

Assignment 1 - Report

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Todo

- finire risposta 4
- check e finire risposta 5
- question 6 mettere una immagine della marginale
- domanda 9, che varianza scegliere nel prior?
- domanda 9 rifare i calcoli per fare un sample delle rette

Question 1

Choosing the gaussian distribution means that the values t_i is distributed symmetrically around the true deterministic function. because the gaussian distribution is a unimodal distribution, which means that has only one mode and for this particular distribution it coincides with the mean. This can be rephrased as assuming a deterministic model $f(\mathbf{x})$ that generates realizations with a random error ε that distributes as $\varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$. This can be written as:

$$\mathbf{t} = f(\mathbf{x}) + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$$

A prior observation about the covariance matrix is that it is constant, it does not depend on the input vector \mathbf{x} . Then the spherical covariance matrix implies two facts:

- All the scalar random variables t_{ij} of the vector \mathbf{t}_i have the same variance σ^2 (called homoscedasticity).
- The fact that the covariance matrix is diagonal means that all the output scalar component t_{ij} of the vector \mathbf{t}_i are independent one another.

Question 2

If we do not assume independence of the samples, we must turn to the joint probability distribution

$$p(\mathbf{T}|f, \mathbf{X}) = p(\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_N|f, \mathbf{X})$$

Question 3

Equation 5 is a linear transformation of a normal distribution which, from its properties, is again a normal distribution equal to:

$$p(\mathbf{t}_i) \sim \mathcal{N}(\mathbf{W} \mathbf{x}_i, \sigma^2 \mathbf{I})$$

Still assuming conditionally independent samples, from Eq. 3 the likelihood is just:

$$p(\mathbf{T}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^N \mathcal{N}(\mathbf{t}_i|\mathbf{W} \mathbf{x}_i, \sigma^2 \mathbf{I})$$

Which we can also write by expanding the whole product, by noting that since all the \mathbf{t}_i have the same variance, the exponents in the probability density function sum up.

$$\begin{aligned} p(\mathbf{T}|\mathbf{X}, \mathbf{W}) &= \prod_{i=1}^N \frac{1}{\sigma^D (2\pi)^{\frac{D}{2}}} \cdot e^{-\frac{1}{2\sigma^2} (\mathbf{t}_i - \mathbf{W} \mathbf{x}_i)^T (\mathbf{t}_i - \mathbf{W} \mathbf{x}_i)} = \\ &= \frac{1}{\sigma^{ND} (2\pi)^{\frac{ND}{2}}} \cdot e^{-\frac{1}{2\sigma^2} \sum_i^N (\mathbf{W} \mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W} \mathbf{x}_i - \mathbf{t}_i)} = \\ &= \frac{1}{\sigma^{ND} (2\pi)^{\frac{ND}{2}}} \cdot e^{-\frac{1}{2\sigma^2} \text{Tr}((\mathbf{X} \mathbf{W}^T - \mathbf{T})(\mathbf{X} \mathbf{W}^T - \mathbf{T})^T)} = \\ &= \mathcal{N}(\mathbf{X} \mathbf{W}^T, \mathbf{I}, \sigma^2 \mathbf{I}) \end{aligned}$$

Where we substituted the expression at the exponent $\sum_i^N (\mathbf{W} \mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W} \mathbf{x}_i - \mathbf{t}_i)$ with $\text{Tr}((\mathbf{X} \mathbf{W}^T - \mathbf{T})(\mathbf{X} \mathbf{W}^T - \mathbf{T})^T)$ by noting that the summation is just the sum of the diagonal of the matrix $(\mathbf{X} \mathbf{W}^T - \mathbf{T})(\mathbf{X} \mathbf{W}^T - \mathbf{T})^T$.

Question 4

The two penalization terms can be obtained from the prior. First let's do the one for the L_2 norm, and then we will generalize to the L_1 . We can write the prior on W as:

$$p(W) = \frac{1}{\tau^2 (2\pi)^{\frac{D}{2}}} \cdot e^{-\frac{\text{tr}((W - W_0)(W - W_0)^T)}{2\tau^2}} = \frac{1}{\tau^2 (2\pi)^{\frac{D}{2}}} \cdot e^{-\frac{\sum_i^N w_i^T \cdot w_i}{2\tau^2}}$$

If we multiply with the expression computed above for the likelihood $p(\mathbf{T}|\mathbf{X}, \mathbf{W})$ we get:

$$p(\mathbf{W}|\mathbf{X}, \mathbf{T}) \propto e^{-\frac{1}{2\sigma^2} \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i) - \frac{1}{2\tau^2} \sum_i^N w_i^T \cdot w_i}$$

Where we have disregarded the multiplicative factor in front of the exponent, because by taking the log will lead to a constant factor. Now we take the negative logarithm:

$$-\log(p(\mathbf{W}|\mathbf{X}, \mathbf{T})) \propto \frac{1}{2\sigma^2} \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i) + \frac{1}{2\tau^2} \sum_i^N w_i^T \cdot w_i$$

Where we can easily see the penalizing factor:

$$\frac{1}{2\tau^2} \sum_i^N w_i^T \cdot w_i = \frac{1}{2\tau^2} \sum_i^N \|w_i\|_{L_2}$$

Of course the proper extension to the L_1 norm will lead to the penalizing term:

$$\frac{1}{2\tau^2} \sum_i^N |w_i| = \frac{1}{2\tau^2} \sum_i^N \|w_i\|_{L_1}$$

Using L_1 norm will perform some kind of dimensionality reduction by setting some variables to 0, while the quadratic term will try to balance the parameter. We can see this effect by inspecting the derivative of the penalizing term: for the L_1 norm it is always constant, while for the L_2 it decreases as we get closer to zero, this means that in L_2 optimizing values that are close to the origin does not get me any decrease in the penalizing term, while if I take a value far away from the origin then this will decrease a lot my penalizing term.

We can also see visually by looking at the iso-contours of these functions in figure 1.

We can see that the corners of the square lie on the axis, so where one of the two variables is zero.

