Bayesian Optimal Design - Weekly Report

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Contents

1 Week 1

1.1 Objective

For week 1, we're going to explore the linear regression problem from a Bayesian perspective. First we are going to state essential model assumptions, from which we can examine the consequences of these using Bayes' rule. This will be used to see how we can incorporate previous knowledge into the model and see how observing new data will change our model. While this is apparent for any regression model, we will also demonstrate how we can actually derive an exact posterior parameter distribution in the case of linear regression.
In the end, we are going to implement a simple linear regression model in Python, and explore how the prior model assumptions affect our resulting model.

1.2 Theory

1.2.1 The regression problem and Bayes' rule

First, we are going to state the regression problem in general: Given a dataset $\mathcal{D} = (\mathbf{d}, \mathbf{y})$, where $\mathbf{d} \in \mathbb{R}^{\ell \times d}$ and $\mathbf{y} \in \mathbb{R}^{\ell}$, we wish to find some function $\phi_\theta \in \mathbb{R}^{\ell \times d} \to \mathbb{R}^{\ell}$ such that

$$\phi(\mathbf{d}) \approx \mathbf{y} \tag{1}$$

where ϕ takes some vector of parameters θ.
In the Bayesian approach, we are going to describe the probability distribution of $\mathbf{y}$ with no additional information as $p(\mathbf{y})$, called the *marginal*. If we have observed any data $\mathbf{d}$ and have some set of parameters θ such that equation 1 is upheld, then we have additional information about the distribution of $\mathbf{y}$. This will be described as the *likelihood* $p(\mathbf{y}|\mathbf{d}, \theta)$.
We might have some prior information on how the parameters θ are distributed - perhaps from prior experiments, domain knowledge or qualified guessing. This can be encoded into the *prior* distribution $p(\theta)$. Given a likelihood, a marginal, and a prior, we can use Bayes' rule to find the *posterior* distribution of θ given the data $\mathbf{d}$ and target values $\mathbf{y}$:

$$p(\theta|\mathbf{d}, \mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{d}, \theta)p(\theta)}{p(\mathbf{y})} \tag{2}$$

What the posterior distribution $p(\theta|\mathbf{d}, \mathbf{y})$ models is the *change of belief* from the prior model $p(\theta)$ given the *evidence* $\mathbf{y}$, $\mathbf{d}$[3]. It gives us a new

best bet for the parameters θ, which we can use to produce a better ϕ for equation 1.

1.2.2 The linear regression problem

In the case of linear regression, we assume that ϕ is a linear function, i.e. $\phi(\mathbf{d}) = \mathbf{d}\theta$ where $\theta \in \mathbb{R}^d$. It is also common to augment the dataset with an additional dimension set to 1, such that ϕ also models the intercept such that $\mathbf{d} \in \mathbb{R}^{\ell \times d+1}$ and $\theta \in \mathbb{R}^{d+1}$. In this case θ_{d+1} will then be the intercept.

We are going to assume that the each target value $\mathbf{y}$ can accurately be described as

$$\mathbf{y}^{(i)} = \mathbf{d}^{(i)}\theta + \epsilon \tag{3}$$

for some $\mathbf{d}$, θ, ϵ, where $\epsilon \sim \mathcal{N}(0, \sigma_{\mathbf{y}}^2)$ is some normally distributed noise term. Thus, the likelihood distribution can be described like a normal distribution.

$$p(\mathbf{y}^{(i)}|\mathbf{d}^{(i)}, \theta) = \mathcal{N}(\mathbf{y}^{(i)}; \mathbf{d}^{(i)}\theta, \sigma_{\mathbf{y}}^2) \tag{4}$$

Assuming that the target values are independent, it must follow that

$$p(\mathbf{y}|\mathbf{d}, \theta) = \prod_{i=0}^{\ell} p(\mathbf{y}^{(i)}|\mathbf{d}^{(i)}, \theta) = \mathcal{N}(\mathbf{y}; \mathbf{d}\theta, \sigma_{\mathbf{y}}^2 I_\ell) \tag{5}$$

When modelling the prior information, one could choose to model the parameter distribution as a multivariate gaussian distribution as well

$$p(\theta) = \mathcal{N}(\theta; \mu_\theta, \Sigma_\theta) \tag{6}$$

where μ_θ, Σ_θ are chosen by the model designer.
The last term of equation 2 is the marginal distribution $p(\mathbf{y})$, which is the probability of observing the target values $\mathbf{y}$ without any additional information. This term is difficult to make any reasonable assumptions about, and can thus hard to compute in practice. Lukily, it mostly acts as a normalization term that makes sure that the posterior distribution integrates to 1, so it can for many use cases be safely ignored. As we will see, for a linear regression problems with these assumptions, we will indeed not need it.

1.2.3 An analytical solution for the posterior distribution

Let us outline a possible derivation for the posterior distribution: Given the likelihood and prior, we can describe the joint distribution $p(\theta, \mathbf{y}|\mathbf{d})$ as

$$p(\theta, \mathbf{y}|\mathbf{d}) = p(\mathbf{y}|\mathbf{d}, \theta)p(\theta|\mathbf{d}) = p(\mathbf{y}|\mathbf{d}, \theta)p(\theta) \tag{7}$$

where the last equality is due to the model parameters being independent from the controlled data points.
From this point, we will need to condition the joint distribution on $\mathbf{y}$:

$$p(\theta|\mathbf{y}, \mathbf{d}) = \frac{p(\theta, \mathbf{y}|\mathbf{d})}{p(\mathbf{y})} \tag{8}$$

To perform these steps, we are going to use some useful lemmas about the multivariate normal distribution.

Lemma 1. *Let* $\mathbf{X} \sim \mathcal{N}(\mu, \Sigma)$ *be a multivariate normal random variable. We can regard these variables in block notation:*

$$\mathbf{X} = \left[\begin{array}{c} \mathbf{X}_1 \\ \hline \mathbf{X}_2 \end{array}\right], \quad \mu = \left[\begin{array}{c} \mu_1 \\ \hline \mu_2 \end{array}\right], \quad \Sigma = \left[\begin{array}{c|c} \Sigma_{11} & \Sigma_{12} \\ \hline \Sigma_{21} & \Sigma_{22} \end{array}\right] \tag{9}$$

then we must have

$$\mu_{2|1} = \mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(X_1 - \mu_1), \quad \Sigma_{2|1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{21}^T \tag{10}$$

Proof. See Krause [3] □

TODO: implement proof

Lemma 2. *For random variables* $\mathbf{X} \sim \mathcal{N}(\mu_\mathbf{X}, \Sigma_\mathbf{X})$, $\mathbf{Y}|\mathbf{X} \sim \mathcal{N}(\mu_\mathbf{Y} + A\mathbf{X}, \Sigma_\mathbf{Y})$, *for some* A, *the joint distribution* $p(\mathbf{X}, \mathbf{Y})$ *is given by*

$$\left[\begin{array}{c} \mathbf{X} \\ \hline \mathbf{Y} \end{array}\right] = \mathcal{N}\left(\left[\begin{array}{c} \mu_\mathbf{X} \\ \hline \mu_\mathbf{Y} + A\mu_\mathbf{X} \end{array}\right], \left[\begin{array}{c|c} \Sigma_\mathbf{X} & \Sigma_\mathbf{X}A^T \\ \hline A\Sigma_\mathbf{X} & A\Sigma_\mathbf{X}A^T + \Sigma_\mathbf{Y} \end{array}\right]\right) \tag{11}$$

Proof. Follows from Lemma 1 and the definition of the multivariate normal distribution. □

