pass the assignment you only need to outline the calculations and show the approach that you would take?*

for a single data $y_i \in \mathbb{R}^D$, we assume a linear and a non-parametric Gaussian process, hence:

$$y_i = Wx_i + \epsilon \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I)$$

The likelihood can be written as:

$$p(y_i | x_i, W) = \mathcal{N}(y_i | Wx_i, \sigma^2 I)$$

We integrate over the latent variables to get the marginal likelihood:

$$p(y_i | W) = \int p(y_i | x_i, W) p(x_i) dx_i$$

where $p(x_i) = \mathcal{N}(0, I)$ is the prior over the latent variables.
The product of 2 Gaussians is a Gaussian, the marginal distribution of the data is also Gaussian. We can derive it by completing the square in the exponent, or just by evaluating the mean and the covariance given that it is a Gaussian:

$$\begin{aligned} \mathbb{E}[y_i | W] &= \mathbb{E}[Wx_i + \epsilon] \\ &= W\mathbb{E}[x_i] + \mathbb{E}[\epsilon] \\ &= 0 \end{aligned}$$

$$\begin{aligned} cov[y_i, y_i | W] &= \mathbb{E}[(y_i - \mathbb{E}[y_i])(y_i - \mathbb{E}[y_i])^T] \\ &= \mathbb{E}[(Wx_i + \epsilon)(Wx_i + \epsilon)^T] \\ &= \mathbb{E}[Wx_i x_i^T W^T] + \mathbb{E}[\epsilon\epsilon^T] \\ &= WW^T + \sigma^2 I \end{aligned}$$

The marginal distribution for each data point is:

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

The marginal distribution for the full data set is:

$$p(Y | W) = \prod_{i=1}^{N} p(y_i | W)$$

2.1.1 Learning

Question 18: *Compare the three estimation procedures above.*

- *How are they different?*
- *How are MAP and ML different when we observe more data?*
- *Why is the two last expressions of Eq. 25 equal?*

- The MAP estimate is the mode of the posterior. Maximum likelihood is equivalent to MAP with a uniform prior. If we write the equations in log space:
  - Maximizing likelihoood is equivalent equivalent to minimizing sum squared error, ie minimizing :
  $$l(w) = -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - W^T x_i^2) + const$$
  - MAP is equivalent to minimizing:
  $$l(w) = -\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - W^T x_i)^2 - \sum w_i^2 + const$$

  MAP is more expensive than ML computationally.
- When we observe more data, the data will dominate the posterior distribution, as it will overwhelm the prior, and the MAP estimate will coverge towards the MLE estimate.
- According to Bayes' rule:
$$p(W|Y,X) = \frac{p(Y|W,X)p(W)}{p(Y|X)} = \frac{p(Y|X,W)p(W)}{\int p(Y|X,W)pW dW}$$

  Since p(Y|X) does not depend on W:
$$argmax_W \ \frac{p(Y|X,W)p(W)}{\int p(Y|X,W)pW dW} = argamx_W \ p(Y|X,W)p(W)$$

Question 19:

1. *Write down the objective function* $-log(p(Y|W)) = \mathcal{L}(W)$
2. *Write down the gradients of the objective with respect to the parameters* $\frac{\partial \mathcal{L}}{\partial W}$

1. The marginal likelihood from Question 17 is, where $y_i \in \mathbb{R}^D$:

$$\begin{aligned} p(Y|W) &= \prod_{i=1}^{N} p(y_i|W) \\ &= \prod_{i=1}^{N} \mathcal{N}(y_i|0, WW^T + \sigma^2 I) \\ ln(p(Y|W)) &= \sum_{i=1}^{N} ln(p(y_i|W)) \\ &= \sum_{i=1}^{N} ln(\frac{1}{2\pi|WW^T + \sigma^2 I|} e - \frac{1}{2}(y_i^T (WW^T + \sigma^2 I)^{-1} y_i) \\ &= -\frac{ND}{2} ln(2\pi) - \frac{N}{2} ln(|WW^T + \sigma^2 I|) - \frac{1}{2} \sum_{i=1}^{N} (y_i^T (WW^T + \sigma^2 I)^{-1} y_i) \\ \mathcal{L}(W) &= \frac{1}{2}(NDln(2\pi) + Nln(|WW^T + \sigma^2 I|) + Tr((WW^T + \sigma^2 I)^{-1} YY^T) \end{aligned}$$