$w^T w$: for the L_2 norm which is just the Frobenius norm $|w|_F$

These two priors will introduce an additive term depending on the model parameter $|w|$, which would be of second order for the L_2 metric, and a first order L_1 for the other one.

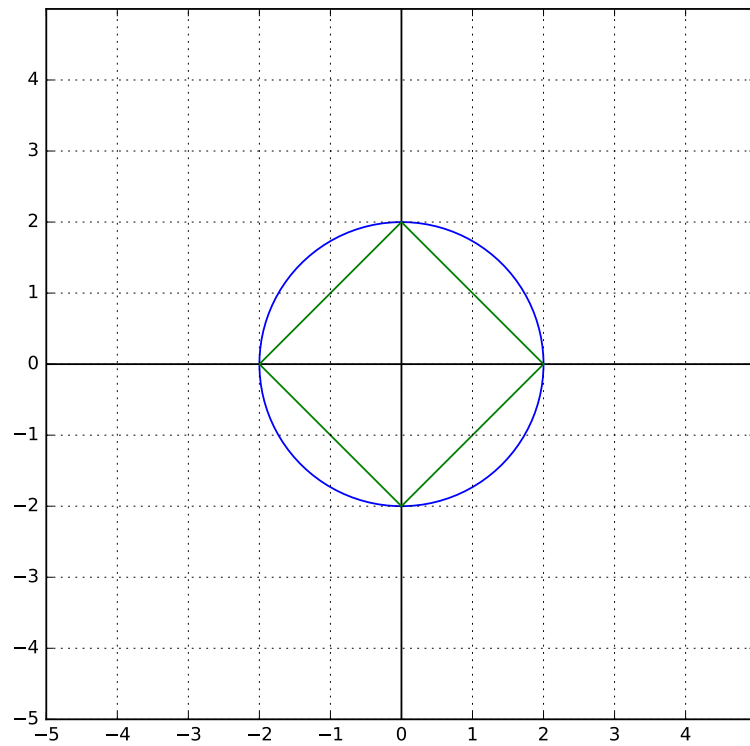


Figure 1: Showing L1 and L2 differences.

Question 5

We will use the square completion to perform this task. So we assume that the output is normal with the following parametrs:

$$\begin{aligned} p(W) &= \frac{1}{\xi} \cdot e^{-\frac{1}{2} \text{tr}(V^{-1}(W-W_0)\Sigma^{-1}(W-W_0)^T)} = \\ &= \frac{1}{\xi} \cdot e^{-\frac{1}{2} \text{tr}(V^{-1}W\Sigma^{-1}W^T)} e^{\text{tr}(V^{-1}W\Sigma^{-1}W_0^T)} e^{-\frac{1}{2} \text{tr}(V^{-1}W_0\Sigma^{-1}W_0^T)} \end{aligned}$$

Where ξ is just the normlaizing factor to make the integral of the function 1.

Now we will take the product of the prior over W , and the likelihood $p(\mathbf{t}_i|\mathbf{x}_i, \mathbf{W})$.

$$\begin{aligned} p(\mathbf{t}_i) &= e^{-\frac{1}{2\sigma^2}(\mathbf{t}_i - W\mathbf{x}_i)^T(\mathbf{t}_i - W\mathbf{x}_i)} \cdot e^{-\frac{1}{2\tau^2} \text{tr}((W-W_0)(W-W_0)^T)} \\ &= e^{-\frac{1}{2\sigma^2} \text{tr}((\mathbf{t}_i - W\mathbf{x}_i)(\mathbf{t}_i - W\mathbf{x}_i)^T)} \cdot e^{-\frac{1}{2\tau^2} \text{tr}((W-W_0)(W-W_0)^T)} \end{aligned}$$

Since they have the same dimensions, we can do merge the two traces:

$$\begin{aligned} p(\mathbf{W}|\mathbf{t}_i, \mathbf{x}_i) &= e^{-\frac{1}{2\sigma^2}(\mathbf{t}_i - W\mathbf{x}_i)^T(\mathbf{t}_i - W\mathbf{x}_i)} \cdot e^{-\frac{1}{2\tau^2} \text{tr}((W-W_0)(W-W_0)^T)} = \\ &= e^{-\frac{1}{2\sigma^2} \text{tr}((\mathbf{t}_i - W\mathbf{x}_i)(\mathbf{t}_i - W\mathbf{x}_i)^T)} \cdot e^{-\frac{1}{2\tau^2} \text{tr}((W-W_0)(W-W_0)^T)} = \\ &= e^{-\frac{1}{2\sigma^2} \text{tr}(\mathbf{t}_i \mathbf{t}_i^T)} e^{\frac{1}{\sigma^2} \text{tr}(W\mathbf{x}_i \mathbf{t}_i^T)} e^{-\frac{1}{2\sigma^2} \text{tr}(W\mathbf{x}_i \mathbf{x}_i^T W^T)} e^{-\frac{1}{2\tau^2} \text{tr}(W W^T)} e^{\frac{1}{\tau^2} \text{tr}(W W_0^T)} e^{-\frac{1}{2\tau^2} \text{tr}(W_0 W_0^T)} = \\ &= e^{-\text{tr}(W(\frac{1}{2\sigma^2} \mathbf{I} + \frac{1}{2\sigma^2} \mathbf{x}_i \mathbf{x}_i^T) W^T)} e^{\text{tr}(W(\frac{1}{\sigma^2} \mathbf{x}_i \mathbf{t}_i^T + \frac{1}{\tau^2} W_0^T))} e^{-\text{tr}(\frac{1}{2\sigma^2} \mathbf{t}_i \mathbf{t}_i^T + \frac{1}{2\tau^2} W_0 W_0^T)} \end{aligned}$$

Then assuming the independence of the t_i we can get to the full posterior.