If we regard the likelihood from equation 5, we can see that it is only dependent of θ in its mean-term. Thus we can use Lemma 2 to get the joint distribution $p(\theta, \mathbf{y}|\mathbf{d})$:

$$\left[\begin{array}{c} \theta \\ \hline \mathbf{y} \end{array}\right] = \mathcal{N}\left(\left[\begin{array}{c} \mu_\theta \\ \hline \mathbf{d}\theta + \mathbf{d}\mu_\theta \end{array}\right], \left[\begin{array}{c|c} \Sigma_\theta & \Sigma_\theta\mathbf{d}^T \\ \hline \mathbf{d}\Sigma_\theta & \mathbf{d}\Sigma_\theta\mathbf{d}^T + \sigma_\mathbf{y}^2 I_\ell \end{array}\right]\right) \tag{12}$$

To get the posterior distribution, we will need to use the conditioning Lemma 1 on a reordered term:

$$\left[\begin{array}{c} \mathbf{y} \\ \hline \theta \end{array}\right] = \mathcal{N}\left(\left[\begin{array}{c} \mathbf{d}\theta + \mathbf{d}\mu_\theta \\ \hline \mu_\theta \end{array}\right], \left[\begin{array}{c|c} \mathbf{d}\Sigma_\theta\mathbf{d}^T + \sigma_\mathbf{y}^2 I_\ell & \mathbf{d}\Sigma_\theta \\ \hline \Sigma_\theta\mathbf{d}^T & \Sigma_\theta \end{array}\right]\right) \tag{13}$$

With the conditioning lemma, we get the posterior distribution $p(\theta|\mathbf{y}, \mathbf{d}) = \mathcal{N}(\theta; \mu_{\theta|\mathbf{y},\mathbf{d}}, \Sigma_{\theta|\mathbf{y},\mathbf{d}})$:

$$\mu_{\theta|\mathbf{y},\mathbf{d}} = \mu_\theta + \Sigma_\theta\mathbf{d}^T(\mathbf{d}\Sigma_\theta\mathbf{d}^T + \sigma_\mathbf{y}^2 I_\ell)^{-1}(\mathbf{y} - \mathbf{d}\theta + \mathbf{d}\mu_\theta) \tag{14}$$

$$\Sigma_{\theta|\mathbf{y},\mathbf{d}} = \Sigma_\theta - \Sigma_\theta\mathbf{d}^T(\mathbf{d}\Sigma_\theta\mathbf{d}^T + \sigma_\mathbf{y}^2 I_\ell)^{-1}\mathbf{d}\Sigma_\theta \tag{15}$$

Thus we have an analytical expression for the posterior distribution.

1.2.4 Using the posterior to optain model parameters

From this distribution, we can optain model parameters in several ways. A common choice is to pick the θ that maximizes the posterior. This is called the *Maximum-a-posteriori* (MAP) estimate, and will for a normal distribution just be the posterior mean $\mu_{\theta|\mathbf{y},\mathbf{d}}$. For other cases than linear regression, one can also use a mean over samples of θ from the posterior distribution, but for our case, this will converge against the posterior mean $\mu_{\theta|\mathbf{y},\mathbf{d}}$. Another solution is to define a distribution called the *posterior*

predictive distribution, that for some new data points $\mathbf{d}_{\text{new}}$ computes the corresponding $\mathbf{y}_{\text{new}}$:

$$p(\mathbf{y}_{\text{new}}|\mathbf{d}_{\text{new}}, \mathbf{d}, \mathbf{y}) = \int p(\theta|\mathbf{y}, \mathbf{d}) p(\mathbf{y}_{\text{new}}|\theta, \mathbf{d}_{\text{new}}) d\theta \tag{16}$$

Integrals like these are usually solved by sampling - examples of this will be seen later. For now, we can use Lemma 2 to get

$$p(\mathbf{y}_{\text{new}}|\mathbf{d}_{\text{new}}, \mathbf{d}, \mathbf{y}) = \mathcal{N}(\mathbf{y}_{\text{new}}; \mathbf{d}_{\text{new}}^T \mu_{\theta|\mathbf{y},\mathbf{d}}, \sigma_{\mathbf{y}}^2 + \mathbf{d}_{\text{new}}^T \Sigma_{\theta|\mathbf{y},\mathbf{d}} \mathbf{d}_{\text{new}}) \tag{17}$$

Having the posterior predictive allows us to both sample a $\mathbf{y}$ for a given $\mathbf{d}$, choose the $\mathbf{y}$ that maximises the distribution, and to give us some measure of the inherent uncertancy in the model [3].

1.2.5 Linear regression being invariant to translation

A relevant side-note worth exploring is the effect of the choice of prior mean μ_θ on the posterior mean $\mu_{\theta|\mathbf{y},\mathbf{d}}$.

TODO: Finish this section with information from Oswin - and edit posterior predictive if needed

1.3 Implementation

Implementing a Bayesian linear regression model is fairly simple. To begin with, one needs to decide on a prior distribution for θ, as well as what the variance of the noise $\sigma_{\mathbf{y}}^2$ should be used to generate the example data. In the real world, $\sigma_{\mathbf{y}}^2$ would be measured from observed data, and the prior would be chosen based on the expected distribution of θ based on as much prior knowledge as possible , but for our toy representation, we are going to play around with many different possible priors and noise parameters. For a toy implementation, one can start by generating some data points $\mathbf{d}$ and noise samples ϵ as well as deciding on some true, underlying weight parameters θ_{true}. Then we can compute $\mathbf{y}$ as in equation 3. From this, we can simply implement the posterior distribution as in equation 14 and 15. In Python, this can be done as follows:

```
1 def posterior_distribution(theta, d, y):
2     mu = cov_prior @ d.T @ np.linalg.inv(d @ cov_prior @ d.T
      ↪  + noise * np.eye(1)) @ y
3     cov = cov_prior - cov_prior @ d.T @ np.linalg.inv(d @
      ↪  cov_prior @ d.T + noise * np.eye(1)) @ d @ cov_prior
4     return stats.multivariate_normal.pdf(theta, mean=mu,
      ↪  cov=cov)
```

1.4 Results

An example of how 20 samples of θ from the posterior changes with the size of the dataset can be seen in Figure 1. As one can see, the posterior becomes

better at estimating the true θ as the number of data points increases, since the lines both become more similar and closer to the mean, as well as how they describe the data better.
An example of how the posterior changes from the prior can be seen in figure 2, where 40 random prior means and covariances are plotted alongside their respective posterior. It can be seen that even when the priors are very different, the posterior usually ends up quite close to the true weight.
An example of how the posterior predictive distribution changes is seen in figure 3. As one can see, the distribution becomes less confident as the noise increases.
Thus we've seen that the Bayesian linear regression model is able to learn the true weight parameters from data, and that it is able to do so even when the prior is very different from the true weight parameters. Now, we will move on to regarding the Bayesian Optimal Design problem.

