CSCI-567: Assignment #3

Due on Friday, October 16, 2015

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Contents

Problem 1

Problem 1: (a)

Let $\sigma(a) = \frac{1}{1+e^{-a}}$ and

$$P(Y=1|X=x) = \sigma(b+w^Tx)P(Y=0|X=x) = 1-\sigma(b+w^Tx)$$

Observe that $Y=1$ when $b+w^Tx \geq 0$ and $Y=0$ when $b+w^Tx < 0$
Thus,

$$\begin{aligned}
P(Y=y|X=x) &= \sigma(b+w^T)^y(1-\sigma(b+w^Tx))^(1-y) \\
\log(P(Y=y|X=x)) &= y\log(\sigma(b+w^Tx))^y + (1-y)\log(1-\sigma(b+w^Tx)) \\
&= y\log(\frac{\sigma(b+w^T)}{1-\sigma(b+w^Tx)}) + \log(1-\sigma(b+w^Tx)) \\
&= y(b+w^Tx) + \log(\frac{e^{-(b+w^Tx)}}{1+e^{-(b+w^Tx)}}) \\
&= y(b+w^Tx) + \log(\frac{1}{1+e^{(b+w^Tx)}}) \\
&= y(b+w^Tx) - \log(1+e^{(b+w^Tx)}) \qquad ([1.1])
\end{aligned}$$

$$\begin{aligned}
\mathcal{L}(w) &= -\log(\prod_{i=1}^{n} P(Y=y_i|X=x_i)) \\
&= -\sum_{i=1}^{n}\log(P(Y=y_i|X=x_i)) \\
&= -\sum_{i=1}^{n}\left(y_i(b+w^Tx_i) - \log(1+e^{(b+w^Tx_i)})\right)
\end{aligned}$$

Consider $(L)(w) = y(b+w^Tx) - \log(1+e^{(b+w^Tx_i)})$

$$\begin{aligned}
\frac{\partial\mathcal{L}(w)}{\partial w} &= -(xy^T) + \frac{e^{(b+w^Tx)}x}{1+e^{(b+w^Tx)}} \\
\frac{\partial^2\mathcal{L}(w)}{\partial w^2} &= 0 + \frac{\partial}{\partial w}(x - \frac{x}{1+e^{(b+w^Tx)}}) \\
\frac{\partial^2\mathcal{L}(w)}{\partial w^2} &= \frac{x(e^{(b+w^Tx)})x^T}{(1+e^{(b+w^Tx)})^2} \geq 0 \ \forall \ x \in \mathbf{R} \\
\frac{\partial^2\mathcal{L}(w)}{\partial w^2} &= x^T\sigma(b+w^Tx)(1-\sigma(b+w^Tx))x \geq 0 \qquad (1.2)
\end{aligned}$$

From (1.2) $\frac{\partial^2\mathcal{L}(w)}{\partial w^2} \geq 0$ and hence, from the definition of convex functions, $\mathcal{L}(w)$ is indeed a convex function.

Problem 1: (b)

When the data is perfectly linearly separable, (assume first $n/2$ of the n training points belong to class 0 and the remaining to class 1), thus our regression model should assign the first $n/2$ points to class with cent percent certainity or with probability 1 and the remaining $n/2$ to class 0 with probability 1. For this to happen, $P(Y = 1|X = X_1) = 1$ and $P(Y = 0|X = X_0) = 1$ where X_1 is the set of points belonging to class 1 and X_0 is the set of points belonging to class 0.
Clearly this scenario is possible when $||w|| \longrightarrow \infty$

Problem 1: (c)

A simple example with two points would be $(0, 0)$, $(1, 1)$. Intuitively the step function's step branches (the horizontals of a sigmooid function) will be located at infinity. Also the line separating the points (0,0) and (1,1) can be anywhere in between 0 and 1, thus there will be multiple solutions.

Problem 1: (d)

$$\mathcal{L}(w) = \sum_{j=1}^{n} \left(-y_j(b + w^T x_j) + \log(1 + e^{(b+w^T x_j)})\right) + \lambda||w||_2^2$$

$$\frac{\partial(\mathcal{L})(w)}{\partial w_i} = \sum_{j=1}^{n} \left(-y_j(x_{ji}) + \frac{x_{ji}e^{(b+w^T x_j)x_{ij}}}{1 + e^{(b+w^T x_j)}}\right) + 2\lambda w_i = 0$$

$$\frac{\partial^2(\mathcal{L})(w)}{\partial w_i^2} = \sum_{j=1}^{n} \left(\frac{x_{ji}^2 e^{(b+w^T x_j)x_{ij}}}{(1 + e^{(b+w^T x_j)})^2}\right) + 2\lambda > 0$$

where the last inequality holds since $\lambda > 0$ Consider $\boldsymbol{f(w_i) = \sum_{j=1}^{n} \left(-y_j(x_{ji}) + \frac{x_{ji}e^{(b+w^T x_j)x_{ij}}}{1+e^{(b+w^T x_j)}}\right) + 2\lambda w_i = 0}$
And u, v are the two solutions of $f(w_i) = 0$, i.e. $f(u) = f(v) = 0$ (Without loss of generality, assume $u < v$)
By Rolle's theorem, If $f(u) = f(v) = 0$ then there exists a point in $[u, v]$ say c such that $f'(c) = 0$ for $c \in [u, v]$
But, $f'(w_i) = \sum_{j=1}^{n} \left(\frac{x_{ji}^2 e^{(b+w^T x_j)x_{ij}}}{(1+e^{(b+w^T x_j)})^2}\right) + 2\lambda > 0$ and hence there exists no such c.
and hence the function is convex, thus the solution to the partial differential $\frac{\partial(\mathcal{L})(w)}{\partial w_i}$ is unique.

