ELEN E4903 Homework 1

Kliment Mamykin UNI 2770

Problem 1

Given a sequence of N observations $X = (x_1, \dots, x_N)$ where $x_i \overset{iid}{\sim} Bern(\pi)$, with p.d.f

$$p(x_i|\pi) = \pi^{x_i}(1-\pi)^{1-x_i} \tag{1}$$

(a) What is the likelihood of the data $(x_1, \dots, x_N)$?

The likelihood of data given parameters of the model (in the case of $Bern(\pi)$ the parameter is a single value π) is:

$$p(X \mid \pi) = p(x_1, \dots, x_N|\pi) = \prod_{i=1}^{N} \pi^{x_i}(1-\pi)^{1-x_i} \tag{2}$$

Where the assumption that the observations are independent allow factorization of the joint distribution into a product of individual observation probabilities.

(b) Maximum likelihood estimate $\hat{\pi}_{ml}$ for π

Maximum likelihood estimate $\hat{\pi}_{ml}$ is defined as

$$\hat{\pi}_{ml} = \arg\max_{\pi} \log p(X \mid \pi) \tag{3}$$

Here $\hat{\pi}_{ml}$ is a point estimate (a scalar), and X is treated as a r.v.. We are selecting a value π that maximizes the log probability of data given model parameters. For the given model ($x_i \sim Bern(\pi)$)

$$\begin{aligned}
\hat{\pi}_{ml} &= \arg\max_{\pi} \log p(x_1, \dots, x_N \mid \pi) \\
&= \arg\max_{\pi} \log \prod_{i=1}^{N} \pi^{x_i} (1-\pi)^{1-x_i} \\
&= \arg\max_{\pi} \log \left(\pi^{\sum_{i=1}^{N} x_i} (1-\pi)^{\sum_{i=1}^{N} (1-x_i)} \right) \\
&= \arg\max_{\pi} \sum_{i=1}^{N} x_i \log \pi + \sum_{i=1}^{N} (1-x_i) \log(1-\pi)
\end{aligned} \tag{4}$$

To find a maximunm of a function, we take a gradient with respect to the parameters of maximization, and find a point where the gradient is 0.

$$\begin{aligned}
0 &= \frac{d}{d\pi} \left(\sum_{i=1}^{N} x_i \log \pi + \sum_{i=1}^{N} (1-x_i) \log(1-\pi) \right) \Big|_{\hat{\pi}_{ml}} \\
&= \frac{\sum_{i=1}^{N} x_i}{\hat{\pi}_{ml}} - \frac{\sum_{i=1}^{N} (1-x_i)}{1-\hat{\pi}_{ml}} \Rightarrow
\end{aligned} \tag{5}$$

$$\hat{\pi}_{ml} = \frac{\sum_{i=1}^{N} x_i}{\sum_{i=1}^{N} x_i + \sum_{i=1}^{N} (1-x_i)} = \frac{\sum_{i=1}^{N} x_i}{N} \tag{6}$$

(c) Maximum a posteriori (MAP) estimate $\hat{\pi}_{MAP}$ for π

MAP estimate $\hat{\pi}_{MAP}$ is defined as

$$\hat{\pi}_{MAP} = \arg\max_{\pi} \log p(\pi \mid X) \tag{7}$$

Here we consider a conditional distribution of parameters of the model, treated as a r.v. conditioned on the data X. X generally is also treated as a r.v. but for conditioning we pick one random instantiation of the dataset. Using Bayes formula we express the posterior through the likelihood, the prior and the data evidence, plug in likelihood of $Bern(\pi)$ and the prior pdf of $Beta(\alpha, \beta)$.