TODO: Make plots nicer, add "true" line for reference, add legend

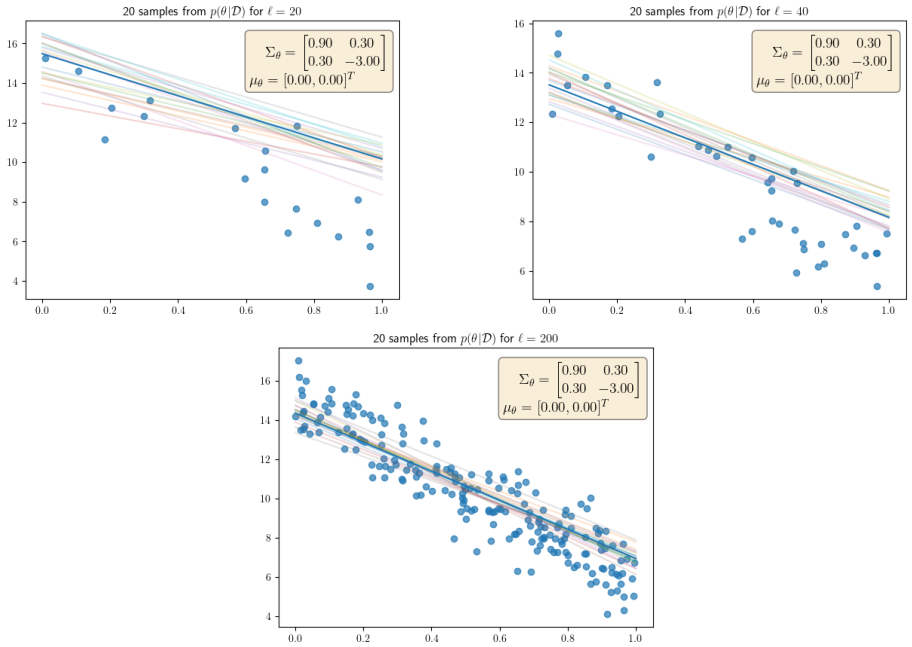
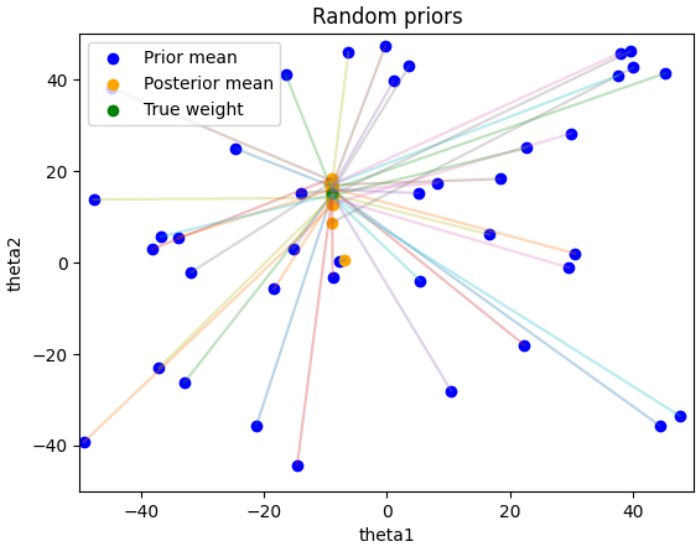
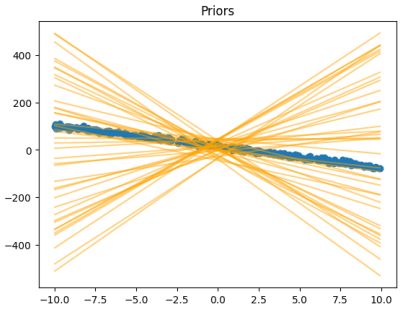


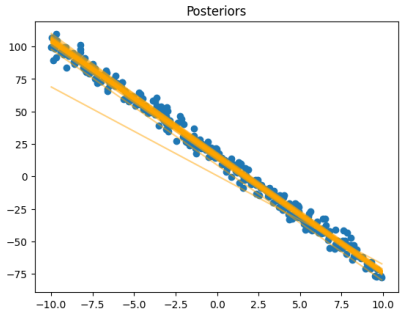
Figure 1: The model trained on data sets with 20, 40 and 200 data points respectively with a fixed prior. The blue line is $\mu_{\theta|\mathcal{D}}$.



(a) Plot showing how the posterior mean changes compared to the prior mean.



(b) Prior mean samples



(c) Posterior mean samples

Figure 2: Priors vs Posteriors for 40 randomly sampled priors on the same data set. Note that the variance is due to random prior covariances.

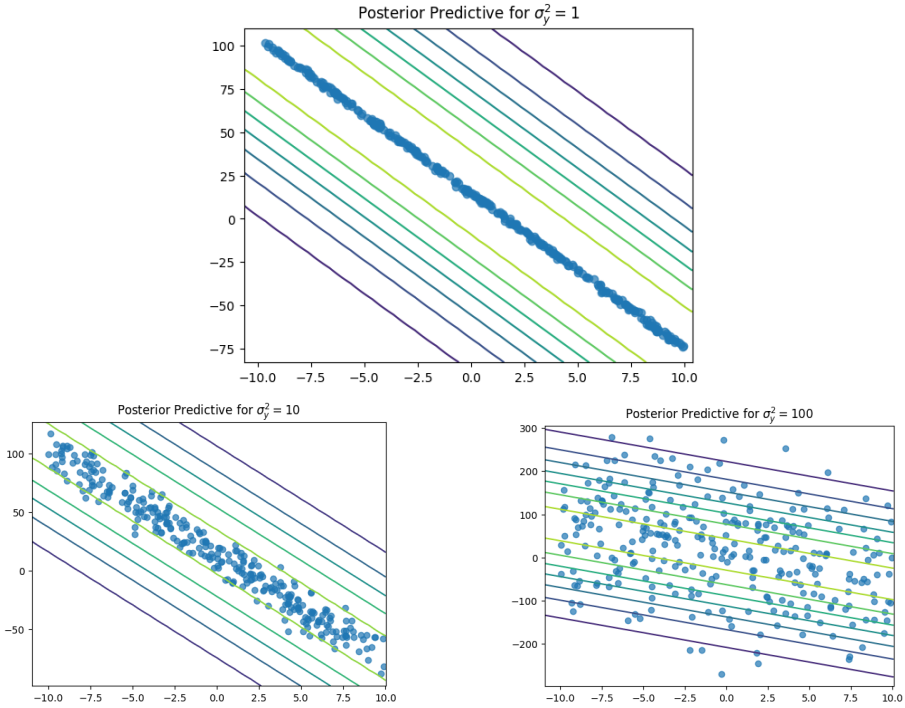


Figure 3: Posterior predictive for different noise levels

2 Week 2

2.1 Objective

For week 2, we are going to regard the *Bayesian Optimal Design* problem for linear regression, and use this to implement a reference implementation, to be used later. We can then also explore the effect of different data sizes, different priors and the difference between estimating an objective function through sampling versus calculating it analytically.

2.2 Theory

2.2.1 Bayesian Optimal Design

Often in scientific contexts as well as other cases, one might have a model that one wishes to strengthen in one way or another using experimental data. Performing the experiments needed to strengthen one's model can be expensive however, so having an efficient strategy to do such can save important ressources. This is where *Bayesian Optimal Design* comes in.

The Bayesian Optimal Design problem is about finding a design $\mathbf{d}$ from a design space $\mathbf{D}$, that optimizes some kind of utility function.[2] For this project, we wish to maximize the expected information gain from the prior to the posterior. To find the optimal design, we want to find a maximizer $\mathbf{d}^*$ defined as such:

$$\mathbf{d}^* = \arg\max_{\mathbf{d}\in\mathbf{D}} I(\mathbf{d}) \tag{18}$$

Where $I(\mathbf{d})$ is the *Mutual Information* between the prior and posterior

when adjusted for data observed at $\mathbf{d}$.