Problem 2

Problem 2

Problem 2: (a)

Consider $||w||_0 = \#i : w_i \neq 0$ for a 1D case. Where, $x_1 = (0)$ and $x_2 = (\epsilon)$ where $0 < \epsilon << 1$
$f(w) = \sum_i I\{w_i \neq 0\}$
Since we are in 1D:

$$\boldsymbol{f(w)} = \begin{cases} \mathbf{0} & \text{if w=0} \\ \mathbf{1} & \text{otherwise} \end{cases}$$

Thus,

$$f(0) = 0$$
$$f(\epsilon) = 1$$
$$f(\lambda \times 0 + (1-\lambda) \times \epsilon) = 1 \forall 0 < \lambda < 1 \tag{2a.1}$$
$$\lambda f(0) + (1-\lambda) f(\epsilon) = 1 - \lambda 0 < 1 - \lambda \qquad < 1 \tag{2a.2}$$

From $(2a.1), (2a.2)$ we see:
$f(\lambda \times 0 + (1-\lambda) \times \epsilon) > \lambda f(0) + (1-\lambda) f(\epsilon)$
Thus, $||w||_0$ is not a convecx function!

Problem 2: (b)

$||w||_1 = \sum_i |w_i|$
Consider two vectors u, v(same dimension say in $\mathbf{R^D}$)
Assume: $0\lambda < 1$

$$\begin{aligned} ||\lambda u + (1-\lambda) v|| &= \sum_{i=1}^{D} |\lambda u_i + (1-\lambda) v_i| \\ &\leq \sum_{i=1}^{D} \big(|\lambda u_i| + |(1-\lambda) v|\big) \ (since\ |a+b| \leq |a| + |b| \forall\ a, b \in R) \\ &= \sum_{i=1}^{D} |\lambda| |u_i| + \sum_{i=1}^{D} |1-\lambda| |v_i| \\ &= \lambda ||u||_1 + (1-\lambda) ||v||_1 \text{ since}(0\lambda < 1) \end{aligned} \tag{2a.1}$$

From $(2b.1)$, we see. $||\lambda u + (1-\lambda) v||_1 \leq \lambda ||u||_1 + (1-\lambda) ||v||_1$
And hence, $||w||_1$ is a convex function.

Problem 2: (c)

Let's redefine(for the sake of easense)x_i to be column vector i.e $x_i \; isD\times 1 \; w^T is1\times D$ and and $Y = (y_1 \dots y_n)$ the equivalent porblem then becomes:

$$min_w \sum_i (y_i - x_i^w)^2$$

$$\min_w \sum_i (y_i - x_i^T w)^2 + \lambda ||w||_1$$

$$\min_w (y - X^T w)^T (y - X^T w) + \lambda ||w||_1$$

$$\min_w (w^T X X^T w - 2Y^T X w + Y^T Y) + \min_w \lambda ||w||_1$$

$$\min_w (w^T X X^T w - 2Y^T X w) + \min_w \lambda ||w||_1$$

We introduce dummy variables t_i such that:

$$||w_i|| \leq t_i \implies t_i \geq w_i \text{and} t_i \geq -w_i$$

Now,

$$\min_w \lambda ||w||_1 \leq \lambda (t_1 + t_2 + \cdots + t_n)$$

Constraint:

$$t_i + w_i \geq$$
$$t_i - w_i \geq -w_i$$

which in the matrix form looks like:

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} t_i \\ w_i \end{pmatrix} \geq 0$$

Now consider this vector,:

$$\begin{pmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots t_n \\ w_1 \\ \vdots w_n \end{pmatrix}$$

The matrix A for reducing this constraicnt to the form $Au < b$ is then given by: Let:

$$B = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & (n-1)zeroes \dots & 1 & 0 \dots \\ 1 & (n-1)zeroes \dots & -1 & 0 \dots \\ 01 & 1 & (n-1)zeroes & -1 \\ & & & -1 \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \\ \vdots t_n \\ w_1 \\ \vdots w_n \end{pmatrix} \geq 0$$

Our optimisation problem now looks like:

$$\begin{pmatrix} t \\ w \end{pmatrix}^T \begin{pmatrix} 0 & 0 \\ 0 & XX^T \end{pmatrix} \begin{pmatrix} t \\ w \end{pmatrix} + \begin{pmatrix} 1 & 1 & \dots (d-2)\text{times } 1 & \text{d times } 0 \dots \end{pmatrix} \begin{pmatrix} t \\ w \end{pmatrix}$$

Problem 3

Problem 3: (a)

$min_w(\sum_i (y_i - w^T x_i)^2 + \lambda ||w||_2^2)$
In more compact matrix notation, let:

$$y_{n\times 1} = (y_1\ y_2\ \cdots\ y_n)^T$$
$$X_{n\times D} = (x_1^T\ x_2^T\ \cdots\ x_n^T)^T$$

This notation, reduces the above function to:
$min_w(||y - w^T X||_2^2 + \lambda ||w||_2^2)$

$$\begin{aligned}
f(w) &= min_w(||y - Xw||_2^2 + \lambda ||w||_2^2) \\
&= (y - Xw)^T (y - Xw) + \lambda w^T w \\
&= (y^T - w^T X^T)(y - Xw) + \lambda w^T w \\
&= y^T y - y^T Xw - w^T X^T y + w^T X^T Xw + \lambda w^T w \\
&= y^T y - (X^T y)^T w - w^T X^T y + w^T X^T Xw + \lambda w^T w \\
\frac{\partial f(w)}{\partial w} &= -X^T y - X^T y + 2\lambda w + (X^T Xw + (XX^T w)) = 0 \\
&= 2\lambda w + 2X^T Xw - 2X^T y = 0 \\
\mathbf{w}(\lambda I_D + X^T w) &= X^T y \\
\mathbf{w} &= (X^T Xw + \lambda I_D)^{-1} X^T y
\end{aligned}$$

Problem 3: (b)

$min_w(||y - w^T \Phi||_2^2 + \lambda ||w||_2^2)$ From the previous part, the solution should be of similar form:
$\mathbf{w} = (\Phi^T \Phi + \lambda I_D)^{-1} \Phi^T y$
Using the identity:
$(P^{-1} + B^T R^{-1} B)^{-1} B^T R^{-1} = PB^T (BPB^T + R)^{-1}$
Thus,
$\big((\lambda I_D + \Phi^T \Phi)^{-1}\big)\Phi^T y = \Phi^T \big(\Phi\Phi^T + \lambda I_N\big)^{-1} y$
$w^* = \Phi^T (\Phi\Phi^T + \lambda I_N)^{-1} y$