$$\begin{aligned}
\hat{\pi}_{MAP} &= \arg\max_{\pi} \log \frac{p(X \mid \pi)p(\pi)}{p(X)} \\
&= \arg\max_{\pi} \log p(X \mid \pi) + \log p(\pi) - \log p(X) \\
&= \arg\max_{\pi} \log \prod_{i=1}^{N} \pi^{x_i}(1-\pi)^{1-x_i} + \log C\pi^{\alpha-1}(1-\pi)^{\beta-1} - \log p(X) \\
&= \arg\max_{\pi} \left((\sum_{i=1}^{N} x_i + \alpha - 1)\log\pi + (\sum_{i=1}^{N}(1-x_i) + \beta - 1)\log(1-\pi) + \log C - \log p(X) \right) \quad (8
\end{aligned}$$

$$\begin{aligned}
0 &= \frac{d}{d\pi}\left((\sum_{i=1}^{N} x_i + \alpha - 1)\log\pi + (\sum_{i=1}^{N}(1-x_i) + \beta - 1)\log(1-\pi) \right)\Big|_{\hat{\pi}_{MAP}} \\
&= \frac{\sum_{i=1}^{N} x_i + \alpha - 1}{\hat{\pi}_{MAP}} - \frac{\sum_{i=1}^{N}(1-x_i) + \beta - 1}{1 - \hat{\pi}_{MAP}} \qquad (9)
\end{aligned}$$

$$\hat{\pi}_{MAP} = \frac{\sum_{i=1}^{N} x_i + \alpha - 1}{\sum_{i=1}^{N} x_i + \alpha - 1 + \sum_{i=1}^{N}(1-x_i) + \beta - 1} = \frac{\sum_{i=1}^{N} x_i + \alpha - 1}{N + \alpha + \beta - 2} \tag{10}$$

(d) Posterior distribution of π

$$
\begin{aligned}
x_i \sim Bernoulli(\pi) \Rightarrow p(X \mid \pi) &= \prod_{i=1}^{N} \pi^{x_i}(1-\pi)^{1-x_i} \\
\pi \sim Beta(\alpha, \beta) \Rightarrow p(\pi) &= C\pi^{\alpha-1}(1-\pi)^{\beta-1} \\
p(\pi \mid X) = \frac{p(X \mid \pi)p(\pi)}{p(X)} &\propto \pi^{\sum_{i=1}^{N} x_i + \alpha - 1}(1-\pi)^{\sum_{i=1}^{N}(1-x_i)+\beta-1} \Rightarrow \\
p(\pi \mid X) = Beta(\alpha', \beta') \qquad \alpha' = \sum_{i=1}^{N} x_i + \alpha \quad \beta' &= \sum_{i=1}^{N}(1-x_i) + \beta \qquad (11)
\end{aligned}
$$

Distribution families sich that when multiplied by a likelihood function produce a re-parameterized distribution from the same family are called conjugate priors. As shown in (11) $Beta(\alpha, \beta)$ is a conjugate prior to $Bern(\pi)$ likelihood. Some other examples: Gaussian distribution is a conjugate prior for the mean in a Gaussian likelihood, Gamma is a prior for Gaussian precision parameter [3].

(e) Mean and variance of π under posterior distribution, relationship to $\hat{\pi}_{MAP}$ and $\hat{\pi}_{ml}$

From (11) we have that posterior $p(\pi) = Beta(\alpha', \beta')$ from which follows (using Beta distribution mean and variance from [2])

$$E[\pi] = \frac{\alpha'}{\alpha' + \beta'} = \frac{\sum_{i=1}^{N} x_i + \alpha}{N + \alpha + \beta} \tag{12}$$

$$Var[\pi] = \frac{\alpha'\beta'}{(\alpha' + \beta')^2(\alpha' + \beta' + 1)} \tag{13}$$

An interpretation of (12) is that the parameters of the prior encode prior belief on the number of successes (α) and failures (β) seen (or believed to be seen) so far, also called *pseudo observations*. And the parameters of the posterior represent an updated belief of the number of success (α') and failues (β') after seeing more data.

Comparing (6) and (10) implies that $\hat{\pi}_{MAP}$ becomes $\hat{\pi}_{ml}$ when prior's parameters $\alpha = \beta = 1$, so the Baysian MAP estimator is a generalization of the maximum likelihood approach with the prior selected as $Beta(1, 1)$

MAP estimator $\hat{\pi}_{MAP}$ picks the mode in the posterior distribution, a point with the highest density. However the follwing derivations show that MAP estimator is biased.