2.2.2 The Nature of the Mutual Information metric

The amount of information of an experiment is often defined as the negative differential entropy defined as such[1]:

$$H(X) = \int_X p(x) \log p(x) dx \tag{19}$$

Thus, the information known before $\mathbf{y}$ is observed from $\mathbf{d}$ is

$$H_1 = \int_\Theta p(\theta) \log p(\theta) d\theta \tag{20}$$

and after is

$$H_2(\mathbf{y}, \mathbf{d}) = \int_\Theta p(\theta|\mathbf{y}, \mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) d\theta \tag{21}$$

The gain of information must thus be

$$H_{\text{gain}}(\mathbf{y}, \mathbf{d}) = H_2(\mathbf{y}, \mathbf{d}) - H_1 \tag{22}$$

If we instead regard equation 20 and 21 as expectations we get

$$= \mathbb{E}_\theta[\log p(\theta|\mathbf{y}, \mathbf{d})] - \mathbb{E}_\theta[\log p(\theta)] = \mathbb{E}_\theta[\log(p(\theta|\mathbf{y}, \mathbf{d})) - \log(p(\theta))] \tag{23}$$

Before we perform the experiment, we do not know what the outcome will be. Instead, we'll just regard the expected outcome by taking the expectation over $\mathbf{y}$:

$$\mathbb{E}_\mathbf{y}[H_{\text{grain}}(\mathbf{y}, \mathbf{d})] = \mathbb{E}_\mathbf{y}[\mathbb{E}_\theta[\log(p(\theta|\mathbf{y}, \mathbf{d})) - \log(p(\theta))]] \tag{24}$$

This expression is called the *Mutual Information* between the prior and posterior, and will be denoted $I(\mathbf{d})$. We can put a new interpretation upon this by expanding equation 24 using Bayes' rule:

$$I(\mathbf{d}) = \mathbb{E}_\mathbf{y}[\mathbb{E}_\theta[\log(p(\mathbf{y}|\theta, \mathbf{d})) - \log(p(\mathbf{y}|\mathbf{d}))]] \tag{25}$$

Then we can use that $\frac{p(\mathbf{y}, \theta|\mathbf{d})}{p(\theta)} = p(\mathbf{y}|\theta, \mathbf{d})$:

$$I(\mathbf{d}) = \mathbb{E}_\mathbf{y}[\mathbb{E}_\theta[\log\left(\frac{p(\mathbf{y}, \theta|\mathbf{d})}{p(\theta)}\right) - \log(p(\mathbf{y}|\mathbf{d}))]] = \mathbb{E}_\mathbf{y}[\mathbb{E}_\theta[\log\left(\frac{p(\mathbf{y}, \theta|\mathbf{d})}{p(\theta)p(\mathbf{y}|\mathbf{d})}\right)]] \tag{26}$$

$$= \text{KL}(p(\mathbf{y}, \theta|\mathbf{d})||p(\theta)p(\mathbf{y}|\mathbf{d}))$$

Two random variables X and Y are said to be *independent* if the product of their distributions is the same as their joint distribution i.e.

$$p(X, Y) = p(X)p(Y) \tag{27}$$

Thus, Mutual Information measures how close the prior and the evidence are to be independent. If $\mathbf{d}$ is picked such that the prior has a high proba-

TODO: check if indeed this is evidence

bility of being able to predict $\mathbf{y}|\mathbf{d}$, then the mutual information is going to be close to 0. If, on the contrary, $\mathbf{d}$ is picked such that the prior has a low probability of being able to predict $\mathbf{y}|\mathbf{d}$, the mutual information is going to be large. Thus one could expect that an optimizer would prefer to pick a $\mathbf{d}$ within an area where the prior is not very representative of the underlying generating function. Of course, in an experimental design context we do not have access to this underlying function as we might not be able to simulate experiments accurately. Instead, the expectation expressions in 24 makes it such that we only regard the expected information gain for any given underlying function.

2.2.3 Evaluating the Mutual Information through sampling

Without using any assumptions about the nature of our model or data, we can utilize Monte Carlo sampling to optain an accurate estimate on the expectations in equation 24. For N samples of $\theta \sim p(\theta)$ and M samples of $\mathbf{y} \sim p(\mathbf{y}|\theta, \mathbf{d})$ this thus looks like

$$I(\mathbf{d}) \approx \frac{1}{NM} \sum_{i=0}^{N} \sum_{j=0}^{M} (\log(p(\theta_i|\mathbf{y}_j, \mathbf{d})) - \log(p(\theta_i))) \tag{28}$$

Picking samples of $\mathbf{y}$ nescessitates that we can simulate the experiment however. Instead, we will use the reparamerization trick to sample M samples of $\mathbf{z} \in \mathcal{N}(0, 1)$ such that

$$\mathbf{y}_{ij} = \mu_{\mathbf{y}|\theta,\mathbf{d}} + A_{\mathbf{y}|\theta,\mathbf{d}}\mathbf{z}_j \tag{29}$$

where $A_{\mathbf{y}}$ is a matrix such that $A_{\mathbf{y}}A_{\mathbf{y}}^T = \Sigma_{\mathbf{y}}$. From equation 5 we have that $p(\mathbf{y}|\theta, \mathbf{d}) = \mathcal{N}(\mathbf{y}; \mathbf{d}\theta, \sigma_{\mathbf{y}}^2 I_n)$ so we must have $A_{\mathbf{y}|\theta,\mathbf{d}} = \sigma_{\mathbf{y}}^2 I_n$ thus

$$I(\mathbf{d}) \approx \frac{1}{NM} \sum_{i=0}^{N} \sum_{j=0}^{M} (\log(p(\theta_i|\mathbf{d}\theta_i + \sigma_{\mathbf{y}}^2\mathbf{z}_j, \mathbf{d})) - \log(p(\theta_i))) \tag{30}$$

2.2.4 Evaluating the Mutual Information through analytical solutions

It also happens that when we transform equation 24 using sum of expectations, one can use the known solution to entropy of multivariate normal distributions:

$$I[(\mathbf{y}, \mathbf{d})] = \mathbb{E}_{\mathbf{y}}[\mathbb{E}_{\theta}[\log(p(\theta|\mathbf{y}, \mathbf{d}))]] - \mathbb{E}_{\theta}[\log(p(\theta))] \tag{31}$$

$$= \mathbb{E}_{\mathbf{y}}[\frac{1}{2} \ln \det(2\pi e \Sigma_{\theta|\mathbf{y},\mathbf{d}})] - \frac{1}{2} \ln \det(2\pi e \Sigma_{\theta})$$

It also happens to be that $\Sigma_{\theta|\mathbf{y},\mathbf{d}}$ is independent from $\mathbf{y}$, as we saw last week, thus we get.

$$I[\mathbf{y}, \mathbf{d}] = \frac{1}{2} \ln \det(2\pi e \Sigma_{\theta|\mathbf{y},\mathbf{d}}) - \frac{1}{2} \ln \det(2\pi e \Sigma_{\theta}) \tag{32}$$

2.2.5 Stochastic Optimization

For the sampling approach here, and in the rest of the project, we will use a stochastic gradient descent algorithm to perform the optimization nescessary to solve 18. From some starting point $\mathbf{d}_0$, iteratively update $\mathbf{d}_i$ by

$$\mathbf{d}_i = \mathbf{d}_{i-1} + \alpha \frac{1}{10^c + i \times 10^{-\beta}} \nabla_{\mathbf{d}} I(\mathbf{d}_{i-1}) \tag{33}$$

where $\alpha, \beta, c \in \mathbb{R}$ are hyperparameters that ensures a slow converges to taylor the natural variance that occurs when using Monte Carlo methods.