Problem 3: (c)

$\hat{y} = w^{*T}\Phi(x)$
$\hat{y} = \left(\Phi^T(\Phi\Phi^T + \lambda I_N)^{-1}y\right)^T\Phi(x) = y^T\left((\Phi\Phi^T + \lambda I_N)^{-1}\right)^T\Phi^T\Phi(x)$
Now using the property, $(A^{-1})^T = (A^T)^{-1}$

$$\begin{aligned}\hat{y} &== y^T\left((\Phi\Phi^T + \lambda I_N)^{-1}\right)^T\Phi^T\Phi(x)\\ &= y^T\left((\Phi\Phi^T + \lambda I_N)^T\right)^{-1}\Phi^T\Phi(x)\\ &= y^T\left((\Phi^T\Phi + \lambda I_N)\right)^{-1}\Phi^T\Phi(x)\\ &= y^T(K + \lambda I_N)^{-1}\kappa(x)\end{aligned}$$

Where $K_{ij} = \Phi_i^T\Phi_j$ and $\kappa(x) = \phi^T\phi^T(x)$

Problem 3: (d)

Kernel ridge regression is $O(n^3)$ for n data points. Linear regression was forumlated as quadratic programing and hence is $O(n^2)$.
The extra n factor comes from the formation of kernel matrix K.

Problem 4

Given: $k_1(.,.)$ and $k_2(.,.)$ are kernel function. Thus, for any vector $y \in \mathbf{R}$, $y^TKy \geq 0$ where $K_{ij} = k(x_i, x_j)$
Mercer's theorem requires K to be positive semi-definite.

Problem 4 continued on next page. . .

Problem 4: (a)

$k_3(x,x') = a_1 k_1(x,x') + a_2 k_2(x,x')$ where$a_1, a_2 \geq 0$
Since $k_1(x,x')$ is positive definite, $\forall y \in \mathbf{R}$,

$$y^T K^{(1)} y \geq 0, \tag{4a.1}$$
$$\text{where}$$
$$K^{(1)}_{ij} = k_1(x_i, x'_j)$$

Similarly,

$$y^T K^{(2)} y \geq 0, \tag{4a.2}$$
$$\text{where}$$
$$K^{(2)}_{ij} = k_2(x_i, x'_j)$$

Thus, from (4a.1) and (4a.2), we get

$$y^T (K^{(1)} + K^{(2)}) y \geq 0 \ \forall y \in \mathbf{R} \implies$$
$$y^T K^{(3)} y \geq 0 \ \forall y \in \mathbf{R}$$
$$\text{where}$$
$$K^{(3)}_{ij} = k_3(x_i, x'_j)$$

Problem 4: (b)

$k_4(x,x') = f(x)f(x')$ Let $K^{(4)}_{ij} = k_4(x_i, x_j) = f(x_i)f(x'_j)$
Since $f(x)$ is a real valued function, consider $K^{(4)}$

$$K^{(4)} = \begin{bmatrix} f(x_1)f(x'_1) & f(x_1)f(x'_2) & \cdots & f(x_1)f(x'_n) \\ \vdots & & & \\ f(x_n)f(x'_1) & f(x_n)f(x'_2) & \cdots & f(x_n)f(x'_n) \end{bmatrix}$$
$$K^{(4)} = F(\vec{x})_{n\times 1} F(\vec{x})^T_{1\times n}$$
$$\text{where}$$
$$F(x)^T_{1\times n} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots f(x_n) \end{pmatrix}$$

Now consider $y^T K^{(4)} y = y^T F(x) F(x)^T y = y^T F(x) (y^T F(x))^T = ||y^T F(x)||_2^2 \geq 0$
Thus, $k_2(.,.)$ is a valid kernel function!.

Problem 4 continued on next page. . .

Problem 4: (c)

$k_5(x, x') = g(k_1(x, x'))$ where g is a polynomial with positive coefficients.
Since g has positive coefficients, $g(x) \geq 0 \forall x \geq 0$
Now consider,

$$y^T K^{(5)} y = (y_1 \ y_2 \cdots y_n) \times \begin{bmatrix} g(k_1(x_1, x_1')) & g(k_1(x_1, x_2')) & \cdots g(k_1(x_1, x_n')) \\ \vdots & & \\ g(k_1(x_n, x_1')) & g(k_1(x_n, x_2')) & \cdots g(k_1(x_n, x_n')) \end{bmatrix} \times \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$y^T K^{(5)} y = y_1 g(k_1(x_1, x_1'))y_1 + y_2 g(k_1(x_1, x_2'))y_2 + \cdots y_n g(k_1(x_n, x_n'))y_n$$

Since $g(k_1(x_i, x_j)) \geq 0$

$$y^T K^{(5)} y \geq 0 \ \forall \ y \in \mathbf{R}$$

Thus k_5 is a kernel

Problem 4: (d)

$k_6(x, x') = k_1(x, x')k_2(x, x')$
Thus, in terms of our earlier defined matrix notation, $K^{(6)} = K^{(1)} \circ K^{(2)}$ where $\circ$ denotes element wise multiplication (also known as the Hadamard product).
Since, k_1 and k_2 are valid kernel function $\exists v_i w_j$ the eigen vectors of matrix K_1 and K_2 defines such that: $K^{(1)} = \sum_i \lambda_i v_i v_i^T$ and $K^{(2)} = \sum_j \mu_j w_j {w_j}^T$
Now,

$$\begin{aligned} K^{(6)} &= K^{(1)} \circ K^{(2)} \\ &= \sum_i \lambda_i v_i v_i^T \circ \sum_j \mu_j w_j {w_j}^T \\ &= \sum_{i,j} \lambda_i \mu_j (v_i v_i^T) \circ w_j {w_j}^T \\ &= \sum_{i,j} \lambda_i \mu_j (v_i \circ w_j)(v_j \circ w_j)^T \\ &\geq 0 \end{aligned}$$

Because $(v_i \circ w_j)(v_j \circ w_j)^T = ||v_i w_j||_2^2 \geq 0$

Problem 4: (e)

$k_7(x, x') = exp(k_1(x, x'))$
Just like subpart (c), here $g(x) = exp(x)$ (it's not a polynomial, though that does not affect the derivation we came up with in part (c)). So this is immediate from part (c).