Calculate $E(\hat{\pi}_{ml})$ and $Var(\hat{\pi}_{ml})$ from (6) considering linearity of expectation of a sum of r.v.'s $E(\sum_{i=1}^{N} a_i X_i) = \sum_{i=1}^{N} a_i E[X_i]$ and for independent r.v.s $Var(\sum_{i=1}^{N} a_i X_i + b) = \sum_{i=1}^{N} a_i^2 Var[X_i]$ and $Var(X \sim Bern(\pi)) = \pi(1 - \pi)$

$$E[\hat{\pi}_{ml}] = E\left[\frac{\sum_{i=1}^{N} x_i}{N}\right] = \frac{\sum_{i=1}^{N} E[x_i]}{N} = \frac{N\pi}{N} = \pi \tag{14}$$

from which we can conclude that $E[\hat{\pi}_{ml}]$ is an unbiased estimate of π with variance

$$Var[\hat{\pi}_{ml}] = Var\left[\frac{\sum_{i=1}^{N} x_i}{N}\right] = \frac{1}{N^2}\sum_{i=1}^{N} Var[x_i] = \frac{1}{N^2} N\pi(1 - \pi) = \frac{1}{N}\pi(1 - \pi) \tag{15}$$

And the same calculations for $\hat{\pi}_{MAP}$ yield:

$$E[\hat{\pi}_{MAP}] = E\left[\frac{\sum_{i=1}^{N} x_i + \alpha - 1}{N + \alpha + \beta - 2}\right] = \frac{\sum_{i=1}^{N} E[x_i] + \alpha - 1}{N + \alpha + \beta - 2} = \frac{N\pi + \alpha - 1}{N + \alpha + \beta - 2} = \frac{\pi + \frac{\alpha - 1}{N}}{1 + \frac{\alpha + \beta - 2}{N}} \tag{16}$$

indicating that $E[\hat{\pi}_{MAP}]$ is a biased estimate of π with variance

$$Var[\hat{\pi}_{MAP}] = Var\left[\frac{\sum_{i=1}^{N} x_i + \alpha - 1}{N + \alpha + \beta - 2}\right] = \frac{1}{(N + \alpha + \beta - 2)^2}\sum_{i=1}^{N} Var[x_i] = \frac{N}{(N + \alpha + \beta - 2)^2}\pi(1 -$$

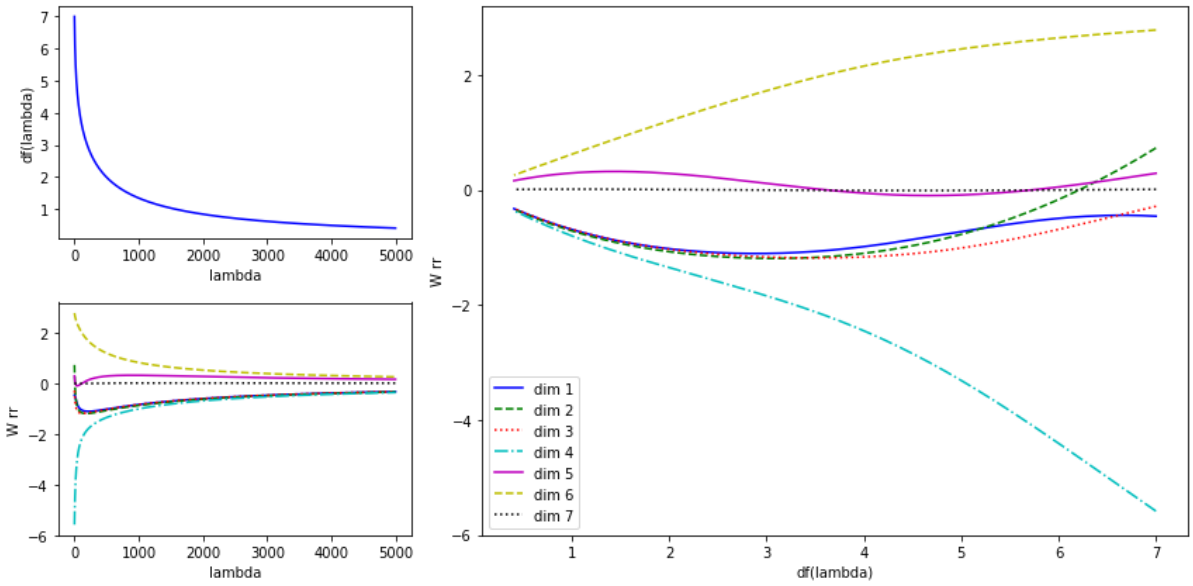
$Var[\hat{\pi}_{MAP}] \leq Var[\hat{\pi}_{ml}]$ implies that on average MAP estimate will be closer to the true but unknown value of π, assuming of course that the prior was selected correctly.