2. Using the following rules[1]:

$$\begin{aligned} \partial ln(det(X)) &= Tr(X^{-1} \partial X) \\ \partial Tr(X) &= Tr(\partial X) \\ \partial X^{-1} &= -X^{-1} (\partial X) X^{-1} \end{aligned}$$

And:

$$\frac{\partial (WW^T + \sigma^2 I)}{\partial W_{ij}} = \frac{\partial WW^T}{\partial W_{ij}}$$

We write the gradient of the objective function:

$$\left(\frac{\partial \mathcal{L}(W)}{\partial W} \right)_{ij} = \frac{\partial \mathcal{L}(W)}{\partial W_{ij}} = \frac{1}{2} Tr(YY^T [-(WW^T + + \sigma^2 I)^{-1} \times \frac{\partial WW^T}{\partial W_{ij}} \times (WW^T + \sigma^2 I)^{-1}]) + \frac{N}{2} Tr[(WW^T + + \sigma^2 I)^{-1} \times \frac{\partial WW^T}{\partial W_{ij}}]$$

Where:

$$\frac{\partial WW^T}{\partial W_{ij}} = J_{ij} W^T + W J_{ij}^T$$

2.1.2 Non-parametric

Question 20: *Explain why it is simpler to marginalise out f than X?*
Suggestion: Draw the graphical model and use this to motivate your explanation.

As we can see in figure 9, in the non-parametric case, the mapping f captures the uncertainty in X and θ, which allows us to have a marginalisation that is a step shorter than if we had integrated out the latent locations X.

[1] Petersen & Pedersen, The Matrix Cookbook, Version: November 15, 2012, Page 8

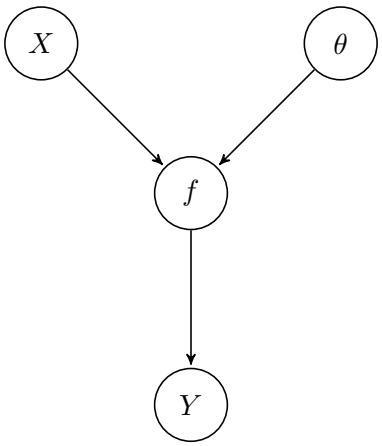


Figure 9: Graphical model for non-parametric representation learning

2.2 Practical

2.2.1 Linear Representation Learning

Question 21: *Plot the representation that you have learned. Explain why it looks the way it does. Was this the result that you expected? Hint: Plot X as a two-dimensional representation.*

We recover the type-II maximum likelihood estimate for the linear mapping W:

$$\hat{W} = argmin_W \, \mathcal{L}(W)$$

We can then write:

$$\begin{aligned} Y &= X'\hat{W}^T \\ Y\hat{W} &= X'\hat{W}^T\hat{W} \\ X' &= Y\hat{W}(\hat{W}^T\hat{W})^{-1} \end{aligned}$$

When comparing the actual X' (figure 11) and the representation of X' that we have learned (figure 10), we can see that while their shapes are similar, one is a rotated version of the other. Since the marginal likelihood that we maximize has the following form:

$$P(Y|W) = \prod_{i=1}^{N} \mathcal{N}(y_i|0, WW^T + \sigma^2 I)$$

For all $\hat{W} = WR$:

$$\begin{aligned} P(Y|\hat{W}) &= \prod_{i=1}^{N} \mathcal{N}(y_i|0, WRR^TW^T + \sigma^2 I) \\ &= \prod_{i=1}^{N} \mathcal{N}(y_i|0, WW^T + \sigma^2 I) \end{aligned}$$

The likelihood is invariant to a rotation of W. Therefore, all the linear mappings $\hat{W} = WR$ are solutions, which explains the difference in the direction of rotation between the actual and the learned X'.