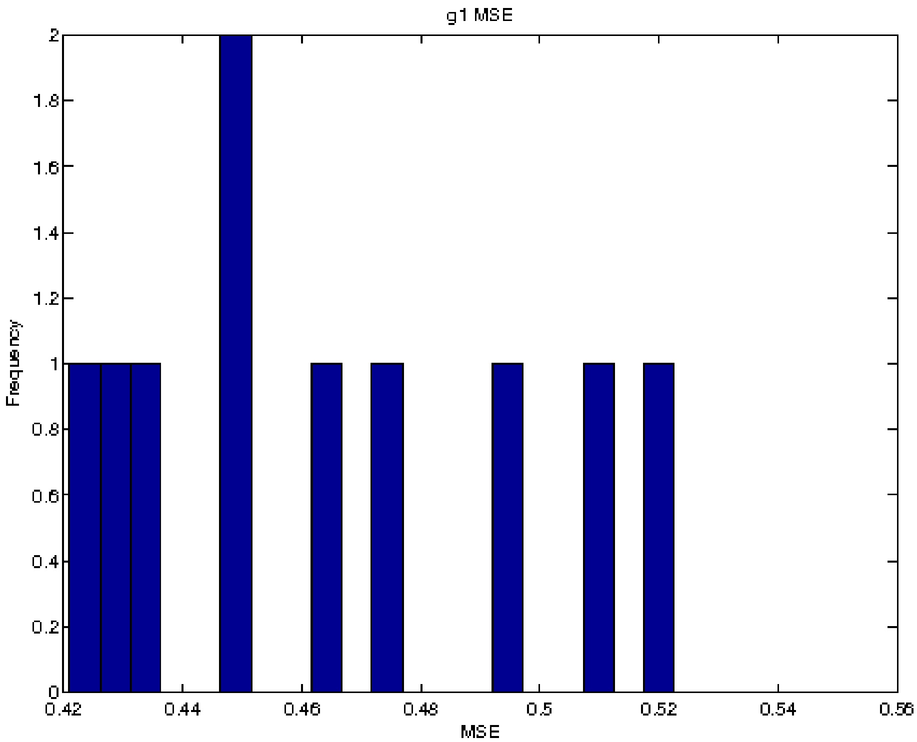

Figure 1: Problem 5.a g_1 MSE

Problem 5

a

——g_1——- MSE:0.463977 Bias Sq:0.108996 Variance:0.000000
——g_2——- MSE:0.356683 Bias Sq:0.002941 Variance:0.003295
——g_3——- MSE:0.354618 Bias Sq:0.002844 Variance:0.007814
——g_4——- MSE:0.004551 Bias Sq:0.000151 Variance:0.003862
——g_5——- MSE:0.005546 Bias Sq:0.000151 Variance:0.004782
—-g_6——- MSE:0.006223 Bias Sq:0.000125 Variance:0.005273

As the model complexity increase the squared bias decreases and the variance increases. However for some reason, the variance attributed with g_3 is a bit more than the normal trend. I could not think of a possible explanation for this.

Problem 5 continued on next page. . .