$$\begin{aligned} p(\mathbf{W}|\mathbf{T}, \mathbf{X}) &= e^{-\text{tr}(W(\frac{1}{2\sigma^2} \mathbf{I} + \frac{1}{2\sigma^2} \sum_i \mathbf{x}_i \mathbf{x}_i^T) W^T)} e^{\text{tr}(W(\frac{1}{\sigma^2} \sum_i \mathbf{x}_i \mathbf{t}_i^T + \frac{1}{\tau^2} W_0^T))} e^{-\text{tr}(\frac{1}{2\sigma^2} \sum_i \mathbf{t}_i \mathbf{t}_i^T + \frac{1}{2\tau^2} W_0 W_0^T)} \\ p(\mathbf{W}|\mathbf{T}, \mathbf{X}) &= e^{-\text{tr}(W(\frac{1}{2\sigma^2} \mathbf{I} + \frac{1}{2\sigma^2} \mathbf{X}^T \mathbf{X}) W^T)} e^{\text{tr}(W(\frac{1}{\sigma^2} \mathbf{X}^T \mathbf{T} + \frac{1}{\tau^2} W_0^T))} e^{-\text{tr}(\frac{1}{2\sigma^2} \mathbf{T}^T \mathbf{T} + \frac{1}{2\tau^2} W_0 W_0^T)} \end{aligned}$$

Where we substituted $\sum_i \mathbf{x}_i \mathbf{t}_i^T$ with $\mathbf{X}^T \mathbf{T}$. This can be demonstrated to be true, and so I do in appendix A.

Now we can retrieve the variance and the mean of our prior.

$$\begin{aligned} \mathbb{E}(\mathbf{W}|\mathbf{T}, \mathbf{X}) &= \\ \text{Var}(\mathbf{W}|\mathbf{T}, \mathbf{X}) &= \end{aligned}$$

λ represents the regularizing term for our posterior distribution and, from Bayes rule, it must be equal to the evidence. But we are not intrested in it for the computation of the posterior, and it does not affect our derivation.

Question 6

This is a prior on functions, where a function is seen as a collection of infinite random variables, and for any subset of it the joint probability is a multivariate gaussian. To comment the prior we will analyze its two components. The least important is the mean, which is set arbitrarily to 0, which means that the functions we'll have zero mean. The most important component is the covariance, that is computed as a kernel function. The kernel function should implement some kind of "closeness measure" between two points x_i and x_j , with the kernel having high values if x_i is similar to x_j , low otherwise. This function sets the correlation between two points, so if x_i and x_j are close, their values will be high correlated, on the opposite side if $k(x_i, x_j) = 0$, then the two values y_i and y_j are independent (works only assuming the distribution normal). Basically the covariance function defines a transfer of information between one point and the other based on their distance.

Put figure(s) here

Question 7

If we also assume that \mathbf{X} and θ are random variables, we can apply the chain rule and easily decompose the formula into:

$$p(\mathbf{T}, \mathbf{X}, \mathbf{f}, \theta) = p(\mathbf{T}, \mathbf{f} | \mathbf{X}, \theta) p(\mathbf{X}, \theta)$$

Moreover it's safe to assume that \mathbf{X} and θ are independent, which lets me factor even more the formula into:

$$p(\mathbf{T}, \mathbf{f} | \mathbf{X}, \theta) p(\mathbf{X}, \theta) = p(\mathbf{T}, \mathbf{f} | \mathbf{X}, \theta) p(\mathbf{X}) p(\theta)$$

I can use the chain rule one again on the first term to get:

$$p(\mathbf{T}, \mathbf{f} | \mathbf{X}, \theta) p(\mathbf{X}) p(\theta) = p(\mathbf{T} | \mathbf{f}, \mathbf{X}, \theta) p(\mathbf{f} | \mathbf{X}, \theta) p(\mathbf{X}) p(\theta)$$

Where we know that $p(\mathbf{f} | \mathbf{X}, \theta)$ is a multivariate normal distribution for the definition of the gaussian processes. While we can get some insights in the term $p(\mathbf{T} | \mathbf{f}, \mathbf{X}, \theta)$ by looking at the relation between t_i and f_i . Since t_i depends on f_i and the latter, being conditioned, is known.

$$p(\mathbf{t}_i = t^* | \mathbf{f} = f^*, \mathbf{X}, \theta) = p(f^* + \varepsilon = t^* | \mathbf{f} = f^*, \mathbf{X}, \theta) = p(\varepsilon = t^* - f^* | \mathbf{f} = f^*, \mathbf{X}, \theta)$$

So this term is also gaussian.

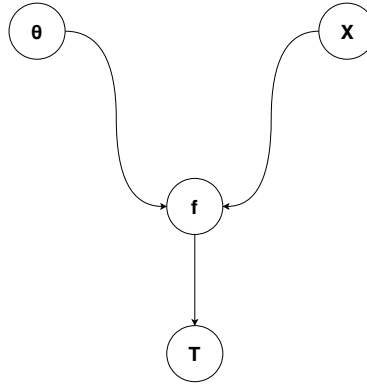


Figure 2: Graphical model of the assumption I made about the variables

Question 8

$$p(\mathbf{T}|\mathbf{X}, \theta) = \int p(\mathbf{T}|\mathbf{f}, \mathbf{X}, \theta) p(\mathbf{f}|\mathbf{X}, \theta) d\mathbf{f}$$

The integral has the meaning of a weighted average of the likelihood of the data over all possible function, where the weight is given by the prior on the functions. The uncertainty is reflected in the covariance matrix of the marginalized distribution, and it has 2 independent components: one comes from the noise ε , and the other comes from the uncertainty we have on the data that is can be seen as uncertainty on the shape of the functions of the gaussian process that we marginalize out. We still condition in θ because we assumed it as a constant, it could be marginalized if we have had assumed it was a random variable. In this form the marginal distribution is a function of θ , which is useful for performing hyperparameter optimization.

Question 9

There are 2 main effects in adding data to my model :

- The first one is the fact that the posterior moves its center towards the true value of my weights pair
- The variance of the posterior shrinks as I add more points

These two effects can be explained easily. The latter occurs because as we get more data we are more certain about the model, our belief increases, and so our variance reduces. This rate of change depends on the noise in our data. The first effect is determined by the fact that our belief changes as we see more points. Starting from the prior at the origin, we move towards the pair that better fits our data. The prior encodes some bias that fades away as we get more and more points.