2.3 Implementation

The mutual information metric can be implemented using the sampling method like so:

```
def mutual_information(d):
  N = 50 # amount of theta samples
  M = 50 # amount of z samples
  thetas = np.random.multivariate_normal(mean_prior,
  ↪  cov_prior, N)
  zs = np.random.randn(M)
  results = []
  for theta in thetas:
    ys = np.array([d @ theta + sigma_y * z for theta in
    ↪  thetas for z in zs])
    for y in ys:
      log_posterior = np.log(posterior_distribution(theta, d,
      ↪  y)) # using posterior_distribution from last week
      log_prior = multivariate_normal.logpdf(theta,
      ↪  mean_prior, cov_prior)
      results.append(log_posterior - log_prior)
  return np.mean(results)
```

And using the analytical solution like so:

```
def mutual_information(d):
  cov_posterior = get_cov_posterior(d) # using method from
  ↪  from last week
  return 0.5 *
  ↪  np.log(np.linalg.det(2*np.pi*np.e*cov_posterior)) - 0.5
  ↪  * np.log(np.linalg.det(2*np.pi*np.e*covariance_prior))
```

Finding the gradient of these solutions can be done using `autograd.grad`. An example of this can be seen in this implementation of the gradient descent algorithm:

```
def optimize(f, d0, alpha, beta, c, iterations):
  d = d0
  g = grad(f)
  for i in range(iterations):
    d = d + alpha / (10**c + i * 10**(-beta)) * g(d)
  return d
```

2.4 Results

If we regard the problem with $\ell = 10$ datapoints and $d = 2$ dimensions with a zero-prior mean and identity prior covariance, we will data that is closer to the optimum to be spread out wider and more evenly in the parameter space. This can be seen if one regards equation 30. If $\mathbf{d}$ is picked such that $\mathbf{d}\theta_i$ has a high probability of being a small number, then $\mathbf{d}\theta_i + \sigma_{\mathbf{y}}^2 \mathbf{z}_j$ is going to get dominated by the noise term $\sigma_{\mathbf{y}}^2 \mathbf{z}_j$. Thus, the log-posterior $\log p(\theta_i | \mathbf{d}_i + \sigma_{\mathbf{y}}^2 \mathbf{z}_j, \mathbf{d})$ will be smaller. If on the other hand, $\mathbf{d}$ is picked such that $\mathbf{d}\theta_i$ has a high probability of being a large number, then $\mathbf{d}\theta_i$ is going to dominate the noise term and the posterior has a higher probability of being a large number.
In figure 4, we can see if start position of 11 datapoints are on top of eachother, all at $(0; 0)$, they will swiftly move to a more spread out formation. Thus we've seen how optimizing over the Mutual Information metric can help find solutions to the Bayesian Optimal Design problem. Now we will move on to exploring how to solve regression problems, even when analytical solutions are not available with the hopes of opening up our Mutual Information optimizer to all kinds of models.

3 Week 3

3.1 Objective

This week, we will study and implement the variational inference framework with the objective of estimating the posterior in a way that is indifferent to the type of regression performed. We are going to pose the problem as an optimization problem and then derive an objective function that we can optimize over. We will then try to implement it and perform some adjustments for efficiency and numerical stability.

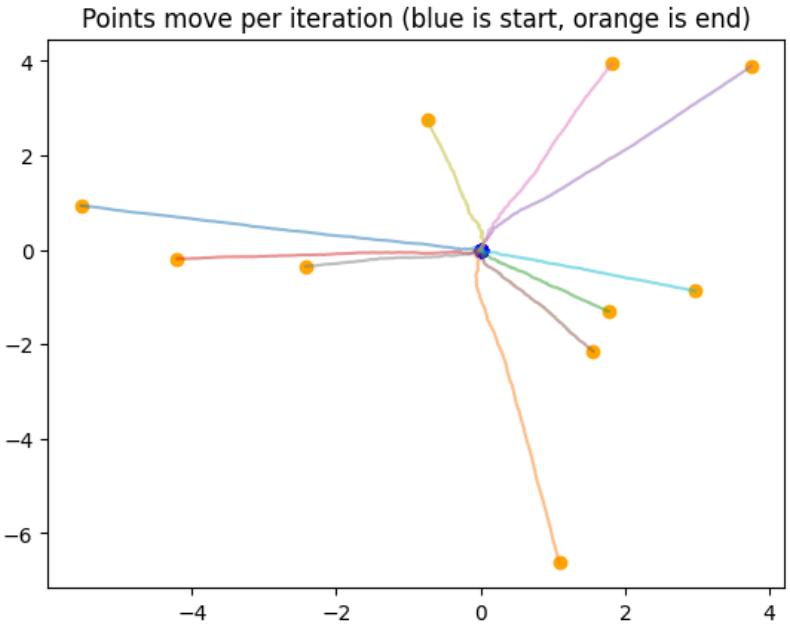


Figure 4: Points moving from their initial position at (0;0) to a more optimal, spread out position.

3.2 Theory

3.2.1 Variational Inference and Variational Families

In week 1, we were able to calculate the exact posterior using the right assumption and conjugacy between the prior and likelihood. This turns out to be a rarity - in most cases, a closed form solution for the posterior is not readily available. A common approach to this problem is to approximate the posterior distribution, using a *variational distribution* q picked from a family of distributions that we might imagine could approximate the posterior. By picking a suitable objective function, we can use optimization techniques to approximate the posterior. This is called *variational inference*.

The point of variational inference is to approximate the posterior distribution $p(\theta|\mathbf{y}, \mathbf{d})$ using optimization techniques. The space of which to optimize in is the parameter space for some distribution $q(\theta)$, which we aim to make as close to the posterior as possible by KL-divergence. For reference, we will recite the definition of our linear model:

$$\theta \sim \mathcal{N}(\mu, \mathbf{\Sigma})$$

$$\epsilon \sim \mathcal{N}(0, \sigma_{\mathbf{y}}^2)$$

$$\mathbf{y}|\mathbf{d}, \theta \sim \theta^T \mathbf{d} + \epsilon$$

The optimization problem we wish to solve is defined like so:

$$q^*(\theta) = \arg\min_{q(\theta)\in\mathcal{L}} \mathrm{KL}(q(\theta)||p(\theta|\mathbf{y}, \mathbf{d}))$$

Computing the KL-divergence is hard though, because it requires computing the evidence $p(\mathbf{y}, \mathbf{d})$, so instead we try to optimize in regards to the

TODO: show why

expectation lower bound (ELBO):

$$\text{ELBO}(q) = \mathbb{E}_{\theta'}[\log p(\theta', \mathbf{d}, \mathbf{y})] - \mathbb{E}_{\theta'}[\log q(\theta')]$$

Let us pick $q(\theta')$ from the family of multivariate normal distributions. This is reasonable, since we expect the posterior to be normally distributed due to conjugacy between the prior and likelihood.
It is possible to rewrite the ELBO into a shape that is easier to optimize:

$$\begin{aligned}
\text{ELBO}(q) &= \mathbb{E}_{\theta'}[\log p(\theta', \mathbf{d}, \mathbf{y})] - \mathbb{E}_{\theta'}[\log q(\theta')] \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})p(\theta'|\mathbf{d})p(\mathbf{d})] - \mathbb{E}_{\theta'}[\log q(\theta')] \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d}) + \log p(\theta'|\mathbf{d}) + \log p(\mathbf{d})] - \mathbb{E}_{\theta'}[\log q(\theta')] \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})] + \mathbb{E}_{\theta'}[\log p(\theta'|\mathbf{d})] + \mathbb{E}_{\theta'}[\log p(\mathbf{d})] - \mathbb{E}_{\theta'}[\log q(\theta')] \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})] + \mathbb{E}_{\theta'}[\log p(\theta')] - \mathbb{E}_{\theta'}[\log q(\theta')] + \text{const} \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})] - (-\mathbb{E}_{\theta'}[\log p(\theta')] + \mathbb{E}_{\theta'}[\log q(\theta')]) + \text{const} \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})] - \mathbb{E}_{\theta'}[\log \frac{q(\theta')}{p(\theta')}] + \text{const} \\
&= \mathbb{E}_{\theta'}[\log p(\mathbf{y}|\theta', \mathbf{d})] - \text{KL}(q||p) + \text{const}
\end{aligned}$$

Since q and p are multivariate normal by assumption, we can use the closed-form solution for $\text{KL}(q||p)$. Thus, we only need to worry about the first part of the expression, which is an integral over the likelihood.
Now, we need to use the assumption about the multivariate normal distribution, that the covariance matrix must satisfy $\Sigma = AA^T$ for some matrix A . This means that

$$\theta \sim \mathcal{N}(\mu_\theta, A_\theta A_\theta^T)$$
$$\theta = \mu_\theta + A_\theta z$$