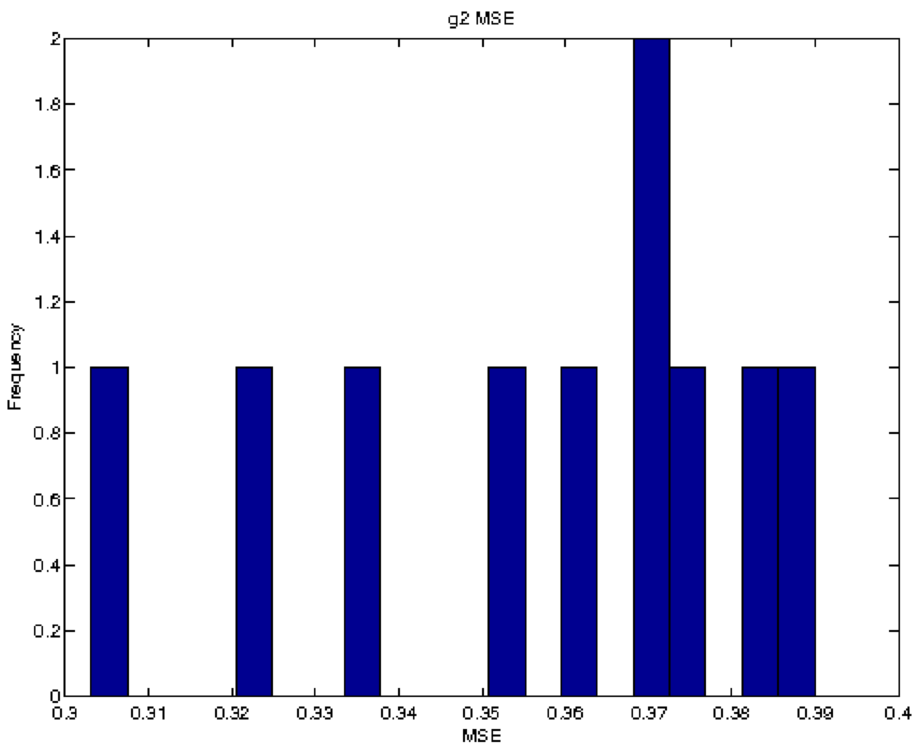

Figure 2: Problem 5.a g_2 MSE

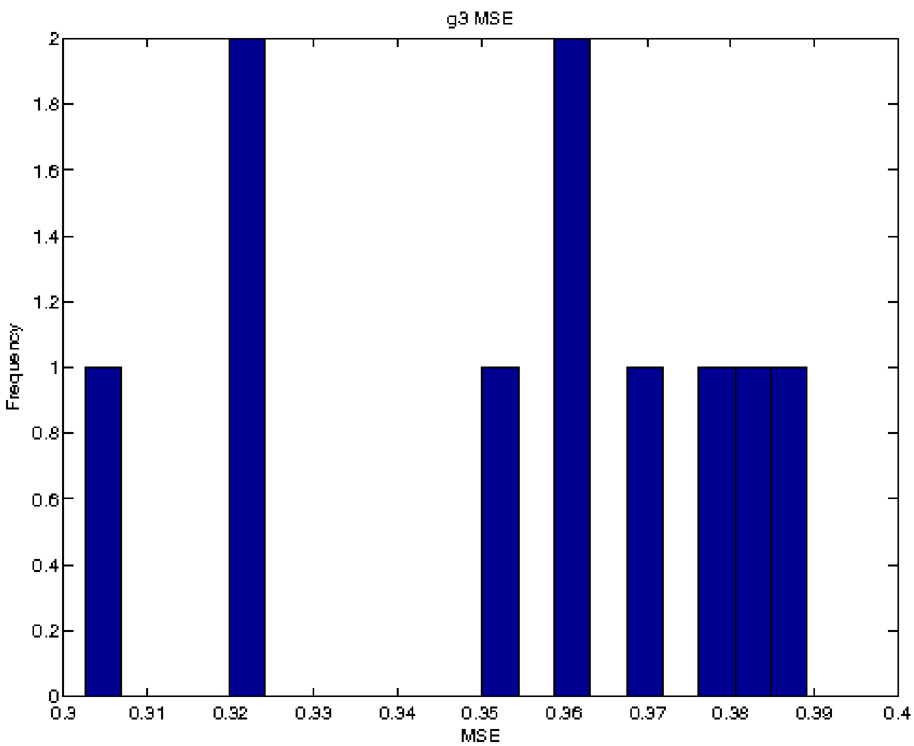

Figure 3: Problem 5.a g_3 MSE

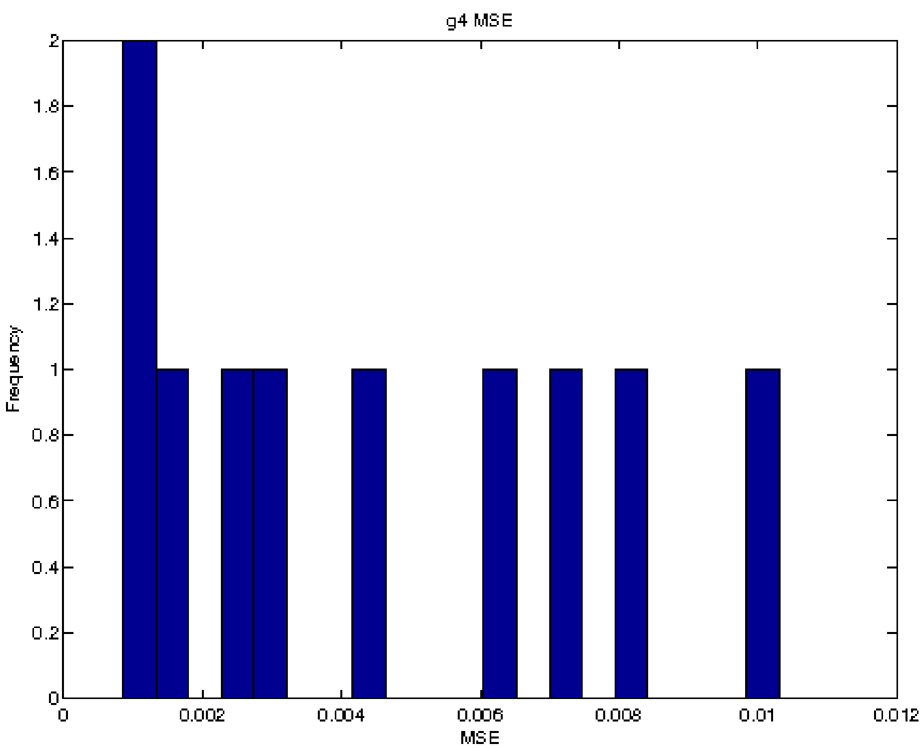

Figure 4: Problem 5.a g_4 MSE

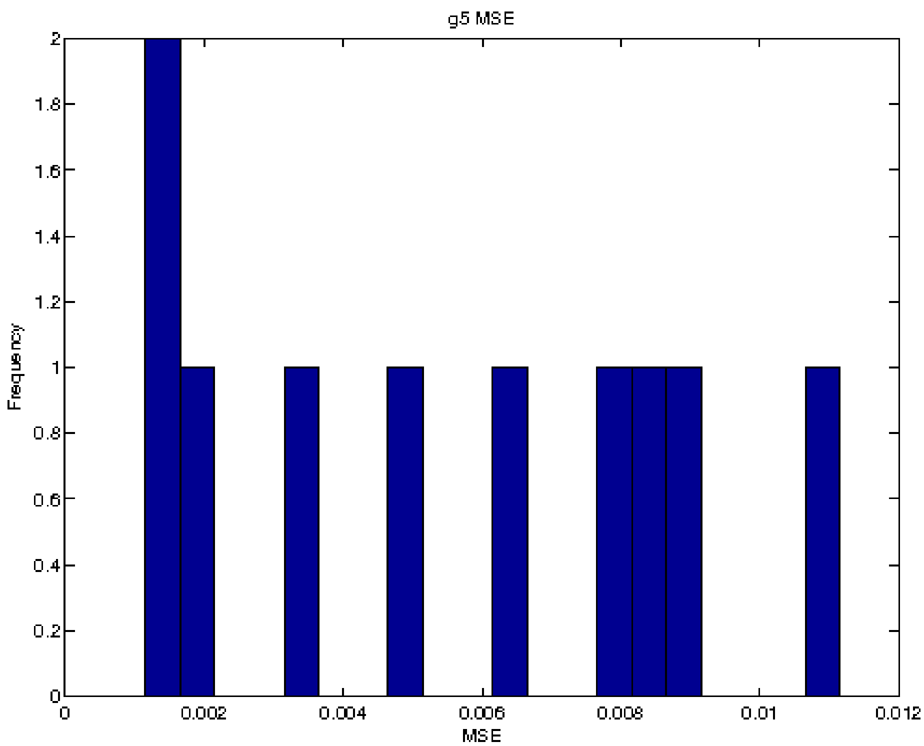

Figure 5: Problem 5.a g_5 MSE

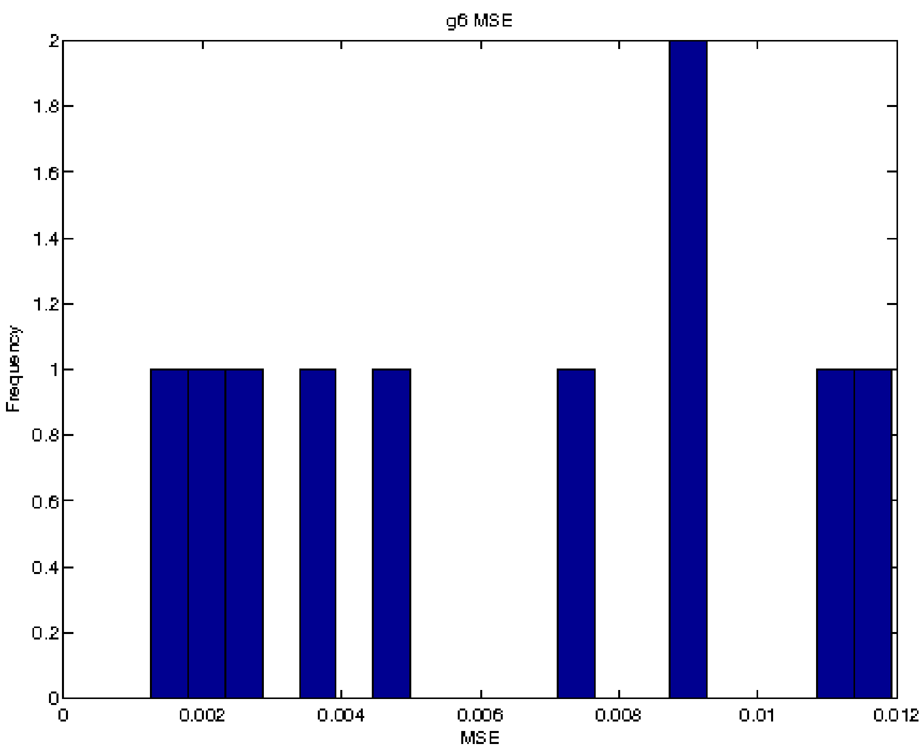

Figure 6: Problem 5.a g_6 MSE

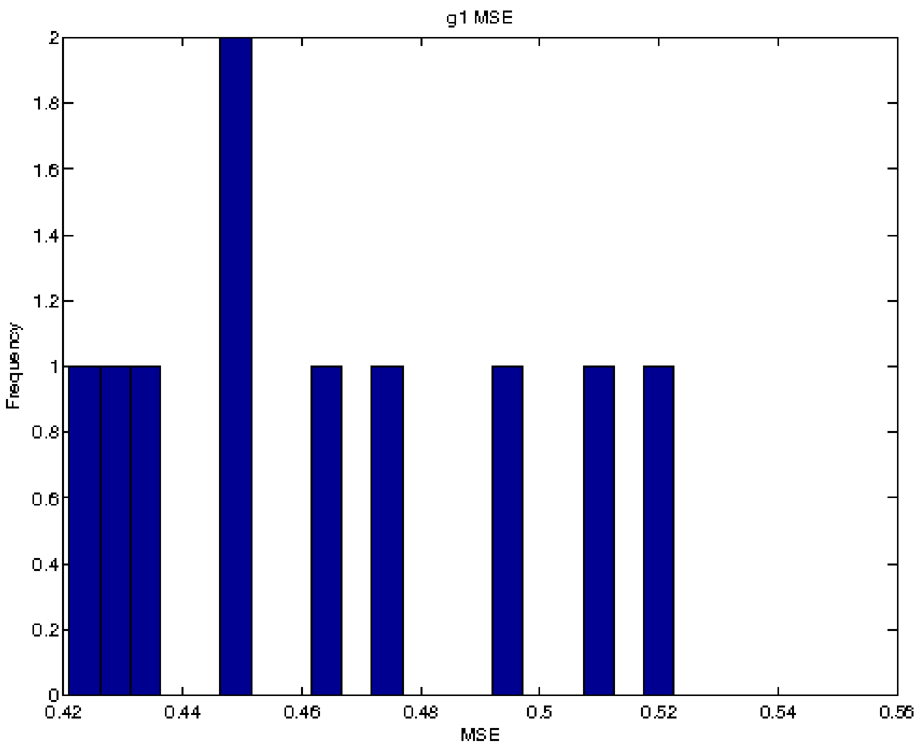

Figure 7: Problem 5.a g_1 MSE

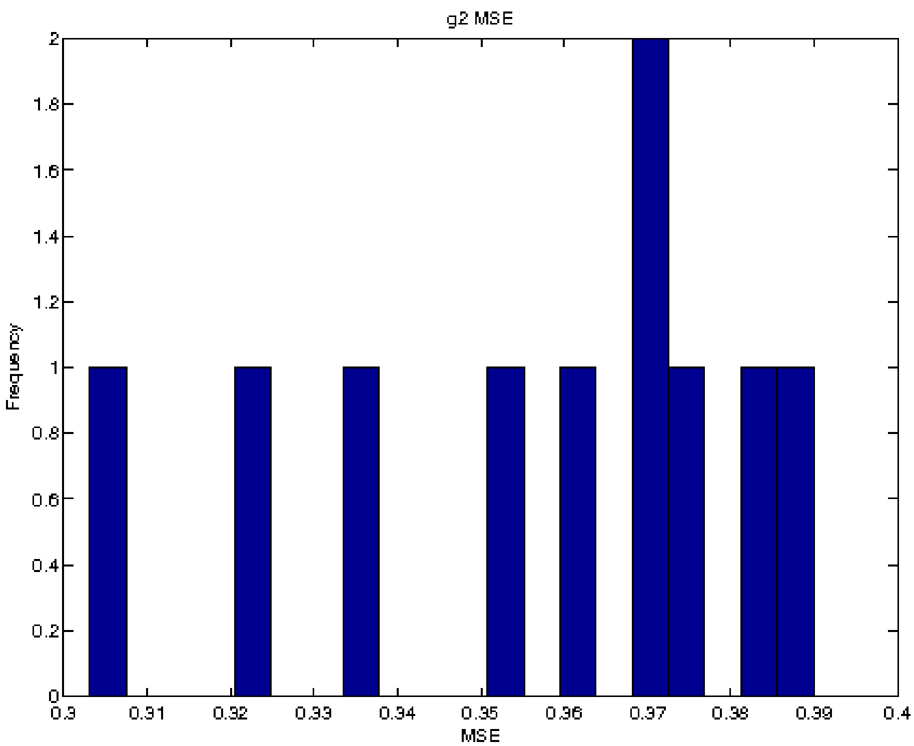

Figure 8: Problem 5.a g_2 MSE

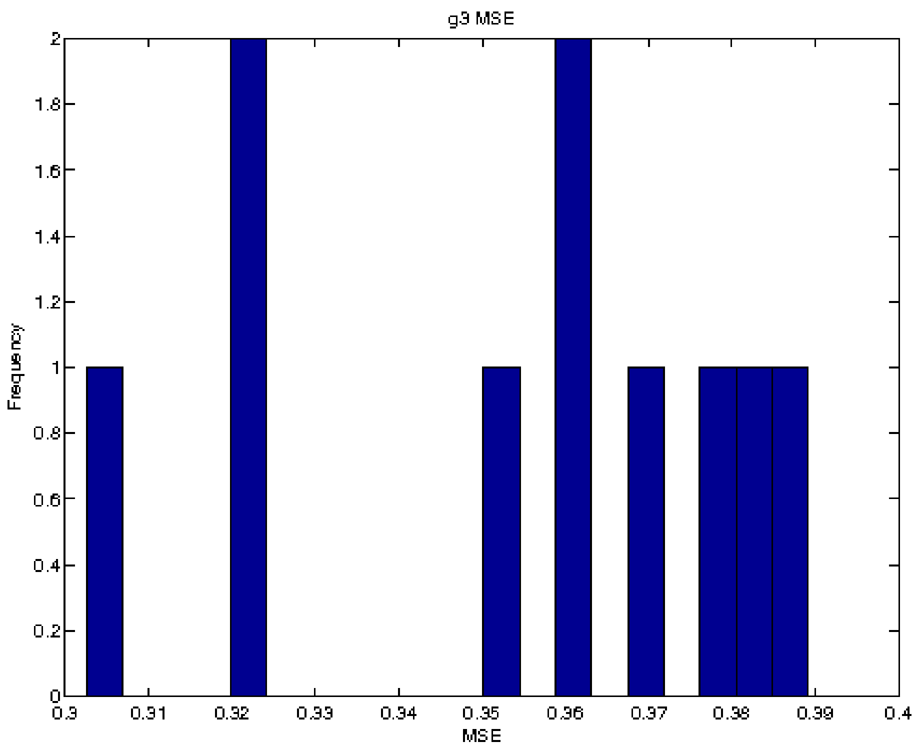

Figure 9: Problem 5.a g_3 MSE

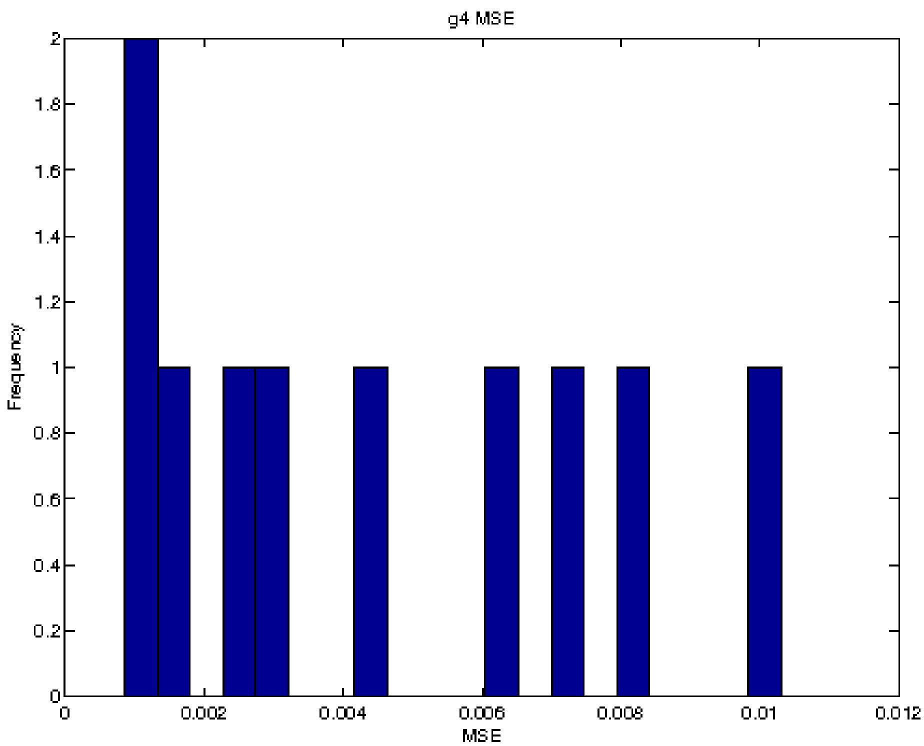

Figure 10: Problem 5.a g_4 MSE

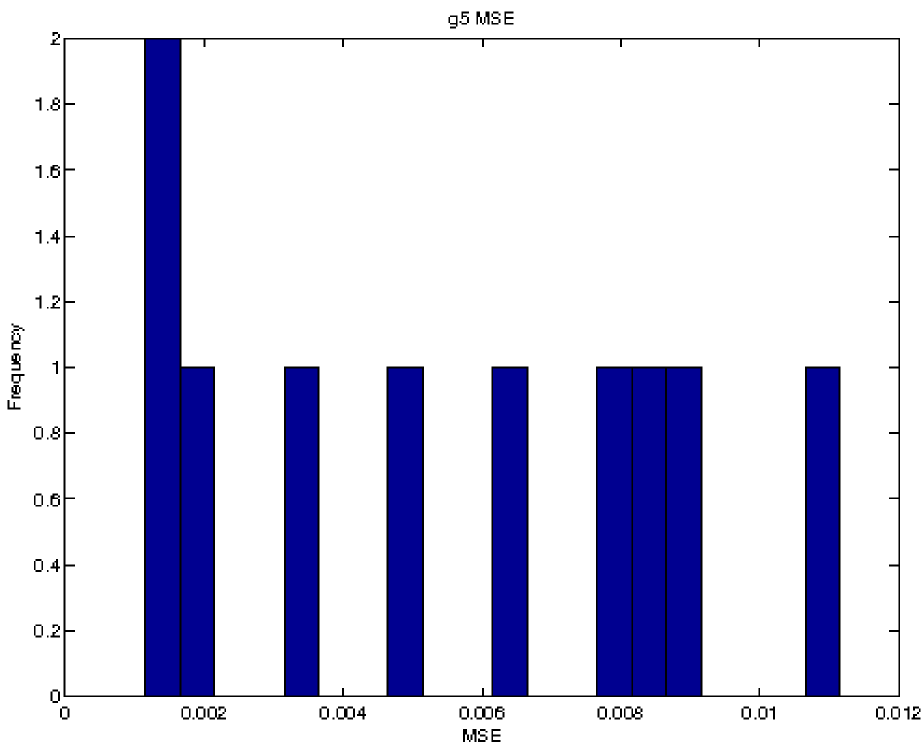

Figure 11: Problem 5.a g_5 MSE

Problem 5 continued on next page...

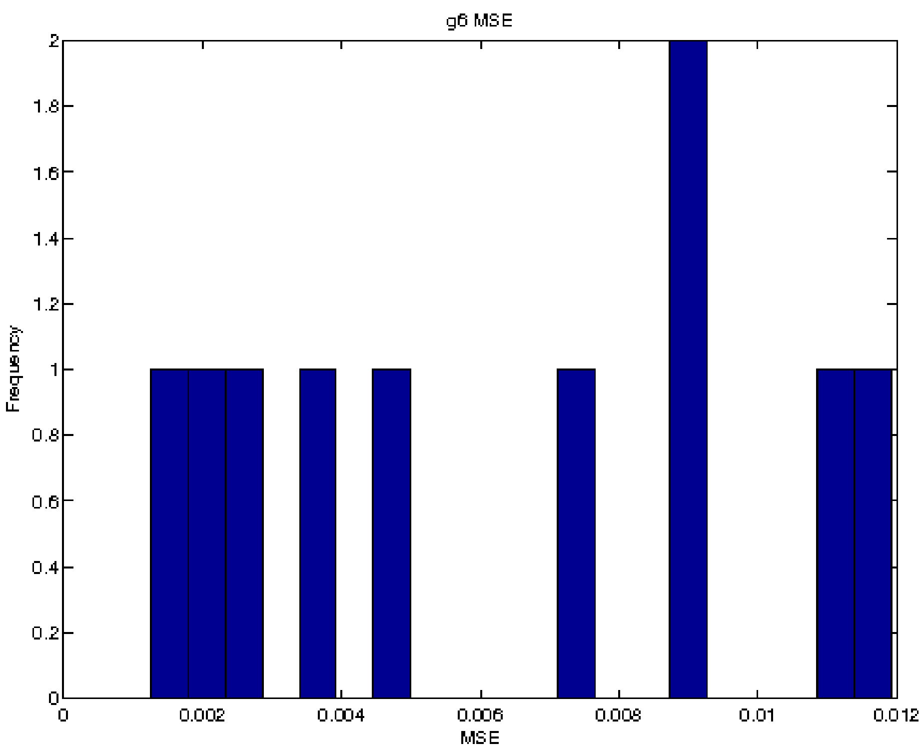

Figure 12: Problem 5.a g_6 MSE

Problem 5 continued on next page. . .

b

Problem 6

Kernel ridge regression with linear kernel does not give the same results, and the thing to realise in this case is that linear kernel projects the data into $N \times N$ dimenisons, while the ridge regression still has the 'kernel' in $D \times D$ dimensions. There is extra information being used here (in cases where $N > D$) In a a siutation where $D > N$ the linear kernl might perform better.(I don't have a proof for this) hoose w such that $||w||_0 = 0$, then $||-w||_0 = 0$.
Thus $||w - w||_0 = ||0||_0 = n > ||w||_0 + ||-w||_0$
So $||w||_0$ is not a convex function.

(b)

Let x, $vcty$ be two vectors and $0 < \lambda < 1$

$$\begin{aligned} ||\lambda x + (1-\lambda)y||_1 &= \sum_i |\lambda x_i + (1-\lambda)y_i| \\ &\leq \sum_i \lambda|x_i| + (1-\lambda)|y_i| \\ &= \lambda||x||_1 + (1-\lambda)||y||_1 \end{aligned}$$

So $||w||_1$ is convex.

(c)

Solving

$$\underset{w}{min} \sum_n (y_i - w^T x_i)^2 + \lambda||w||_1 = \underset{w}{min}\, ||y - xw||_2 + \lambda||w||_1$$

Which is to minimize $||y - xw||_2$ for some bounded $\lambda||w||_1$
Which transforms to

$$\underset{w}{min}\, w^T x x^T w - 2y^T x w$$
$$\text{subject to } \lambda||w||_1 \leq c$$

Introduce additional D variables $t_1, t_2, \cdots t_D$ and $|w_i| \leq t_i$. Then $||w||_1 = \sum_i w_i \leq \sum_i t_i$ which gives the upper bound of $||w||_1$
Let $u = (w, t)^T$, then the problem transform to

$$\underset{u}{min}\, u^T Q u - c^T u$$

Where $Q = \begin{pmatrix} xx^T & 0 \\ 0 & 0 \end{pmatrix}$ and $c^T = \lambda(2y^T x, 1)$
Subject to

$$Au \leq b$$

where $A = \begin{pmatrix} I_D & -I_D \\ -I_D & -I_D \end{pmatrix}$ and $b = 0$ which corresponds to $w_i \leq t_i$ and $-w_i \leq t_i$