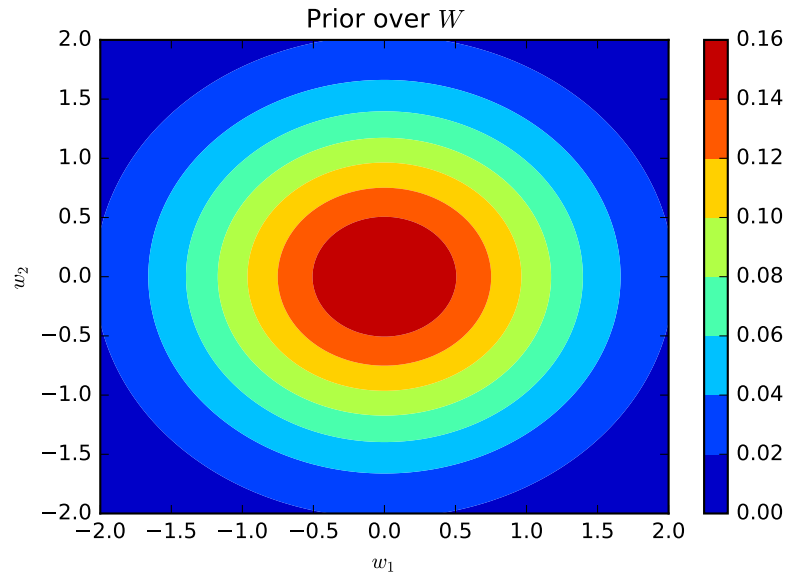


Figure 3: Prior over the parameters

Question 10

The lengthscale defines a “unit of measure” between the two points. Since it divides the difference between two points, if the lengthscale is low the two points will be less correlated, if the value of the lengthscale is high, then they will be highly correlated.

Question 11

Question 12

The preference is that our variable X is a normal distribution whose elements are independent, and distribute around zero.

Question 13

Since the model is:

$$\mathbf{y}_i = \mathbf{W}\mathbf{x}_i + \varepsilon$$

The mean of each \mathbf{y}_i is :

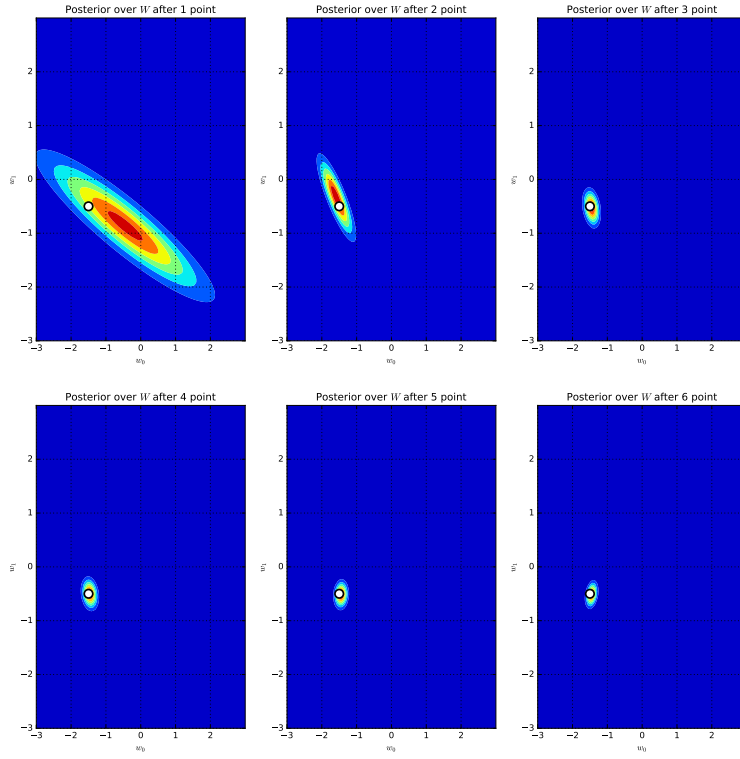


Figure 4: Posterior over the parameters after observing one point with $\sigma = 0.1$