Problem 2

In [1]:
```
%load_ext autoreload
%autoreload 2
%matplotlib inline
from hw1 import regression
```

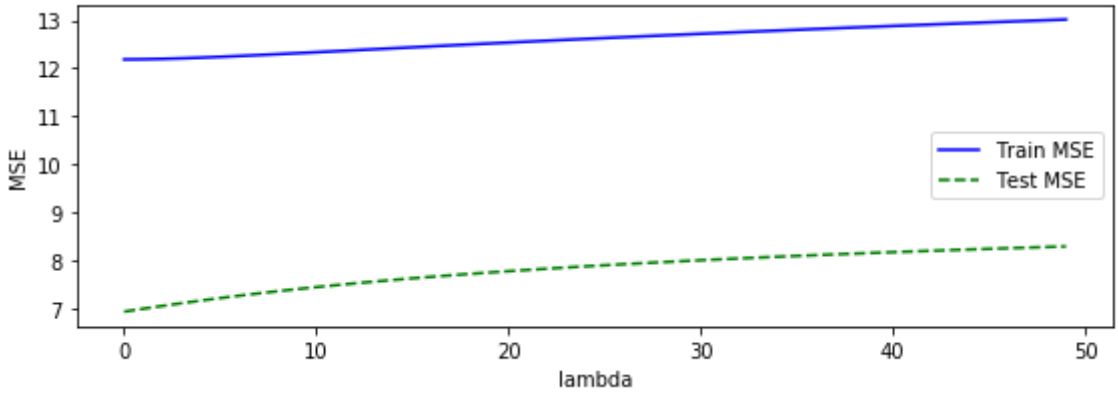
Part 1

In [4]:
```
regression.part1a()
```

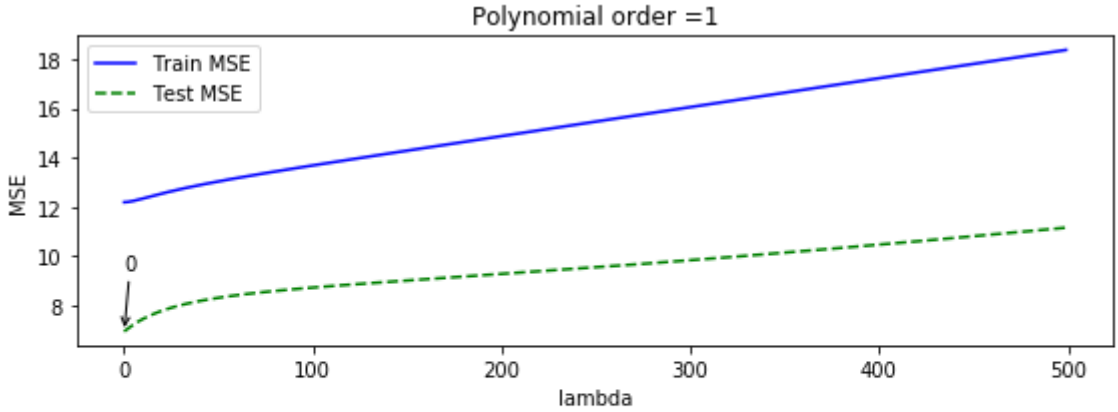


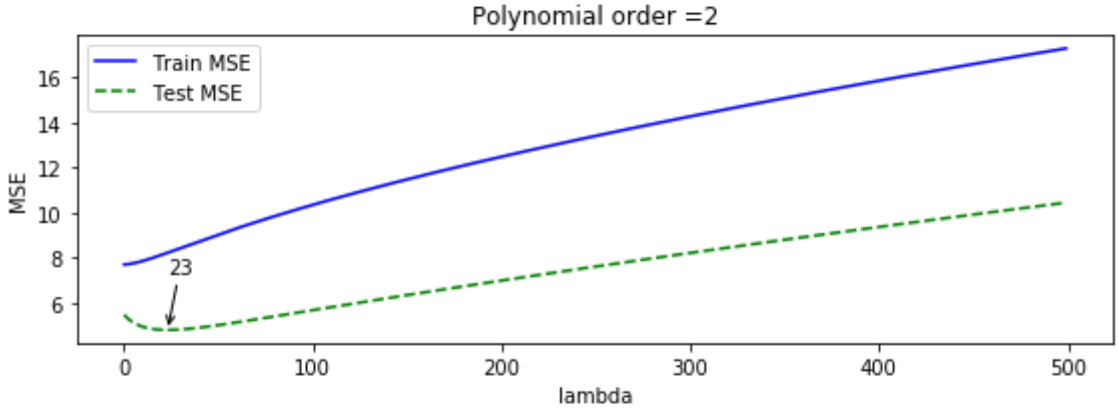
When degrees of freedom = 7, which corresponds to $\lambda = 0$ or no regularization, the magnitude of weights, especially for dim 2 and dim 6 are larger then the other dimentions. This means that dim 2 and dim 6 are more correlated to the outcome of the model. When there is no regularization, the wights are allowed to grow unconstrained, as long as the model fits training data well. With ridge regularization, as λ increases and $df(\lambda)$ decreases, the magnitudes of all weights are shrunk to small values.