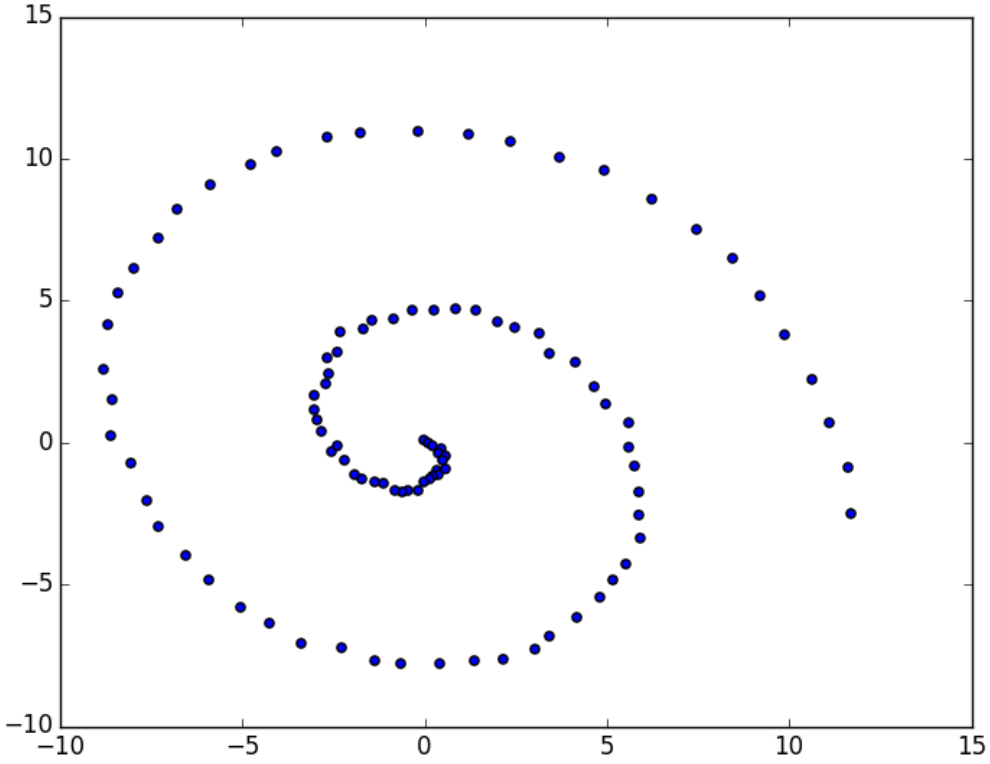


Figure 10: Learned representation of X'

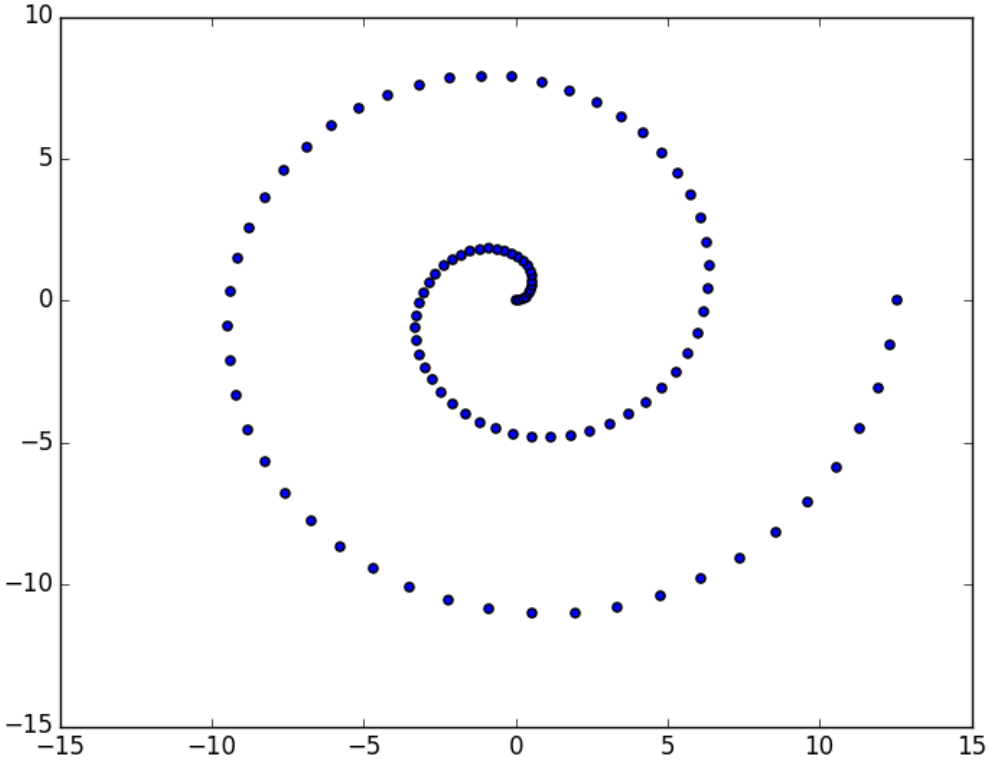


Figure 11: Actual $X' = [X \odot sin(X), X \odot cos(X)]$ where $X = [0...4\pi]^T$

3 The Evidence $p(Y)$

3.1 Theory

3.1.1 Data

3.1.2 Models

Question 22: *Why is this the simplest model, and what does it actually imply? Discuss its implications, why is this a bad model and why is it a good model.*

M_0 is the simplest model because it has no free parameters: it assigns all datasets an equal probability of $\frac{1}{152}$. It has the advantage of having the largest evidence over all the range of possible data-sets, but it since it uses no information about the actual data-set, it is unable to assign much probability mass to simple data-sets.

Question 23: *Explain how each separate model works? In what way is this model more or less flexible compared to M0? How does this model spread its probability mass over D?*

Given θ_i, each model gives see how well a point x^i is separable by the decision boundary $\theta_1^1 x^i = 0$ where one side of which has $y = 1$ and the other one has $y = -1$. If y^i corresponds to the right position of the point with respect to the boundary then, $p \geq 0.5$.
M_1 is similar to standard logistic regression but it only takes into account the first dimension of x. M_1 will give a higher probability to data-sets with sharp linear decision boundaries that are a function of x_1, and not x_2: it means that it is more adaptable to this category of data-sets. M_1 concentrates its probability mass around this limited number of data-sets, while M_0 predicts that the data will be drawn from a large number of data-sets, thus spreading its unit probability mass over a wider range.

Question 24: *How have the choices we made above restricted the distribution of the model? What data sets are each model suited to model? What does this actually imply in terms of uncertainty? In what way are the different models more flexible and in what way are they more restrictive? Discuss and compare the models to each other?*

M_2 will give a higher probability to data-sets with decision boundaries crossing the origin, while M_3 with the bias term θ_0 allows decision boundaries to be offset from the origin. M_3, is the most complex model of the four in the sense that it has the most parameters and can realize the other models by setting some of its parameters to zero. This means that we expect it to spread the important part of its unit probability mass over a wider range of data sets than the other models. However, this flexibility means that when the observed data can be explained by a simpler model, M_3 will be penalized since it has spent its probability mass elsewhere.

Question 25: *Explain the process of marginalisation. Discuss its implications.*

Being Bayesians, we express our believes about the parameter θ by specifying a prior over θ. We then find the evidence of the model $p(D|M_i)$ by averaging $p(D|M_i, \theta)$ over all possible values of the parameter θ,

using the prior $p(\theta)$ as a weight for each of these values: we average according to our beliefs. The evidence can also be viewed as the probability of generating the data set D from a model whose parameters are sampled randomly from the prior.

Question 26: *What does this choice of prior imply? How does the choice of the parameters of the prior μ and Σ affect the model?*

The prior on the parameters $p(\theta|M_i) = \mathcal{N}(0, 10^3 I)$ implies :

- The components (dimensions) of the vector θ are independent.
- The standard deviation is $10^{\frac{3}{2}}$: it means that we favour settings of the parameter θ which correspond in x space to sharp linear boundaries. Therefore we assume data-sets with sharp linear boundaries to be typical.

Question 27: *For each model sum the evidence for the whole of D what numbers do you get? Explain these numbers for all the models and relate them to each other.*

By construction of $p(D|M, \theta)$ for all possible data-sets, the evidence sums to one (for each model).

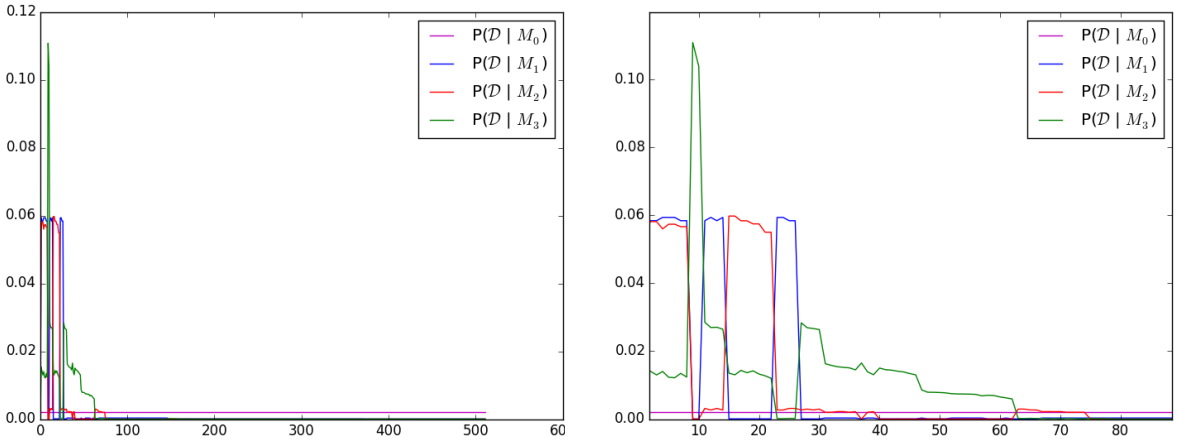
Question 28: *Plot the evidence over the whole data set for each model. The x-axis index the different instances in D and each models evidence is on the y-axis. How do you interpret this, relate this to the parametrisation of each model.*

The evidence plot in figure 12 confirms that M_0 has the largest evidence over all the range of possible data-sets.
We can also see that the models M_1, M_2 and M_3 are nested in the sense that a model with a higher number of parameters could represent another by setting some of its parameters to 0. Therefore, we can see that M_3 assigns probability mass to all the data-sets predicted by M_1 and M_2, but it is outperformed by them in some ranges that would correspond to data-sets with simple decision boundaries.
The range where the evidence given by M_2 and M_3 is maximal and similar ($D \leq 10$) would correspond to data-sets with vertical or almost vertical boundaries that are well-modeled by both, with an advantage for M_1 that is simpler and therefore has more probability mass to assign to them. When the evidence given by M_2 is maximal, the data-sets would still have simple boundaries(linear and crossing the origin), but with orientations that cannot be captured by M_1 because it is only a function of x_1.
When ($D \geq 25$), we are in the range of data-sets with more complex boundaries that can only be modeled by M_3 because it's the only model with a bias term.

Question 29: *Find using np.argmax and np.argmin which part of the D that is given most and least probability mass by each model. Plot the data-sets which are given the highest and lowest evidence for each model. Discuss these results, does it make sense?*

Model 0

All data-sets have the same probability under M_0



(a) Plot over all possible data-sets

(b) zoom over a subset of possible data-sets

Figure 12: Plots of evidence for possible data-sets $\mathcal{D}$ for the models

Model 1

M_1 captures decision boundaries that are functions of x_1 and not x_2. The data-set in table 2 has a simple boundary that is a function of x1 (since the different point has $x_1 = 0$, which explains why M_1 would give it a high probability.

The data-set in table 3 has a complex boundary (the points are non-linearly separable), which explains why it has a low probability.

Table 1: Model 1

Table 2: Most probable data-set

O	O	X
O	O	X
O	X	X

Table 3: Least probable data-set

O	X	O
X	X	O
O	X	X

Model 2

M_2 is standard logistic regression without the bias term θ_0, so it models decision boundaries that cross the origin. It makes sens that the data-set in table 5 has a high probability under M_2.

Similarly to M_1, the data-set with the lowest probability for M_2 (table 6) has a complex non-linear boundary.

Table 4: Model 2

Table 5: Most probable data-set

O	O	O
X	O	O
X	X	X

Table 6: Least probable data-set

X	O	O
X	O	X
O	O	O

Model 3

M_3 has a bias term that allows decision boundaries to be offset from the origin; the prior on the parameter θ_3, has width $10^{\frac{3}{2}}$, which favors sharp linear boundaries (possibly large intercepts), both of which are consistent with the data-set in table 8.

Table 7: Model 3

Table 8: Most probable data-set

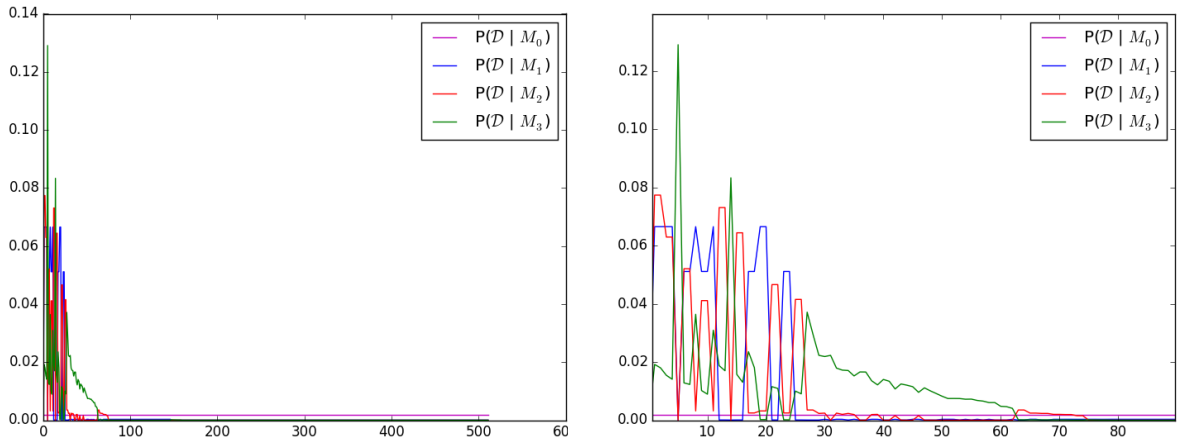
X	X	X
X	X	X
X	X	X

Table 9: Least probable data-set

O	X	O
O	O	X
X	O	O

Question 30: *What is the effect of the prior $p(\theta)$.*

- *What happens if we change its parameters?*
- *What happens if we use a non-diagonal covariance matrix for the prior?*
- *Alter the prior to have a non-zero mean, such that $\mu = [5, 5]^T$?*
- *Redo evidence plot for these and explain the changes compared to using zero-mean.*



(a) Plot over all possible data-sets

(b) zoom over a subset of possible data-sets

Figure 13: Evidence for possible data-sets $\mathcal{D}$ with $p(\theta|M_i) = \mathcal{N}(\mu, \Sigma)$, where $\mu = [5, 5]^T$

- We saw from our experiments that a prior with a large variance favored sharp decision boundaries, which happens for large settings of the parameters θ. If we had chosen a prior with a smaller variance, then the models would have given a more uniform evidence, similarly to M_0.
- With a non-diagonal covariance matrix for the prior, the parameters θ_n (components of the vector θ) become dependent. Certain data-sets would become more or less probable depending on the value and sign of the correlation between the parameters. For example in M_3, if θ_1 and θ_2 are

positively correlated with each other and negatively correlated with θ_0, the data-sets with a slope and and intercept that have different signs will be assigned a higher probability.

- The evidence plot for a prior with a non-zero mean (figure 13) show evidence distributions that are more peaked around certain data-sets for all models. We can therefore conclude that a non-zero mean assigns a larger probability mass to specific data-sets, for which the boundaries correspond to parameter values around this mean.