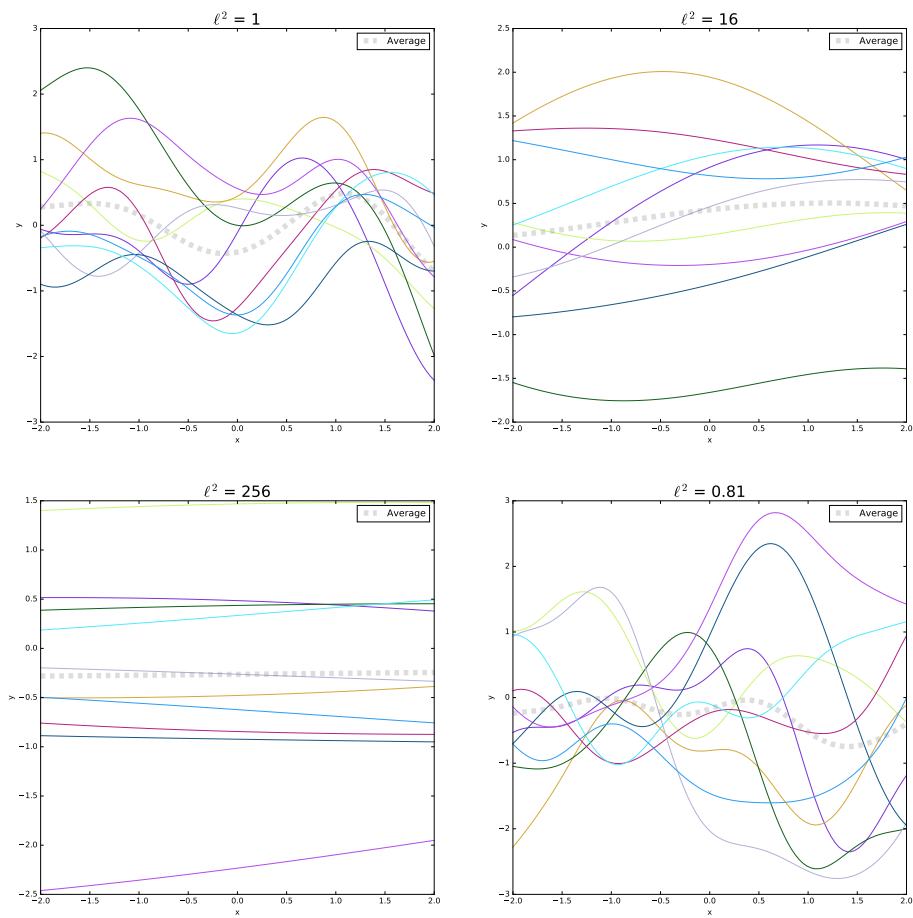


Figure 5: Samples from a gaussian process

$$\begin{aligned}
\mathbb{E}(\mathbf{y}_i) &= \mathbb{E}(\mathbf{W}\mathbf{x}_i + \varepsilon) \\
\mathbb{E}_X(\mathbf{y}_i) &= \mathbf{W} \mathbb{E}_X(\mathbf{x}_i) + \mathbb{E}_X(\varepsilon) \\
\mathbb{E}_X(\mathbf{y}_i) &= 0 + 0
\end{aligned}$$

We can describe the probability by only the first 2 moments of the random variable:

$$\text{Var}(\mathbf{y}_i) = \text{Var}(\mathbf{W}\mathbf{x}_i + \varepsilon)$$

Since they are uncorrelated, we can write:

$$\begin{aligned}
\text{Var}(\mathbf{y}_i) &= \text{Var}(\mathbf{W}\mathbf{x}_i) + \text{Var}(\varepsilon) \\
\text{Var}(\mathbf{y}_i) &= \mathbf{W}\text{Var}(\mathbf{x}_i)\mathbf{W}^T + \sigma^2\mathbf{I} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}
\end{aligned}$$

Since each y_i is independent with each other, we can combine the results we got into the distribution:

$$p(\mathbf{Y}|\mathbf{W}) = \prod_i^N \mathcal{N}(\mathbf{y}_i | \mathbf{0}, \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})$$

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

Question 14

MLE

From the derived distribution in question 3 we can compute the log likelihood:

$$\begin{aligned}
\log(p(\mathbf{Y}|\mathbf{X}, \mathbf{W})) &= \log \left(\frac{1}{\sigma^2(2\pi)^{\frac{D}{2}}} \cdot e^{-\frac{1}{2\sigma^2} \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)} \right) = \\
&= -\log \left(\sigma^2(2\pi)^{\frac{D}{2}} \right) - \frac{1}{2\sigma^2} \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)
\end{aligned}$$

In the maximization we disregard the constant factor $-\log \left(\sigma^2(2\pi)^{\frac{D}{2}} \right)$, and then remove also the multiplicative constant in the second term $\frac{1}{2\sigma^2}$. So we are left with the maximization of:

$$\arg \max_W - \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)$$

Which is clearly the generalization of the sum of residual square for vectorial outputs.

MAP

We can derive the expression starting from the previous part of the question.

$$\log(p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) \cdot p(\mathbf{W})) = \log(p(\mathbf{Y}|\mathbf{X}, \mathbf{W})) + \log(p(\mathbf{W}))$$

The first term of the summation is the MLE term from before, while the second one I have already computed in question 4 as:

$$\log(p(\mathbf{W})) = -\log\left(\tau^2(2\pi)^{\frac{D}{2}}\right) - \frac{1}{2\tau^2} \sum_i^N (\mathbf{w}_i)^T (\mathbf{w}_i)$$

Again we can disregard the constant term at the beginning, but we need to keep the multiplicative terms both for the prior and for the least square. Putting everything together we get:

$$\arg \max_W \left\{ -\frac{1}{2\sigma^2} \sum_i^N (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i)^T (\mathbf{W}\mathbf{x}_i - \mathbf{t}_i) - \frac{1}{2\tau^2} \sum_i^N (\mathbf{w}_i)^T (\mathbf{w}_i) \right\}$$

Where the second term acts as a regularizing term.

Type II ML

$$\begin{aligned} \log \left(\int p(\mathbf{Y}|\mathbf{X}, \mathbf{W}) p(\mathbf{X}) d\mathbf{X} \right) &= \log(p(\mathbf{Y}|\mathbf{W})) = \\ \log \left(\prod_{i=0}^N p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{W}) \right) &= \\ = \sum_{i=0}^N \log(p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{W})) &= \end{aligned}$$

If we substitute with the expression for $p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{W})$ we still have a log of a normal distribution.

$$= -\sum_{i=0}^N \log \left((\det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I}) 2\pi^D)^{\frac{1}{2}} \right) - \sum_{i=0}^N \mathbf{y}_i^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{y}_i$$

The two expression in equation 25 are equal because the denominator (the evidence) is constant for any choice of the model parameter W . The evidence only changes if we choose another model.

Type-II Maximum-Likelihood is a sensible way of learning the parameters because we first use the bayesian approach to avoid the overfit on data, and then we maximize the hyperparameter, which cannot overfit, because it is not backed by data.

Question 15

$$\begin{aligned} \mathcal{L}(\mathbf{W}) &= -\log \left(\prod_{i=0}^N \frac{1}{(2\pi^D \cdot \det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I}))^{1/2}} e^{-\frac{1}{2} \mathbf{y}_i^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{y}_i} \right) = \\ &= \sum_{i=0}^N \frac{1}{2} \log (2\pi^D \cdot \det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})) + \sum_{i=0}^N \frac{1}{2} \mathbf{y}_i^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{y}_i = \\ &= \frac{ND}{2} \log (2\pi^D) + \frac{N}{2} \log (\det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})) + \frac{1}{2} \sum_{i=0}^N \mathbf{y}_i^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{y}_i = \\ &= \frac{ND}{2} \log (2\pi^D) + \frac{N}{2} \log (\det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})) + \frac{1}{2} \text{Tr} (\mathbf{Y}^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{Y}) \end{aligned}$$

We can remove the constant terms, and remove 1/2 by multiplying by 2.

$$\mathcal{L}(\mathbf{W}) = N \log (\det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})) + \text{Tr} (\mathbf{Y}^T (\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{Y})$$