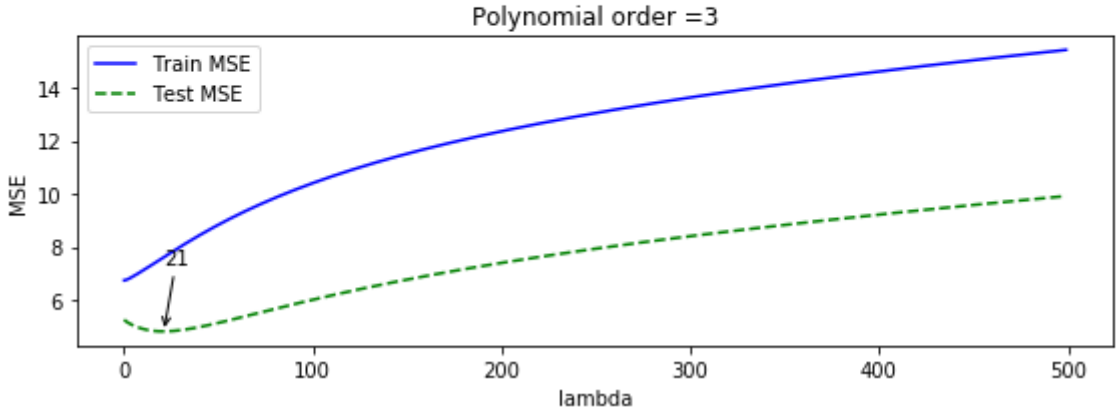
In [6]:
```
regression.part1c()
```



In [5]:
```
regression.part2a()
```





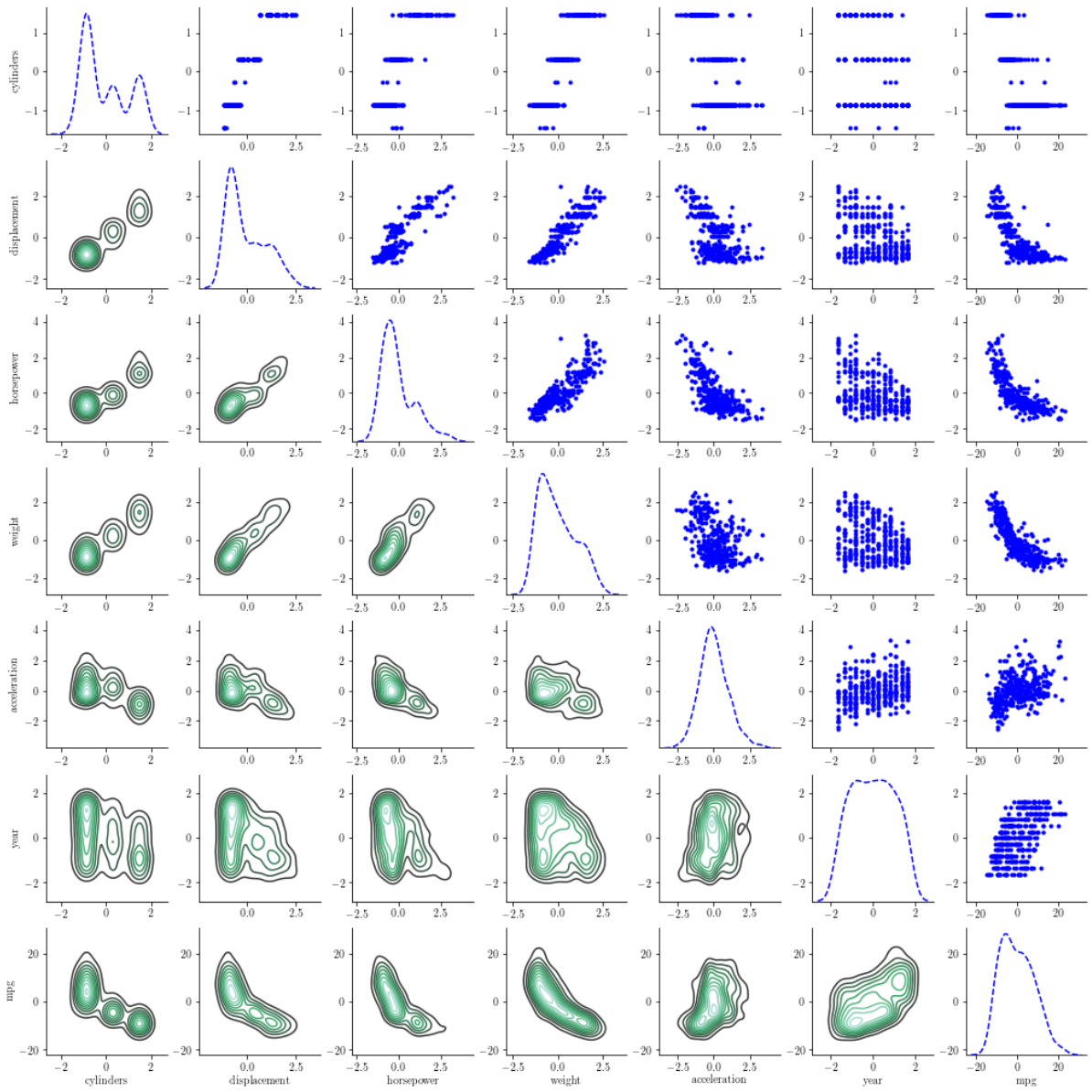


References

1. Lars Buitinck et all, "API design for machine learning software: experiences from the scikit-learn project", https://arxiv.org/pdf/1309.0238.pdf (https://arxiv.org/pdf/1309.0238.pdf)
2. Beta Distribution, Wikipedia, https://en.wikipedia.org/wiki/Beta_distribution (https://en.wikipedia.org/wiki/Beta_distribution)
3. Conjugate Prior, Wikipedia, https://en.wikipedia.org/wiki/Conjugate_prior (https://en.wikipedia.org/wiki/Conjugate_prior)

In [3]:
```
regression.pairplot(regression.make_dataframe(X_train, y_train))
```

```
/Users/kmamykin/anaconda3/envs/hearts/lib/python3.6/site-packages/matplotlib/contour.py:967: UserWarning: The following kwargs were not used by contour: 'label', 'color'
  s)
```



In [4]:
```
regression.pairplot(regression.make_dataframe(X_test, y_test))
```

```
/Users/kmamykin/anaconda3/envs/hearts/lib/python3.6/site-packages/matpl
otlib/contour.py:967: UserWarning: The following kwargs were not used b
y contour: 'label', 'color'
  s)
```