TODO: add this assumption to week 1

where

$$z \sim \mathcal{N}(0, 1)$$

TODO: why? (see eq 25 from lecture notes)

Thus we can rewrite our ELBO function as

$$\text{ELBO}(q) = \mathbb{E}_z[\log p(\mathbf{y}|\mu_\theta + A_\theta z, \mathbf{d})] - \text{KL}(q||p) + \text{const}$$

thus the log-likelihood is independent of θ'.
Now consider the first expectation:

$$\begin{aligned}
&\mathbb{E}_z[\log p(\mathbf{y}|\mu_\theta + A_\theta z, \mathbf{d})] \\
&= \int_z p(z) \log p(\mathbf{y}|\mu_\theta + A_\theta z, \mathbf{d}) \; dz \\
&\approx \frac{1}{N} \sum_{i=1}^{N} p(z^{(i)}) \log p(\mathbf{y}|\mu_\theta + A_\theta z^{(i)}, \mathbf{d})
\end{aligned}$$

where $N \in \mathbb{Z}$ and $z_i \sim \mathcal{N}(0, 1)$.

3.3 Design

The implementation is heavily utilizes the `autograd` library, which automatically calculates the gradient of the ELBO. To do this, it was nescessary to manually implement the PDF for the likelihood, since the one provided by Autograd doesn't support optimizing over the mean of the distribution. Several measures were taken to ensure numerical stability in this implementation including using the log-sum-exp trick as well as using the logarithm of the determinant instead of the actual determinant. It is also nescessary to make sure that enough samples are drawn of $\mathbf{z}$ to ensure our expectation over the log-likelihood is accurate enough. 100 samples were used in this implementation. Another issue that arises is that sometime the log-likelihood becomes a very small negative number (often denoted as $-\infty$ by Numpy). This happens when a sample z is picked such that the log-likelihood $p(\mathbf{y}|\mu_\theta + A_\theta z^(i), \mathbf{d})$ becomes very close to zero. This was solved by simply rejecting any sample that results in such a log-likelihood.

Another problem that arises is overflows when the amount of datapoints become larger. To handle this, it first of all makes sense to work directly with the log of the likelihood instead of first calculating the likelihood and then taking the log of it.

$$-\frac{1}{2}(n\log(2\pi) + \log(\det(\Sigma)) + (x-\mu)^T\Sigma^{-1}(x-\mu))$$

This also means that we don't need to apply the log-sum-exp trick, since we are working directly with logarithms. A disadvantage with this method is first of all that we can't guarantee that the covariance has an inverse, and secondly that computing the inverse of large matrices is very inefficient. To solve the first issue, we can try regularize the covariance matrix by adding a small constant to the diagonal. The second could potentially be solved by using some sort of approximation like Cholesky decomposition, but this was not regarded for now. The stop condition for the optimization is decided by the default gradient tolerance of the scipy-implementation, but in practice the optimization is stopped when the precision of the gradient is lost due to the stocastic nature of the objective function. This typically happens when trying to take small steps around the minimum, but as can be seen in Figure ... the precision is increased when the amount of datapoints is increased.

