Homework 2

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Problem 1

Consider a data set in which each data point t_n is associated with a weighting factor $r_n > 0$, so that the sum-of-squares error function becomes

$$E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} r_n \left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right)^2 \tag{1}$$

Find an expression for the solution $\mathbf{w}^*$ that minimizes this error function. Give two alternative interpretations of the weighted sum-of-squares error function in terms of (i) data dependent noise variance and (ii) replicated data points

Solution. To minimize the error function, we take the derivative with respect to $\mathbf{w}$.

$$\frac{\partial}{\partial \mathbf{w}} E_D(\mathbf{w}) = -\sum_{n=1}^{N} r_n \left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right) \phi(\mathbf{x}_n)$$

Setting the derivative to zero, we get

$$\begin{aligned}
\sum_{n=1}^{N} r_n \left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right) \phi(\mathbf{x}_n) &= 0 \\
\sum_{n=1}^{N} r_n \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top \mathbf{w} &= \sum_{n=1}^{N} r_n \phi(\mathbf{x}_n) t_n \\
\mathbf{w} &= \left(\sum_{n=1}^{N} r_n \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top\right)^{-1} \sum_{n=1}^{N} r_n \phi(\mathbf{x}_n) t_n
\end{aligned}$$

Problem 2

We showed in the class that the conjugate prior for a Gaussian distribution with unknown mean and unknown precision (inverse variance) is a normal-gamma distribution. This property also holds for the case of the conditional Gaussian distribution $p(t|x, w, \beta)$ of the linear regression model. If we consider the likelihood function (3.10),

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^\top \phi(\mathbf{x}_n), \beta^{-1}) \tag{2}$$

then the conjugate prior for $\mathbf{w}$ and β is given by

$$p(\mathbf{w}, \beta) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \beta^{-1}\mathbf{S}_0)\text{Gamma}(\beta|a_0, b_0) \tag{3}$$

Show that the corresponding posterior distribution takes the same functional form, so that

$$p(\mathbf{w}, \beta|\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \beta^{-1}\mathbf{S}_N)\text{Gamma}(\beta|a_N, b_N) \tag{4}$$

and find expressions for the posterior parameters $\mathbf{m}_N$, $\mathbf{S}_N$, a_N, and b_N.

Solution. We already know that the conjugate prior is given by

$$p(\mathbf{w}, \beta) = \frac{\sqrt{\beta}}{\sqrt{2\pi}|\mathbf{S}_0|} \exp\left(-\frac{1}{2}\beta(\mathbf{w} - \mathbf{m}_0)^\top S_0^{-1}(\mathbf{w} - \mathbf{m}_0)\right) \frac{\beta^{a_0-1}}{\Gamma(a_0)} b_0^{a_0} \exp(-b_0\beta)$$

And with the relationship that posterior $\propto$ likelihood $\times$ prior, it is clear that the family of the posterior distribution would be Gaussian-gamma distribution. However, the format might be different. Now, we want to show that for some constant k,

$$kp(\mathbf{t}|\mathbf{w}, \beta)p(\mathbf{w}, \beta) = p(\mathbf{w}, \beta|\mathbf{t})$$

What left is to evaluate the likelihood which is given by

$$\begin{aligned} p(\mathbf{t}|\mathbf{w}, \beta) &= \prod_{n=1}^{N} \mathcal{N}(t_n|\mathbf{w}^\top \phi(\mathbf{x}_n), \beta^{-1}) \\ &= \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\beta^{-1}}} \exp\left(-\frac{1}{2}\beta\left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right)^2\right) \end{aligned}$$

Now, we can evaluate the posterior distribution,

$$\begin{aligned} p(\mathbf{w}, \beta|\mathbf{t}) &= k\frac{\sqrt{\beta}}{\sqrt{2\pi}|\mathbf{S}_0|} \exp\left(-\frac{1}{2}\beta(\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0)\right) \frac{\beta^{a_0-1}}{\Gamma(a_0)} b_0^{a_0} \exp(-b_0\beta) \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi\beta^{-1}}} \exp\left(-\frac{1}{2}\beta\left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right)^2\right) \\ &= k\frac{b_0^{a_0} \exp(-b_0\beta)\beta^{a_0+N/2-1}}{\Gamma(a_0)\sqrt{2\pi}|\mathbf{S}_0|} \exp\left(-\frac{1}{2}\beta\left[(\mathbf{w} - \mathbf{m}_0)^\top \mathbf{S}_0^{-1}(\mathbf{w} - \mathbf{m}_0) + \sum_{n=1}^{N}\left(t_n - \mathbf{w}^\top \phi(\mathbf{x}_n)\right)^2\right]\right) \end{aligned}$$