Moving on to the derivative:

$$\frac{\partial \mathcal{L}(\mathbf{W})}{\partial W_{ij}} = N \frac{\partial \log (\det(\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I}))}{\partial W_{ij}} + \frac{\partial \text{Tr} ((\mathbf{W}\mathbf{W}^T + \sigma^2 \mathbf{I})^{-1} \mathbf{Y}^T \mathbf{Y})}{\partial W_{ij}} =$$

Let's expand one term at a time:

$$\begin{aligned}\frac{\partial \log(\det(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}))}{\partial W_{ij}} &= Tr \left((\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot \frac{\partial (\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})}{\partial W_{ij}} \right) = \\ \frac{\partial \log(\det(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}))}{\partial W_{ij}} &= Tr \left((\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot \frac{\partial (\mathbf{W}\mathbf{W}^T)}{\partial W_{ij}} \right) \\ \frac{\partial (\mathbf{W}\mathbf{W}^T)}{\partial W_{ij}} &= \frac{\partial (\mathbf{W})}{\partial W_{ij}} \cdot \mathbf{W}^T + \mathbf{W} \cdot \frac{\partial (\mathbf{W}^T)}{\partial W_{ij}}\end{aligned}$$

Where the derivation $\frac{\partial (\mathbf{W})}{\partial W_{ij}}$ give rise to the single-entry element J_{ij}^1 .

$$\frac{\partial (\mathbf{W}\mathbf{W}^T)}{\partial W_{ij}} = \mathbf{J}_{ij} \cdot \mathbf{W}^T + \mathbf{W} \cdot \mathbf{J}_{ij}^T = \mathbf{J}_{ij} \cdot \mathbf{W}^T + (\mathbf{J}_{ij} \cdot \mathbf{W}^T)^T$$

The next term to derive is:

$$\frac{\partial Tr((\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \mathbf{Y}^T \mathbf{Y})}{\partial W_{ij}} = Tr \left(\frac{\partial (\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \mathbf{Y}^T \mathbf{Y}}{\partial W_{ij}} \right)$$

Using the identity:

$$\partial \mathbf{X}^{-1} = \mathbf{X}^{-1} \cdot \partial \mathbf{X} \cdot \mathbf{X}^{-1}$$

Mi sono dimenticato un meno

We get to:

$$\begin{aligned}Tr \left(\frac{\partial [(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \mathbf{Y}^T \mathbf{Y}]}{\partial W_{ij}} \right) &= Tr \left((\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot \frac{\partial (\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})}{\partial W_{ij}} \cdot (\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot \mathbf{Y}^T \mathbf{Y} \right) = \\ Tr \left(\frac{\partial [(\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \mathbf{Y}^T \mathbf{Y}]}{\partial W_{ij}} \right) &= Tr \left((\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot [\mathbf{J}_{ij} \cdot \mathbf{W}^T + \mathbf{W} \cdot \mathbf{J}_{ij}^T] \cdot (\mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})^{-1} \cdot \mathbf{Y}^T \mathbf{Y} \right)\end{aligned}$$

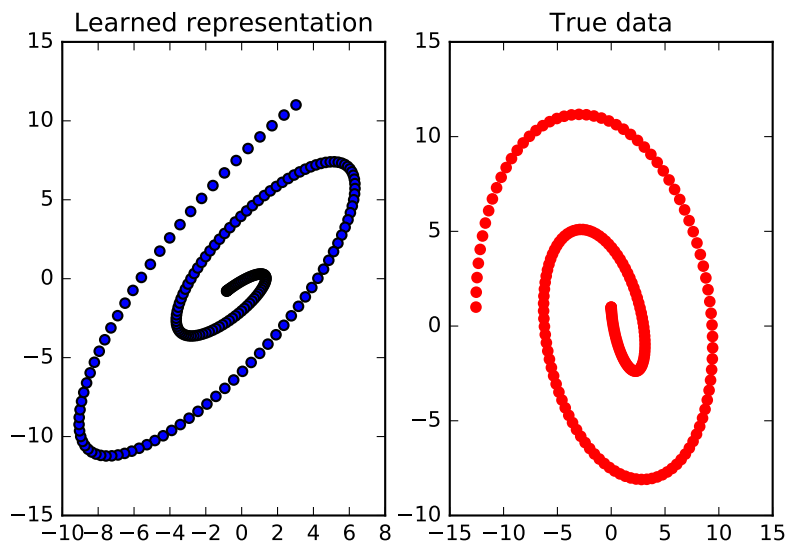


Figure 6: Representation learned

Question 16

Here is the representation I have learned, and beside the true data.

There is an invariance in the parameter matrix \mathbf{W} with respect to the dot product of any Orthogonal matrix, that is all possible rotation. We can see mathematically, if

$$\mathbf{W}'_{\text{opt}} = \mathbf{W}_{\text{opt}} \mathbf{R}$$

In the likelihood formula the parameter \mathbf{W} is present only in the form $\mathbf{W} \cdot \mathbf{W}^T$. So substituting both \mathbf{W}_{opt} and \mathbf{W}'_{opt} :

$$\mathbf{W}'_{\text{opt}} \cdot (\mathbf{W}'_{\text{opt}})^T = \mathbf{W} \mathbf{R} \cdot \mathbf{R}^T \mathbf{W}^T = \mathbf{W} \cdot \mathbf{W}^T$$

We can conclude that $\mathcal{L}(\mathbf{W}_{\text{opt}}) = \mathcal{L}(\mathbf{W}'_{\text{opt}})$, and so both are valid optimal solutions.

¹This notation is taken from the wikipedia page.

Question 17

This model is the simplest because it does not have any parameter and so its probability density function is fixed. In particular this model spreads all its probability equally over all dataset which means that the model does not have a more common dataset, one that it can “explain” the most. The lack of parameter means that we cannot also tune the model, we cannot make it learn or adapt to our data.