TODO: Why is log-pdf true? prove in theory

3.4 Results

TODO: Make subplots

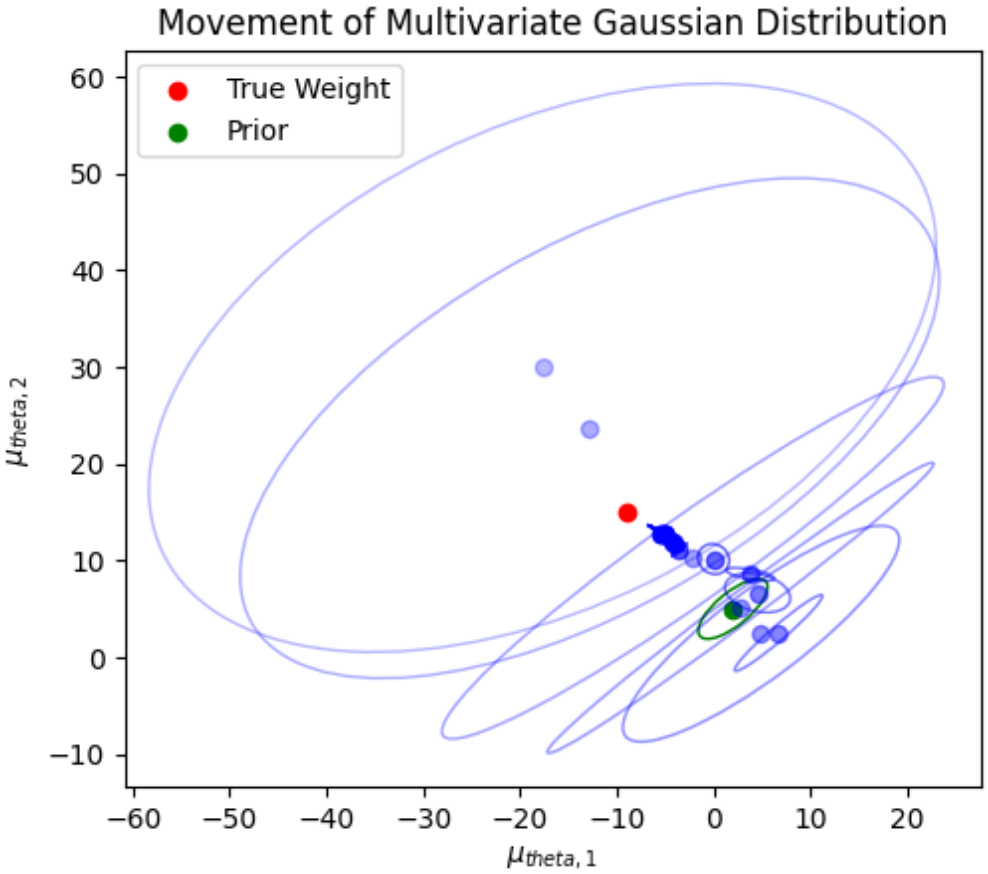


Figure 5: Optimization over the ELBO for 50 datapoints

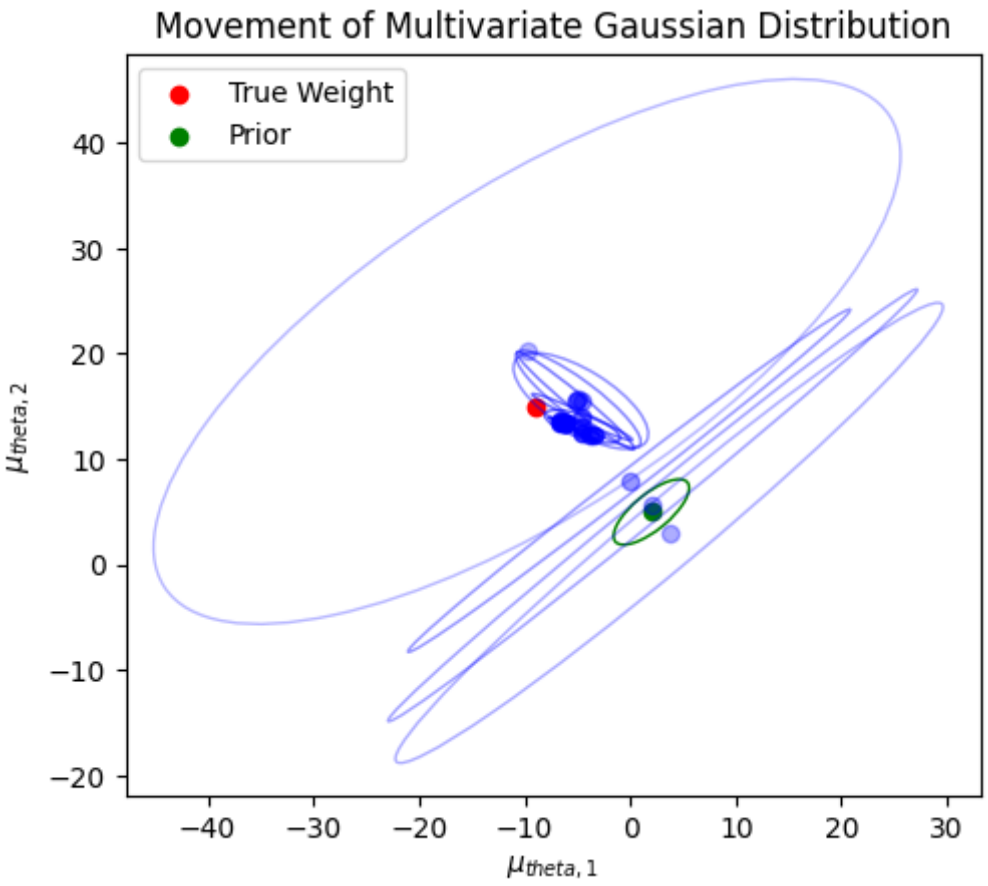


Figure 6: Optimization over the ELBO for 100 datapoints

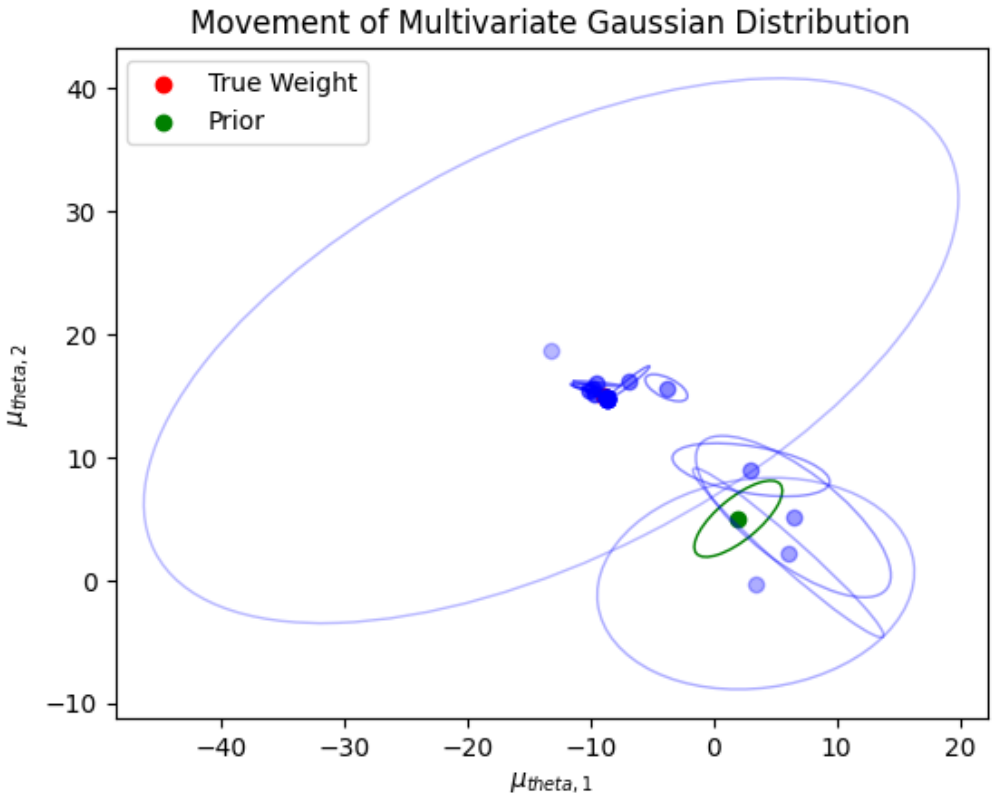


Figure 7: Optimization over the ELBO for 300 datapoints

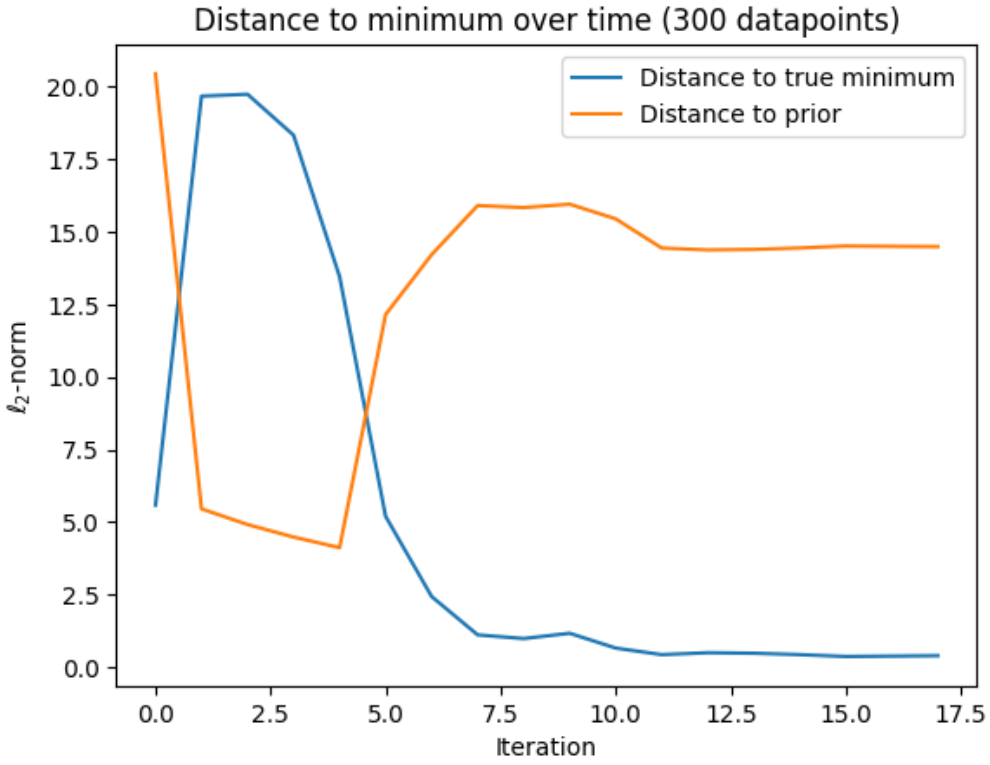


Figure 8: Optimization over the ELBO for 300 datapoints

As one can see, the optimization converges quite close to the true weights when the amount of datapoints increases as expected. First, the algorithm quickly moves towards the prior, and then slowly moves towards the true minimum. If the prior is close to the true minimum, one could expect that the algorithm would converge faster. It is also seen that the covariance of the parameters quickly become very small.

TODO: Interpret this - what does that mean?

3.5 Evaluation

The algorithm presented here seems to work - although it is not as efficient as the analytical solution, it represents a framework that could be more useful for other problems. From this we've also learned a bit about how we can expect the movement of the distribution - first towards the prior, then towards the minimum. It has also shown the importance of numerical stability as well as how we can use the reparameterization trick for efficient computation.

4 Week 4

4.1 Objective

The objective of this week is to integrate our Bayesian Optimal Design optimizer from week 2 with our linear regression variational inference optimizer from week 3.