it is clear that from the multiplication, $\mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top$ and $\mathbf{m}_N = \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \sum_{n=1}^{N} \phi(\mathbf{x}_n)t_n\right)$ Thus,

$$\begin{aligned} \mathbf{S}_N &= \left(\mathbf{S}_0^{-1} + \sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top\right)^{-1} \\ \mathbf{m}_N &= \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{m}_0 + \sum_{n=1}^{N} \phi(\mathbf{x}_n)t_n\right) \end{aligned}$$

and for a_N and b_N, we have

$$a_N = a_0 + \frac{N}{2}$$
$$b_N = b_0 + \frac{1}{2}\sum_{n=1}^{N}\left(t_n - \mathbf{w}^\top\phi(\mathbf{x}_n)\right)^2 + \frac{1}{2}\mathbf{m}_0^\top\mathbf{S}_0^{-1}\mathbf{m}_0 - \frac{1}{2}\mathbf{m}_N^\top\mathbf{S}_N^{-1}\mathbf{m}_N$$

Problem 3

Show that for a linearly separable data set, the maximum likelihood solution for the logistic regression model is obtained by finding a vector $\mathbf{w}$ whose decision boundary $\mathbf{w}^\top\phi(\mathbf{x}) = 0$ separates the classes and then taking the magnitude of $\mathbf{w}$ to infinity

Solution. Intuitively, we can see that $\mathbf{w}^\top\phi(\mathbf{x}) \geq 0$ for all $\mathbf{x}$ corresponding to a class y_i. Thus, the decision boundary would be $\mathbf{w}^\top\phi(\mathbf{x}) = 0$. Looking at the likelihood function of this Bernoulli process,

$$p(\mathbf{x}|y_i, \mathbf{w}) = \prod_{i=1}^{n}\left(\frac{1}{1+e^{-w^T x_i}}\right)^{y_i}\left(1 - \left(\frac{1}{1+e^{-w^T x_i}}\right)\right)^{1-y_i}$$
$$\ln p(\mathbf{x}|y_i, \mathbf{w}) = \sum_{i=1}^{n}\left(y_i \ln\left(\frac{1}{1+e^{-w^T x_i}}\right) + (1-y_i)\ln\left(1 - \left(\frac{1}{1+e^{-w^T x_i}}\right)\right)\right)$$

to maximize the log-likelihood here, it is clear that the magnitute of $\mathbf{w}$ should be as large as possible.

Problem 4

Show that the Hessian matrix $\mathbf{H}$ for the logistic regression model, given by (4.97),

$$\mathbf{H} = \nabla\nabla E(\mathbf{w}) = \sum_{n=1}^{N} y_n(1-y_n)\phi_n\phi_n^\top = \mathbf{\Phi}^\top\mathbf{R}\mathbf{\Phi} \tag{5}$$

is positive definite. Here $\mathbf{R}$ is a diagonal matrix with elements $y_n(1-y_n)$, and y_n is the output of the logistic regression model for input vector $\mathbf{x}_n$. Hence show that the error function is a concave function of $\mathbf{w}$ and that it has a unique minimum.

Solution. It is clear that $y_n(1-y_n)$ is positive for all n. Thus, $\mathbf{R}$ is positive definite. Thus, $\mathbf{H}$ is positive definite. And as we know, a function is concave if its Hessian is positive definite. Thus, the error function is a concave function of $\mathbf{w}$. Also, with the concavity, we know that the error function has a unique minimum.

Problem 5 (Likelihood Estimate for Gamma regression)

Gamma distribution is defined by

$$f(x|\alpha,\beta) = \frac{\beta^\alpha}{\Gamma(\alpha)}x^{\alpha-1}e^{-\beta x} \tag{6}$$

1. Write down the probability in general form of the exponential distribution family, and find natural parameter η, $u(x)$, $h(x)$, and $g(\eta)$.