Question 18

Each of the next model resembles the logistic regression model, in fact we have in all setting a logistic sigmoid of a linear function in X and y .

$$\frac{1}{1 + \exp(-y_i \cdot (\mathbf{w}^T \cdot \mathbf{x}))}$$

So each model gives more probability mass to the dataset for which the quantity $y_i \cdot (\mathbf{w}^T \cdot \mathbf{x})$ is positive and (possibly) large. This quantity has a geometric meaning: the quantity is the distance between the line given by $\mathbf{w}^T \cdot \mathbf{x} = 0$ and the point \mathbf{x} , having the sign of y_i if \mathbf{x} lies on the side of the line “pointed” by \mathbf{w} , the opposite otherwise.

Model M1

Here we only focus the value of x_1 and we don’t consider x_2 , the line induced by w is orthogonal to the x_1 axis.

Model M2

Here we also care about the value of x_2 , and the resulting line can have any orientation, but it still pass through the origin.

Model M3

Here we also have a bias term w_3 , and the resulting line can have any orientation and intercept. This is the most general linear model, we cannot have more degrees of freedom.

Put image here

Question 19

Question 20

Marginalization is the process through which we can obtain the probability distribution of a random variable, from a joint probability distribution containing it. This process effectively “removes” the other variables, the marginalized ones, by a process that looks like a weighted average, in fact the formula:

$$\int_{\theta} p(D|M_i, \theta) p(\theta) d\theta$$

Expresses an average of models $p(D|M_i, \theta)$, by the probability of the model parameters $p(\theta)$. So we are averaging models taking into account the probability density function of θ .

Question 21

Again, by choosing that distribution for the prior we again assume that all the parameters are independent, because of the diagonal covariance matrix. And then we can relate the chosen parameters μ and σ^2 to the orientation of the lines defined by the expression $\mathbf{w}^T \cdot \mathbf{x}$ that we talked about in Question 18. The mean is zero, which means that the value of the parameters θ_i will distribute around zero, but their variance is very high, which means that is not unlikely the event of having a parameter far from zero. Since the parameter spread around zero, the average resulting line will be one

Question 22

If we sum up the evidence over all dataset, for each model we get 1 (obviously in practice there is a small error, in my case on the order of 10^4). That is because this is a probabilistic distribution, and so must sum up to 1. We can interpret this distribution from a generative perspective: if we would sample the model parameters at random, the probability of generating dataset D_i is $p(D_i|M_i)$.

There are a few comments about figure , where we can see that the left plot is symmetric, and given how the datasets are indexed in that figure, that means that the probability of a dataset doesn't change if we flip the sign to all the y_i in a dataset. This of course makes sense because the only thing that changes is the separating line sign, and since the distribution of the parameter is symmetric the probability of obtaining θ_i or $-\theta_i$ is the same.

Another comment is the shape of the plot on the right side. We see that M_3 has a higher peak in some datasets, while M_2 has its maximum value lower than the one of M_3 , but on a wider range in the dataset axis. The same consideration for

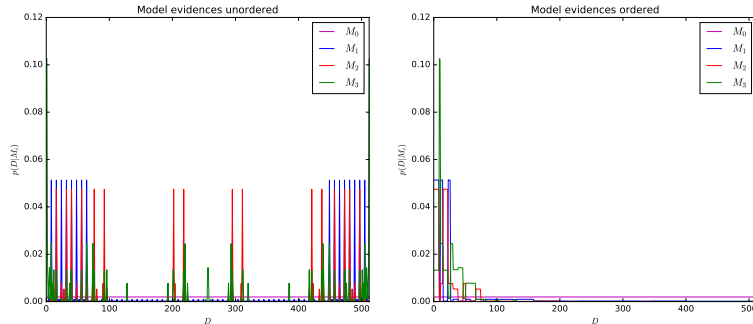


Figure 7: Shown here are the plots of the evidence of each dataset per each model. On the left using the order of the datasets as they were generated, on the right using the same ordering procedure proposed in the paper.

M_1 with respect to M_2 , while M_0 is completely flat at a constant value of $1/512$. We also see that M_3 assigns some probability distribution to the datasets where most of the probability mass of M_2 and M_1 lies, but the probability of M_3 is lower than the one assigned by M_2 or M_1 . Here lies the automatic Occam’s razor, we choose the model that puts the most probability on the datasets that we are interested in, which is usually the simplest.

Question 23

We can comment the most likely and the least likely for each models, represented in figure 8. Of course we do not have a maximum and minimum in the M_0 case, since all the models are equally probable, so they are not shown in the figure. For M_1 the most likely is one that can be separated by a vertical line, that is the model that it encodes. For M_2 the most likely is one that can be separated by a line that passes through the origin, again because the model it represents divide the space with a line crossing the origin. For M_3 the most likely is the one with all $+1$ (or -1). This is because we have also the bias term, and having a big variance this can move the line very far away from the square $[-1, 1] \times [-1, 1]$ where the data lies. If the line don’t cut in half the data it “classifies” all points as -1 or $+1$. While for the least probable dataset we see that it represent non-linearly separable configuration, which means that none of the model is likely to generate since they represent lines.

Question 24

The prior encodes the preferences about the parameter of the linear boundaries that each model encodes. So changing the mean, will make the “average”

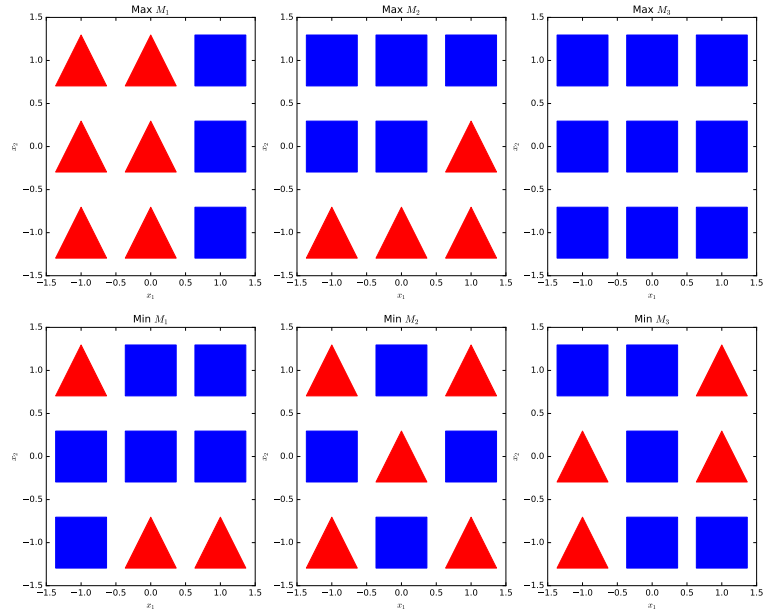


Figure 8: Representation of the most and least likely datasets, as said before, because of simmetricity we don't care if triangles represent +1 or -1. in the first row are the most probable datasets, and in the second one the least.