4.2 Theory

4.2.1 Finding the gradient of the Mutual Information

This is a working draft and should be sectioned into a more readable format, as well as have made notation consistent Let us first regard our mutual information objective function from week 2:

$$MI(\mathbf{d}) = \int_{\Theta}\int_{\mathbf{Y}} p(\theta, \mathbf{y}|\mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) d\mathbf{y} d\theta - \int_{\Theta} p(\theta) \log p(\theta) d\theta$$

Since we are optimizing, let us throw away the second term, since it is constant in terms of $\mathbf{d}$:

$$= \int_{\Theta}\int_{\mathbf{Y}} p(\theta, \mathbf{y}|\mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) d\mathbf{y} d\theta$$

To optimize the mutual information, we will need the derivative of it in terms of $\mathbf{d}$:

$$\frac{\partial}{\partial \mathbf{d}} MI(\mathbf{d}) = \frac{\partial}{\partial \mathbf{d}} \int_{\Theta}\int_{\mathbf{Y}} p(\theta, \mathbf{y}|\mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) d\mathbf{y} d\theta$$

$$= \int_{\Theta}\int_{\mathbf{Y}} \frac{\partial}{\partial \mathbf{d}} p(\theta, \mathbf{y}|\mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) d\mathbf{y} d\theta$$

Let us then use the product rule

$$= \int_\Theta \int_{\mathbf{Y}} (\frac{\partial}{\partial \mathbf{d}} p(\theta, \mathbf{y}|\mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d})) + (p(\theta, \mathbf{y}|\mathbf{d}) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d})) d\mathbf{y} d\theta$$

TODO: maybe change left derivative

Now, let us use the fact that $\frac{\partial}{\partial \mathbf{d}} p(\theta, \mathbf{y}|\mathbf{d}) = p(\theta, \mathbf{y}|\mathbf{d}) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d})$

TODO: prove this lemma

$$= \int_\Theta \int_{\mathbf{Y}} p(\theta, \mathbf{y}|\mathbf{d}) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d}) \log p(\theta|\mathbf{y}, \mathbf{d}) + p(\theta, \mathbf{y}|\mathbf{d}) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d}) d\mathbf{y} d\theta$$

$$= \int_\Theta \int_{\mathbf{Y}} p(\theta, \mathbf{y}|\mathbf{d}) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d}) (\log p(\theta|\mathbf{y}, \mathbf{d}) + 1) d\mathbf{y} d\theta$$

$$= \int_\Theta \int_{\mathbf{Y}} p(\mathbf{y}|\theta, \mathbf{d}) p(\theta) \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d}) (\log p(\theta|\mathbf{y}, \mathbf{d}) + 1) d\mathbf{y} d\theta$$

Solving this double integral can be hard. Let us consider it as an expectation of the form

$$\mathbb{E}[f(\theta, \mathbf{y})] = \int_{(\theta, \mathbf{y})} p(\theta, \mathbf{y}) f(\theta, \mathbf{y}) d(\theta, \mathbf{y})$$

with $p(x) = p(\mathbf{y}|\theta, \mathbf{d}) p(\theta)$ and $f(x) = \frac{\partial}{\partial \mathbf{d}} \log p(\theta|\mathbf{y}, \mathbf{d}) (\log p(\theta|\mathbf{y}, \mathbf{d}) + 1)$. We can then approximate this expectation by sampling by reducing the expectation to:

$$\mathbb{E}[f(x)] \approx \frac{1}{N} \sum_{i=0}^{N} f(\theta_i, \mathbf{y}_i), \quad (\theta_i, \mathbf{y}_i) \sim p(\theta_i, \mathbf{y}_i)$$

which leads to

TODO: Figure out specific notation here

$$\frac{\partial}{\partial \mathbf{d}} MI(\mathbf{d}) = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{d}} \log p(\theta_i|\mathbf{y}_i, \mathbf{d}) (\log p(\theta_i|\mathbf{y}_i, \mathbf{d}) + 1)$$

where $(\theta_i, \mathbf{y}_i) \sim p(\mathbf{y}_i|\theta_i, \mathbf{d}) p(\theta_i)$. Sampling θ_i is easy from our prior, and we can do reparameterization to sample $\mathbf{y}_{ij} = \theta_i^T \mathbf{d} + z_j$ where $z_j \sim \mathcal{N}(0, \sigma_{\mathbf{y}}^2)$.

4.2.2 Finding the gradient of the posterior

Notation:
$\vartheta = \mu_\theta$ and A_θ for use in q_ϑ
$\mathbf{y_d} = \mathbf{y}$ calculated from $\mathbf{d}$.
Now, let us consider the posterior $p(\theta_i|\mathbf{y}, \mathbf{d})$. This is the distribution that we try to approximate when performing variational inference. Thus we can expect our variational distribution $q(\theta_i)$ to reasonably approximate it after our inference algorithm has run. We will denote the optimal parameters found $\vartheta^*(\mathbf{d}, \mathbf{y_d}) = \arg\max_\vartheta \text{ELBO}_{\mathbf{d}, \mathbf{y}(\mathbf{d})}(q_\vartheta)$ such that $q_{\vartheta^*}(\theta_i) \approx p(\theta_i|\mathbf{y_d}, \mathbf{d})$.
In our refactored expression for mutual information, we have a term containing $\frac{\partial}{\partial \mathbf{d}} \log p(\theta_i|\mathbf{y_d}, \mathbf{d})$.

$$\frac{\partial}{\partial \mathbf{d}} \log p(\theta_i|\mathbf{y_d}, \mathbf{d}) \approx \frac{\partial}{\partial \mathbf{d}} \log q_{\vartheta^*}(\theta_i)$$

Since ϑ^* is a function of $\mathbf{d}$, and q^* is a function of θ^*, then we can use the chain rule.

$$= \frac{\partial}{\partial \vartheta^*} \log q_{\vartheta^*}(\theta_i) \frac{\partial}{\partial \mathbf{d}} \vartheta^*(\mathbf{y_d}, \mathbf{d})$$

4.2.3 Using The Implicit Function Theorem for finding the indirect gradient

Let $\mathcal{D}$ be $(\mathbf{d}, \mathbf{y})$ encoded in some vector.
If for some $(\mathcal{D}', \vartheta')$, $\frac{\partial}{\partial \vartheta} \text{ELBO}_{\mathcal{D}'}(q_\vartheta)\Big|_{\mathcal{D}=\mathcal{D}', \vartheta=\vartheta'} = 0$ and the Jacobian is invertible, then there exists an open set of datapoints $\mathcal{D} \in \mathcal{X} \times \mathcal{Y}$ such that there exists a function $\vartheta^* \colon \mathcal{X} \times \mathcal{Y} \to \Theta$ such that

TODO: add reference! very similar to litterature

$$\vartheta^*(\mathcal{D}') = \vartheta' \text{ and } \forall \mathcal{D} \in \mathcal{X} \times \mathcal{Y}, \frac{\partial}{\partial \vartheta} \text{ELBO}_{\mathcal{D}}(q_\vartheta)\Big|_{\mathcal{D}, \vartheta^*(\mathcal{D})} = 0$$

Another consequence of this is that we can write

$$\frac{\partial \vartheta^*}{\partial \mathbf{d}}\Big|_{\mathbf{d}'} = \left(- \left[\frac{\partial^2 \text{ELBO}_{\mathbf{d}, \mathbf{y}_i}(q_\vartheta)}{\partial \vartheta \partial \vartheta^T} \right]^{-1} \times \frac{\partial^2 \text{ELBO}_{\mathbf{d}, \mathbf{y}_i}(q_\vartheta)}{\partial \vartheta \partial \mathbf{d}^T} \right) \Big|_{\mathbf{d}', \vartheta^*(\mathbf{d}', \mathbf{y}_i')}$$

Where $\mathbf{y}_i' = \theta^T \mathbf{d}' + \mathbf{z}$. Now we have the indirect gradient.

4.3 Design

4.4 Results

4.5 Evalution

References

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