Solution.

$$
\begin{aligned}
f(x|\alpha,\beta) &= h(x)g(\eta)\exp(\eta^\top u(x)) \\
\eta &= [\alpha-1, -\beta]^\top \\
u(x) &= [\ln x, -x]^\top \\
h(x) &= 1 \\
g(\eta) &= \frac{\beta^\alpha}{\Gamma(\alpha)}
\end{aligned}
$$

2. Let's assume we have a set of data points (t_i, x_i) $i = 1, \ldots, N$, and we assume t_i follows a Gamma distribution where its mean is defined by

$$y_k = \exp(w_0 + w_1 x_k) \tag{7}$$

and the conditional distribution is

$$f(t_k|y_k) = \frac{1}{\Gamma(\nu)}\left(\frac{\nu t_k}{y_k}\right)^\nu \frac{1}{y_k} e^{-\frac{\nu t_k}{y_k}} \tag{8}$$

discuss how you can find maximum likelihood estimates of w_0 and w_1 using a gradient ascent algorithm. Derive the gradient and discuss whether the likelihood function is a concave function of the w_0 and w_1 or not.

Solution. We can see that $f(t_k|y_k)$ is a Gamma distribution with parameters $\alpha = \nu$ and $\beta = \nu/y_k$. Thus, we can write down the log-likelihood function as Given that Gamma distribution is in the exponential family, we can write down the log-likelihood function as

$$p(\mathbf{t}|\mathbf{y}) = \sum_{k=1}^{N}\left(\ln\left(\frac{\nu}{y_k}\right) - \frac{\nu t_k}{y_k} - \ln\Gamma(\nu)\right)$$

Substituting $y_k = \exp(w_0 + w_1 x_k)$, we have

$$
\begin{aligned}
p(\mathbf{t}|\mathbf{y}) &= \sum_{k=1}^{N}\left(\ln\left(\frac{\nu}{\exp(w_0+w_1x_k)}\right) - \frac{\nu t_k}{\exp(w_0+w_1x_k)} - \ln\Gamma(\nu)\right) \\
&= \sum_{k=1}^{N}\left(\ln(\nu) - (w_0+w_1x_k) - \nu t_k \exp(w_0+w_1x_k) - \ln\Gamma(\nu)\right)
\end{aligned}
$$

Find the gradient of the log-likelihood function with respect to w_0 and w_1:

$$
\begin{aligned}
\frac{\partial p(\mathbf{t}|\mathbf{y})}{\partial w_0} &= -\sum_{k=1}^{N}\left(\nu t_k \exp(w_0+w_1x_k) + 1\right) \\
\frac{\partial p(\mathbf{t}|\mathbf{y})}{\partial w_1} &= -\sum_{k=1}^{N}\left(\nu t_k x_k \exp(w_0+w_1x_k) + x_k\right)
\end{aligned}
$$

As exponential function is convex, its negative is concave. Thus, the log-likelihood function is concave. That means, we can use the gradient ascent to find the maximum likelihood estimates of w_0 and w_1. This can be done by updating the parameters w_0 and w_1 as

$$
\begin{aligned}
w_0 &\leftarrow w_0 + \eta\frac{\partial p(\mathbf{t}|\mathbf{y})}{\partial w_0} \\
w_1 &\leftarrow w_1 + \eta\frac{\partial p(\mathbf{t}|\mathbf{y})}{\partial w_1}
\end{aligned}
$$

for some learning rate η.

Problem 6 (Laplacian Prior)

Laplacian prior for the weights of a linear (or logistic) regression will turn into Lasso regularization. Laplacian distribution on w is defined by

$$p(\mathbf{w}) = \frac{1}{2b} \exp\left(-\frac{|\mathbf{w}|}{b}\right) \tag{9}$$

which can be defined for weights of the model (except the intercept), where we assume different weigths are independent. b is a hyperparameter.

1. Let's assume we have $D = \{(\mathbf{x}_i, t_i)|i = 1, \ldots, N\}$ and we want to build a linear regression model with the Laplacian prior on the model weights. Define the likelihood and prior term here, and show it turns to a lasso regression. You can assume weights share the same hyperparameter.

   Solution. Let say we have a linear regression model with Laplacian prior on the weights. The likelihood term is

   $$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2}{2\sigma^2}\right)$$

   and the prior term is

   $$p(\mathbf{w}) = \frac{1}{2b} \exp\left(-\frac{|\mathbf{w}|}{b}\right)$$

   The posterior distribution is proportional to the likelihood and prior term

   $$p(\mathbf{w}|\mathbf{X}, \mathbf{t}) \propto p(\mathbf{t}|\mathbf{X}, \mathbf{w}) p(\mathbf{w})$$

   or

   $$p(\mathbf{w}|\mathbf{X}, \mathbf{t}) \propto \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2}{2\sigma^2}\right) \frac{1}{2b} \exp\left(-\frac{|\mathbf{w}|}{b}\right)$$

   MAP estimation would be

   $$\begin{aligned}
   \mathbf{w}^* &= \arg\max_{\mathbf{w}} p(\mathbf{w}|\mathbf{X}, \mathbf{t}) \\
   &= \arg\max_{\mathbf{w}} \ln p(\mathbf{w}|\mathbf{X}, \mathbf{t}) \\
   &= \arg\max_{\mathbf{w}} \ln \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2}{2\sigma^2}\right) \frac{1}{2b} \exp\left(-\frac{|\mathbf{w}|}{b}\right) \\
   &= \arg\max_{\mathbf{w}} \sum_{i=1}^{N} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2}{2\sigma^2} + \ln \frac{1}{2b} - \frac{|\mathbf{w}|}{b} \\
   &= \arg\max_{\mathbf{w}} -\frac{1}{2} \sum_{i=1}^{N} \frac{(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2}{2\sigma^2} + \frac{2|\mathbf{w}|}{b}
   \end{aligned}$$

   which shows the sum-of-squares error with penalty term in the lasso regression.

2. Lasso regression is defined by

   $$E_D(\mathbf{w}) = -\frac{1}{2} \sum_{i=1}^{N} (t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2 - \lambda \sum_{j=1}^{M} |w_j| \tag{10}$$

We can use a gradient descent algorithm to find the model parameters, but the issue is that derivative of $|\mathbf{w}|$ has a discontinuity at zero. A remedy is to rewrite the optimization by

$$E_D(\mathbf{w}) = -\frac{1}{2}\sum_{i=1}^{N}(t_i - \mathbf{w}^\top \phi(\mathbf{x}_i))^2 - \lambda \sum_{j=1}^{M} \frac{w_j^2}{|w_j|} \tag{11}$$

where, you replace the term in denominator of the regularization term by a known value. Let's assume, you are in the r^{th} iteration of a gradient descent algorithm (r represents the iteration), and your partial derivative for j^{th} weight is defined by

$$\frac{\partial E_D^{(r)}(\mathbf{w})}{\partial w_j} \approx \sum_{i=1}^{N} \phi(\mathbf{x}_i)\left(t_i - \mathbf{w}^{(r)\top}\phi(\mathbf{x}_i)\right) - \lambda \frac{w_j^{(r)}}{\max\left\{\epsilon, |w_j^{(r-1)}|\right\}} \tag{12}$$

where, ϵ has a small value, like 0.0001. Complete the update rule for all other weights in the model and show its result in a simulated data.

Solution. The update rule for the j^{th} weight is

$$w_j^{(r+1)} = w_j^{(r)} - \eta\left(\sum_{i=1}^{N} \phi(\mathbf{x}_i)\left(t_i - \mathbf{w}^{(r)\top}\phi(\mathbf{x}_i)\right) - \lambda \frac{w_j^{(r)}}{\max\left\{\epsilon, |w_j^{(r-1)}|\right\}}\right) \tag{13}$$

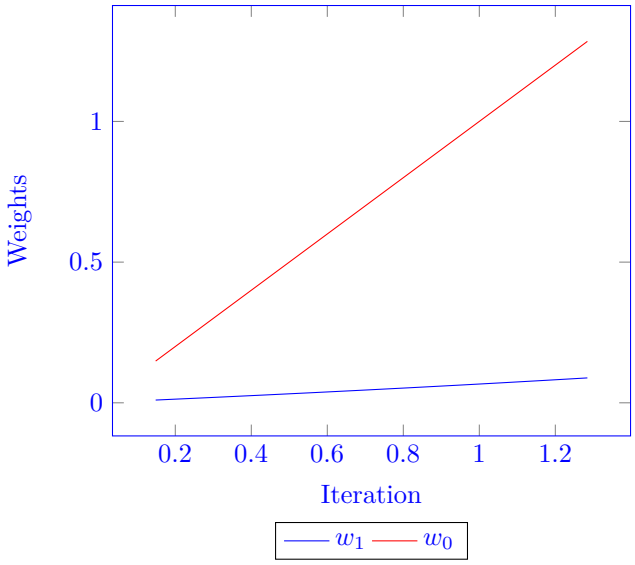
and the update rule for all other weights is the same. The simulation code is given below.

```
import numpy as np
np.random.seed(0)
N = 100
x = np.random.randn(N, 1)
y = 3 + 2 * x + np.random.randn(N, 1)
phi = x
alpha = 0.01
lambda_ = 0.1
max_iter = 10
w = np.zeros((2, 1))
weights = np.zeros((max_iter, 2))
obj = np.zeros((max_iter, 1))
for r in range(max_iter):
    for i in range(w.size):
        obj[r] = 0.5 * np.sum((y[i] - np.dot(phi[i], w[i])) ** 2) +
        lambda_ * np.sum((w[i] ** 2)/ np.abs(w[i]))
        grad = -np.dot(phi[i], y[i] - np.dot(phi[i], w[i])) +
        lambda_ * w[i]/max(np.abs(w[i]), 0.0001)
        w[i] = w[i] - alpha * grad
        weights[r,i] = w[i]
```

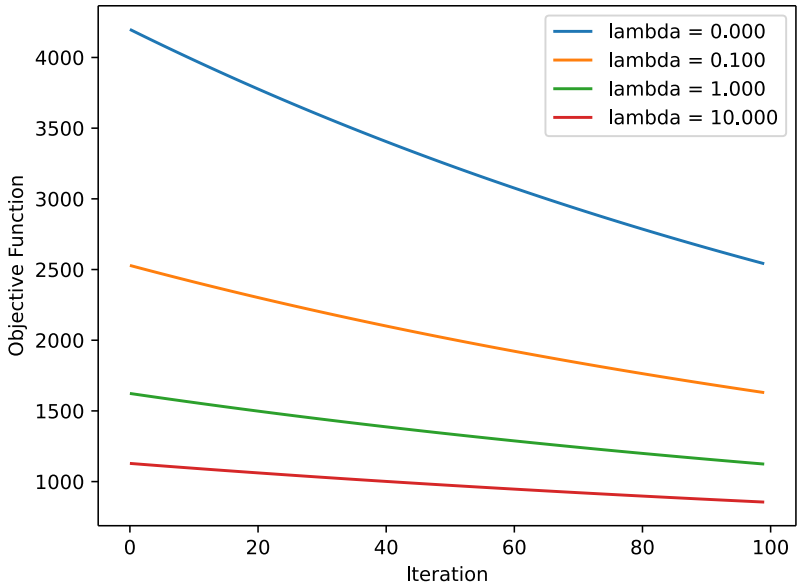
3. Create 100 sample data points for $t_i = 1 + 0.001\mathbf{x}_i - 2\mathbf{x}_i^2 + \epsilon_k$ where ϵ_k has normal distribution with a mean zero and variance of 0.1. Show how the estimated weights will change as a function of λ. For x, you can draw 100 random values from a normal distribution with mean 0 and variance 1. To find the model parameters you can use the gradient descent algorithm we discussed here.

Solution. The simulation code is given below.

```
import numpy as np
import matplotlib.pyplot as plt
np.random.seed(0)
```




```
N = 1000
x = np.random.randn(N, 1)
epsilon = np.random.randn(N, 1) * np.sqrt(0.1)
t = 1 + 0.001 * x - 2 * x ** 2 + epsilon
phi = np.hstack((np.ones((N, 1)), x, x ** 2))
alpha = 1e-6
lambda_ = np.array([0, 0.1, 1, 10])
max_iter = 100
w = np.zeros((3, 1))
obj = np.zeros((len(lambda_), max_iter))
for i, l in enumerate(lambda_):
    for r in range(max_iter):
        obj[i, r] = 0.5 * np.sum((t - np.dot(phi, w)) ** 2) +
        l * np.sum(np.abs(w[1:]))
        grad = -np.dot(phi.T, t - np.dot(phi, w)) +
        l * np.vstack((0, l * np.sign(w[1:])))
        w = w - alpha * grad
for i in range(len(lambda_)):
    plt.plot(range(max_iter), obj[i, :], label='lambda = {:.3f}'.format(lambda_[i]))
plt.xlabel('Iteration')
plt.ylabel('Objective Function')
plt.legend()
plt.show()
```


lambda = 0.000
lambda = 0.100
lambda = 1.000
lambda = 10.000
Objective Function
Iteration
4000
3500
3000
2500
2000
1500
1000
0
20
40
60
80
100