boundary the one having as parameter, the one specified by the mean. If we change the covariance, we introduce some dependance in the parameters of the decision boundary, which can cause the line to have a “preferred” direction. The result of changing the mean to 5, are depicted in figure 9. First of all we can see that we have lost the symmetricity in the left plot, because a having changed the mean, we encoded some preference in the direction of the normal of the decision boundary, so we will prefer datasets for which negative y_i lies below the line. Moreover the right plot is a little bit squashed toward the y_axis compared to the one of figure , we can see a scaled version in figure 10.

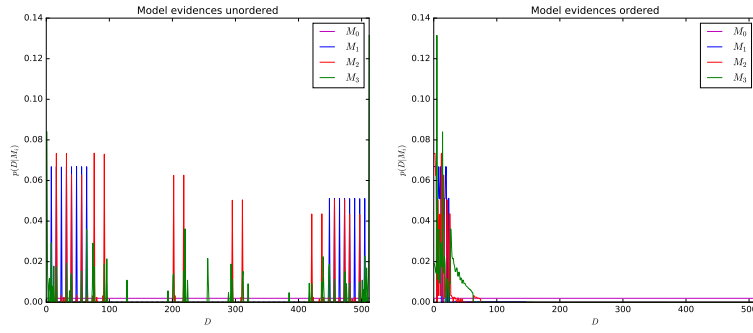


Figure 9:

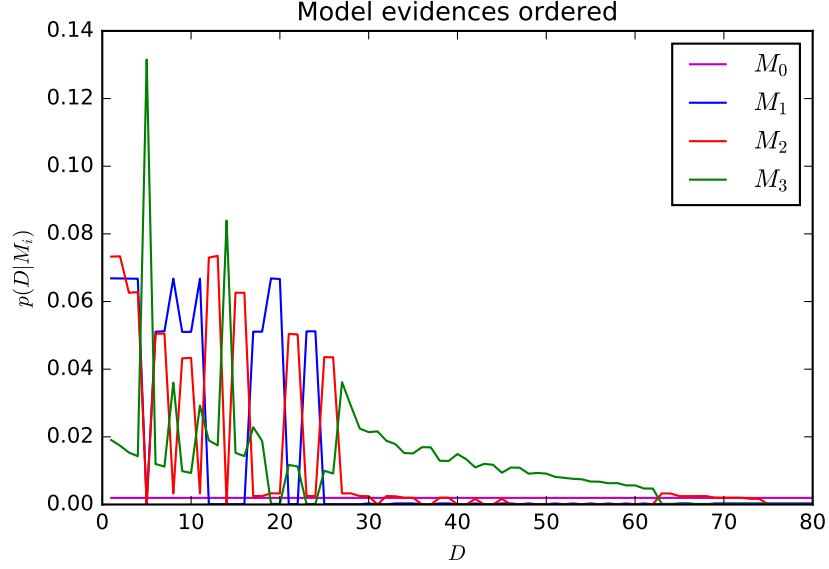


Figure 10:

Appendix A

Demonstration of $\sum_i \mathbf{x}_i \mathbf{x}_i^T = \mathbf{X}^T \mathbf{X}$

Suppose we have a matrix \mathbf{X} :

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix}$$

We can decompose this matrix as:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{0}^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} + \begin{bmatrix} \mathbf{0}^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} + \cdots + \begin{bmatrix} \mathbf{0}^T \\ \mathbf{0}^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix}$$

From the previous it immediately follows that its transpose can be expressed as:

$$\mathbf{X}^T = [\mathbf{x}_1 \quad \mathbf{0} \quad \cdots \quad \mathbf{0}] + [\mathbf{0} \quad \mathbf{x}_2 \quad \cdots \quad \mathbf{0}] + \cdots + [\mathbf{0} \quad \mathbf{0} \quad \cdots \quad \mathbf{x}_n]$$

Now if we multiply the decomposed version of the matrix \mathbf{X}^T together with \mathbf{X} and apply the distributive property we get:

$$\mathbf{X}^T \mathbf{X} = ([\mathbf{x}_1 \ \mathbf{0} \ \dots \ \mathbf{0}] + \dots + [\mathbf{0} \ \mathbf{0} \ \dots \ \mathbf{x}_n]) \cdot \left(\begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{0}^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} + \begin{bmatrix} \mathbf{0}^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} + \dots + \begin{bmatrix} \mathbf{0}^T \\ \mathbf{0}^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \right)$$

From which we can see that the multiplication of any corresponding matrices containing the same vector \mathbf{x}_i we get:

$$[\mathbf{0} \ \dots \ \mathbf{x}_i \ \dots \ \mathbf{0}] \cdot \begin{bmatrix} \mathbf{0}^T \\ \vdots \\ \mathbf{x}_i^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} = \mathbf{x}_i \cdot \mathbf{x}_i^T$$

While by multiplying two matrices containing different vectors we get:

$$[\mathbf{0} \ \dots \ \mathbf{x}_j \ \dots \ \mathbf{0}] \cdot \begin{bmatrix} \mathbf{0}^T \\ \vdots \\ \mathbf{x}_i^T \\ \vdots \\ \mathbf{0}^T \end{bmatrix} = \mathbf{0}$$

We can therefore conclude that:

$$\mathbf{X}^T \mathbf{X} = \sum_i \mathbf{x}_i \mathbf{x}_i^T$$

If we have 2 different matrices \mathbf{X} and \mathbf{Y} we can repeat the procedure and conclude that: