

Homework 3

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1) (a)

$$\begin{aligned}\ell(\mathbf{w}) &= \sum_{i=1}^n -y_i \log\left(\frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}_i}}\right) - (1 - y_i) \log\left(\frac{e^{-\mathbf{w}^T \mathbf{x}_i}}{1 + e^{-\mathbf{w}^T \mathbf{x}_i}}\right) \\ &= \sum_{i=1}^n [y_i \log(1 + e^{\mathbf{w}^T \mathbf{x}_i}) - (1 - y_i)(-\mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \log(1 + e^{-\mathbf{w}^T \mathbf{x}_i})] \\ &= \sum_{i=1}^n [-y_i \mathbf{w}^T \mathbf{x}_i + \log(1 + e^{\mathbf{w}^T \mathbf{x}_i})]\end{aligned}$$

So,

$$\begin{aligned}\nabla \ell(\mathbf{w}) &= \sum_{i=1}^n \left[\mathbf{x}_i \left(-y_i + \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}_i}} \right) \right] \\ &= \sum_{i=1}^n [\mathbf{x}_i (-y_i + h(\mathbf{x}_i))]\end{aligned}$$

(b)

$$\begin{aligned}\nabla^2 \ell(\mathbf{w}) &= \frac{\partial^2 \ell}{\partial \mathbf{w} \partial \mathbf{w}^T} \\ &= \sum_{i=1}^n \mathbf{x}_i \frac{\partial h}{\partial \mathbf{w}^T} \\ &= \sum_{i=1}^n \mathbf{x}_i \frac{\partial h}{\partial (e^{-\mathbf{w}^T \mathbf{x}_i})} \frac{\partial (e^{-\mathbf{w}^T \mathbf{x}_i})}{\partial (\mathbf{w}^T \mathbf{x}_i)} \frac{\partial (\mathbf{w}^T \mathbf{x}_i)}{\partial \mathbf{w}^T} \\ &= \sum_{i=1}^n \mathbf{x}_i \cdot \frac{-1}{(1 + e^{\mathbf{w}^T \mathbf{x}_i})^2} \cdot (-e^{\mathbf{w}^T \mathbf{x}_i}) \cdot \mathbf{x}_i^T \\ &= \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T \frac{e^{-\mathbf{w}^T \mathbf{x}_i}}{(1 + e^{-\mathbf{w}^T \mathbf{x}_i})^2} \\ &= \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T h(\mathbf{x}_i) (1 - h(\mathbf{x}_i))\end{aligned}$$

So for any vector $\mathbf{u} \in \mathbb{R}^d$

$$\begin{aligned}\mathbf{u}^T \nabla^2 \ell(\mathbf{w}) \mathbf{u} &= \mathbf{u}^T \left[\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T h(\mathbf{x}_i) (1 - h(\mathbf{x}_i)) \right] \mathbf{u} \\ &= \sum_{i=1}^n \mathbf{u}^T \mathbf{x}_i \mathbf{x}_i^T \mathbf{u} h(\mathbf{x}_i) (1 - h(\mathbf{x}_i)) \\ &= \sum_{i=1}^n (\mathbf{x}_i^T \mathbf{u})^2 h(\mathbf{x}_i) (1 - h(\mathbf{x}_i))\end{aligned}$$

Since $0 < h(\mathbf{x}_i) < 1$, $\mathbf{u}^T \nabla^2 \ell(\mathbf{w}) \mathbf{u} \geq 0$ for any vector $\mathbf{u} \in \mathbb{R}^d$.

So $\nabla^2 \ell(\mathbf{w})$ is positive semi-definite, and thus $\ell(\mathbf{w})$ is convex and has no local minimum other than the global one.

(c) The algorithm takes 10 iterations to converge, the final coefficient \mathbf{w} is

$$\mathbf{w} = [-4.738783 \quad 4.402149 \quad -1.515217]$$

The error curve is shown below:

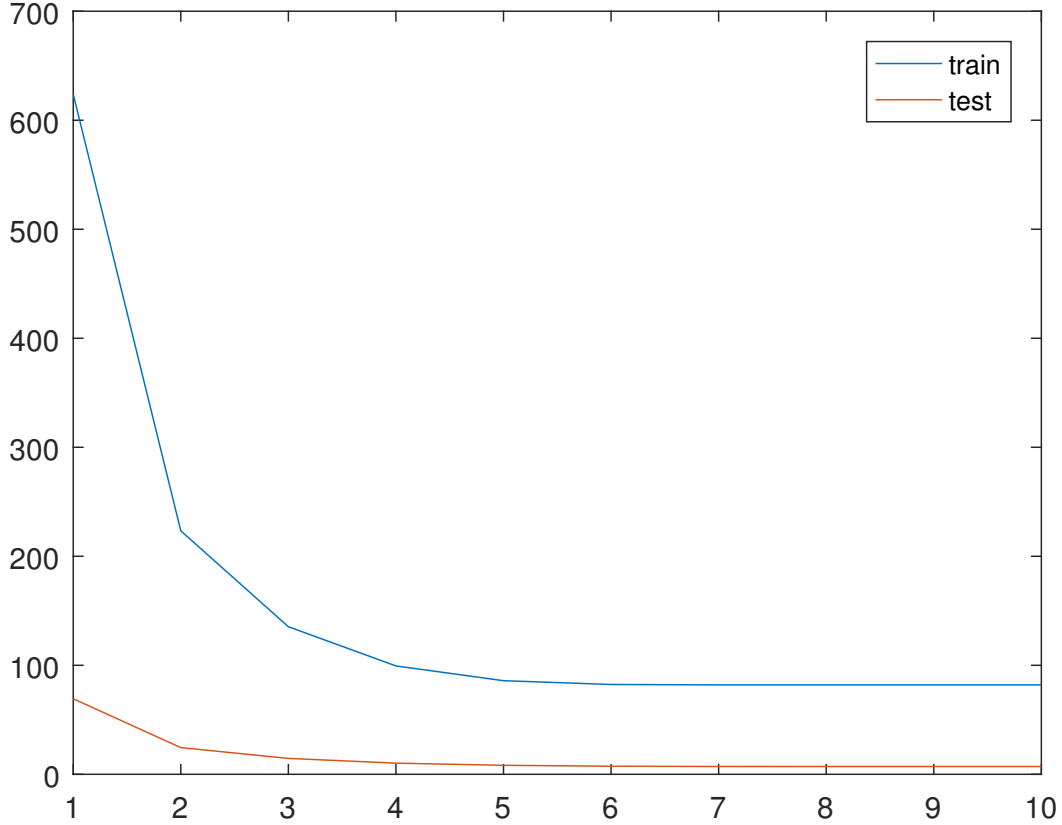


Figure 1: Error on training and test set

Following is the implementation:

```

1 w = [0 0 0];
2 train_data = [ones(size(train_x0)) train_x0 train_x1];
3 train_label = train_y;
4
5 test_data = [ones(size(test_x0)) test_x0 test_x1];
6 test_label = test_y;
7
8 loss = zeros(2, 1);
9 loss(1) = getLoss(train_data, train_label, w);
10 loss(2) = loss(1) + 1;
11
12 eps = 1e-8;
13 training_losses = [loss(1)];
14 test_losses = [getLoss(test_data, test_label, w)];
15
16 while (abs(loss(1) - loss(2)) > eps)
17     loss(1) = loss(2);
18
19     h_w = h(train_data, w)';
20     delta_w = sum(-train_data .* repmat(train_label - h_w, 1, 3));
21     hessian_w = zeros(3, 3);
22     for i = 1 : size(train_data, 1)
23         hessian_w = hessian_w + train_data(i, :) * train_data(i, :) *
24             h_w(i) * (1 - h_w(i));
25     end
26     w = w - (inv(hessian_w) * delta_w)';
27     loss(2) = getLoss(train_data, train_label, w);
28     test_losses = [test_losses getLoss(test_data, test_label, w)];
29     training_losses = [training_losses, loss(2)];
30 end
31 fprintf('Takes %d iterations to converge.\n', size(training_losses, 2));
32 fprintf('%f\n', w);
33 x = 1 : size(training_losses, 2);
34 plot(x, training_losses, x, test_losses);
35 legend('train', 'test');

```

2) a)

$$L(\theta) = \prod_{i=1}^n f(x_i; \theta) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i - \alpha)^2}{2\sigma^2}\right)$$

So,

$$\begin{aligned}
 \ell(\theta) &= \sum_{i=1}^n \left[\log \frac{1}{\sqrt{2\pi\sigma^2}} + \left(-\frac{(x_i - \alpha)^2}{2\sigma^2} \right) \right] \\
 &= n \log \frac{1}{\sqrt{2\pi\sigma^2}} + \sum_{i=1}^n \left(-\frac{(x_i - \alpha)^2}{2\sigma^2} \right)
 \end{aligned}$$

Thus,

$$\begin{aligned}\frac{\partial \ell}{\partial \alpha} &= \sum_{i=1}^n \left(\frac{2(x_i - \alpha)}{2\sigma^2} \right) \\ \frac{\partial \ell}{\partial \sigma^2} &= -\frac{n}{2} \frac{1}{2\pi\sigma^2} + \sum_{i=1}^n \left(\frac{(x_i - \alpha)^2}{2\sigma^4} \right)\end{aligned}$$

We let

$$\frac{\partial \ell}{\partial \alpha} = \frac{\partial \ell}{\partial \sigma^2} = 0$$

Then we can get the maximum likelihood estimates of α and σ^2 :

$$\begin{aligned}\hat{\alpha} &= \frac{1}{n} \sum_{i=1}^n x_i \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\alpha})^2\end{aligned}$$

b)

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^n \left[-\frac{1}{2} \log \left((2\pi)^d |\Sigma| \right) + \left(-\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}_i - \boldsymbol{\mu}) \right) \right] \\ &= \sum_{i=1}^n \left[-\frac{1}{2} \left(d \log(2\pi) + \log |\Sigma| + \mathbf{x}_i^T \Sigma^{-1} \mathbf{x}_i - 2\boldsymbol{\mu}^T \Sigma^{-1} \mathbf{x}_i + \boldsymbol{\mu}^T \Sigma^{-1} \boldsymbol{\mu} \right) \right]\end{aligned}$$

So,

$$\frac{\partial \ell}{\partial \boldsymbol{\mu}} = \sum_{i=1}^n \frac{\partial}{\partial \boldsymbol{\mu}} \left[-\frac{1}{2} \left(2\Sigma^{-1} \mathbf{x}_i + (\Sigma^{-1} + (\Sigma^{-1})^T) \boldsymbol{\mu} \right) \right]$$

We let

$$\frac{\partial \ell}{\partial \boldsymbol{\mu}} = 0$$

Then we obtain

$$\hat{\boldsymbol{\mu}} = \frac{2\Sigma^{-1} \sum_{i=1}^n \mathbf{x}_i}{n(\Sigma^{-1} + (\Sigma^{-1})^T)}$$

Since Σ is a symmetric matrix, we have

$$\Sigma^{-1} = (\Sigma^{-1})^T$$

Thus, the maximum likelihood estimate of $\boldsymbol{\mu}$ will be

$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$$

3) a) *Proof.* In definition,

$$I(X, Y) = \iint p(X, Y) \log \left(\frac{p(X, Y)}{p(X)p(Y)} \right) dX dY$$

So we can obtain,

$$\begin{aligned} H(X) - H(X|Y) &= - \int p(X) \log p(X) dX + \iint p(X, Y) \log p(X|Y) dX dY \\ &= - \int \log p(X) \int p(X, Y) dY dX + \iint p(X, Y) \log \frac{p(X, Y)}{p(Y)} dX dY \\ &= \iint p(X, Y) \log \frac{p(X, Y)}{p(X)p(Y)} dX dY \\ &= I(X, Y) \end{aligned}$$

and

$$\begin{aligned} H(Y) - H(Y|X) &= - \int p(Y) \log p(Y) dY + \iint p(X, Y) \log p(Y|X) dY dX \\ &= - \int \log p(Y) \int p(X, Y) dX dY + \iint p(X, Y) \log \frac{p(X, Y)}{p(X)} dY dX \\ &= \iint p(X, Y) \log \frac{p(X, Y)}{p(X)p(Y)} dX dY \\ &= I(X, Y) \end{aligned}$$

Therefore,

$$I(X, Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$

□

b) *Proof.* If $X = f(Y)$ and $Y = f^{-1}(X)$, then we can obtain

$$\begin{aligned} p(X = f^{-1}(Y)|Y) &= p(Y = f(X)|X) = 1 \\ p(X \neq f^{-1}(Y)|Y) &= p(Y \neq f(X)|X) = 0 \end{aligned}$$

Thus,

$$\begin{aligned} H(X|Y) &= - \iint p(X, Y) \log p(X|Y) dX dY \\ &= - \iint_{X=f^{-1}(Y)} p(X, Y) \log p(X|Y) dX dY - \iint_{X \neq f^{-1}(Y)} p(X, Y) \log p(X|Y) dY dX \\ &= 0 \\ H(Y|X) &= - \iint p(X, Y) \log p(Y|X) dY dX \\ &= - \iint_{Y=f(X)} p(X, Y) \log p(Y|X) dY dX - \iint_{Y \neq f(X)} p(X, Y) \log p(Y|X) dY dX \\ &= 0 \end{aligned}$$

Therefore,

$$I(X, Y) = H(X) - H(X|Y) = H(Y) - H(Y|X) = H(X) = H(Y)$$

□

c) *Proof.* For the maximum likelihood estimation of $q(x|\theta)$, the loss function will be

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^N \log q(x = x_i|\theta) \\ \hat{\theta}_{ML} &= \operatorname{argmax}_{\theta} \sum_{i=1}^N \log q(x = x_i|\theta)\end{aligned}$$

And

$$\begin{aligned}- \int \hat{p}(x) \log \frac{q(x|\theta)}{\hat{p}(x)} dx &= - \int \hat{p}(x) \log[q(x|\theta)] - \hat{p}(x) \log[\hat{p}(x)] dx \\ &= - \int \hat{p}(x) \log[q(x|\theta)] dx + \int \hat{p}(x) \log[\hat{p}(x)] dx\end{aligned}$$

Since $\hat{p}(x) = \frac{1}{N} \sum_{i=1}^N \mathbb{I}[x = x_i]$, we can obtain

$$\begin{aligned}\int \hat{p}(x) \log[q(x|\theta)] dx &= \int \frac{1}{N} \sum_{i=1}^N \mathbb{I}[x = x_i] \log[q(x|\theta)] dx \\ &= \sum_{i=1}^N \log[q(x = x_i|\theta)] \\ &= \ell(\theta)\end{aligned}$$

Because $\int \hat{p}(x) \log[\hat{p}(x)]$ is irrelevant to θ , minimizing the Kullback-Leibler divergence is equivalent to maximizing the likelihood function $\ell(\theta)$, which produces θ_{ML} .

Therefore, the minimum Kullback-Leibler divergence can be obtained by maximum likelihood estimate θ_{ML} given the data. □

d) *Proof.* We can start from getting the maximum of $H(p)$ for any PDF that satisfies following constraints:

$$\int p(x) dx = 1 \tag{1}$$

$$\int xp(x) dx = \mu \tag{2}$$

$$\int (x - \mu)^2 dx = \sigma^2 \tag{3}$$

So the Lagrangian function can be written as

$$L(p(x), \alpha, \beta, \gamma) = - \int p(x) \log[p(x)] dx + \lambda_1 \left(\int p(x) dx - 1 \right) \\ + \lambda_2 \left(\int xp(x) dx - \mu \right) + \lambda_3 \left(\int (x - \mu)^2 p(x) dx - \sigma^2 \right)$$

So,

$$\frac{\partial L}{\partial p(x)} = -\log[p(x)] + 1 + \lambda_1 + \lambda_2 x + \lambda_3 (x - \mu)^2$$

Let $\frac{\partial L}{\partial p(x)} = 0$, we can obtain

$$p(x) = \exp(1 + \lambda_1 + \lambda_2 x + \lambda_3 (x - \mu)^2)$$

Put the $p(x)$ back to the constraints Eqn. (1) - (3), we can get the value of Lagrangian multiplier.

$$\lambda_1 = -\frac{1}{2} \log(2\pi\sigma^2) - 1 \\ \lambda_2 = 0 \\ \lambda_3 = -\frac{1}{2\sigma^2}$$

So the $p(x)$ that maximize $H(p)$ will be $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$, which is the PDF of Gaussian distribution.

Therefore, Gaussian distribution has the maximum entropy $H(p)$. \square

4) a)

$$\ell(\mathbf{w}) = \log P(Y|\tilde{\mathbf{X}}; \mathbf{w}) \\ = \sum_{i=1}^n c_i \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(y_i - \mathbf{w}^T \tilde{\mathbf{x}}_i)^2}{2\sigma^2} \right) \\ = \sum_{i=1}^n c_i \log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{i=1}^n c_i (y_i - \mathbf{w}^T \tilde{\mathbf{x}}_i)^2$$

So it is equivalent to minimizing $J(\mathbf{w}) = \sum_{i=1}^n c_i (y_i - \mathbf{w}^T \tilde{\mathbf{x}}_i)^2$

Let

$$\frac{\partial J}{\partial b} = \sum_{i=1}^n -2c_i (y_i - \beta^T \mathbf{x}_i - b) = 0$$

we can obtain

$$\hat{b} = \frac{\sum_{i=1}^n c_i (y_i - \beta^T \mathbf{x}_i)}{\sum_{i=1}^n c_i} = \bar{y} - \beta^T \bar{\mathbf{x}}$$

where $\bar{\mathbf{x}}$ and \bar{y} are weight averages,

$$\bar{\mathbf{x}} = \frac{\sum_{i=1}^n c_i \mathbf{x}_i}{\sum_{i=1}^n c_i}, \quad \bar{y} = \frac{\sum_{i=1}^n c_i y_i}{\sum_{i=1}^n c_i}$$

Denote $\tilde{\mathbf{x}}_i = \mathbf{x}_i - \bar{\mathbf{x}}$, $\tilde{y}_i = y_i - \bar{y}$,

$$\begin{aligned} J(\mathbf{w}) &= \sum_{i=1}^n c_i (y_i - \bar{y} - \beta^T (\mathbf{x}_i - \bar{\mathbf{x}}))^2 \\ &= \sum_{i=1}^n c_i (\tilde{y}_i - \beta^T \tilde{\mathbf{x}}_i)^2 \\ &= (\tilde{Y} - \tilde{\mathbf{X}} \beta)^T C (\tilde{Y} - \tilde{\mathbf{X}} \beta) \\ &= \tilde{Y}^T C \tilde{Y} - 2 \tilde{Y}^T C \tilde{\mathbf{X}} \beta + (\tilde{\mathbf{X}} \beta)^T C (\tilde{\mathbf{X}} \beta) \\ &= -\frac{1}{2} \beta^T A \beta + U^T \beta + V \end{aligned}$$

where

$$\tilde{\mathbf{X}} = \begin{bmatrix} \tilde{\mathbf{x}}_1 \\ \vdots \\ \tilde{\mathbf{x}}_n \end{bmatrix}, \quad \tilde{Y} = \begin{bmatrix} \tilde{y}_1 \\ \vdots \\ \tilde{y}_n \end{bmatrix}, \quad A = \tilde{\mathbf{X}}^T C \tilde{\mathbf{X}}, \quad U = -\tilde{\mathbf{X}}^T C \tilde{Y}, \quad V = \frac{1}{2} \tilde{Y}^T C \tilde{Y}$$

So,

$$\hat{\beta} = -A^{-1}U = (\tilde{\mathbf{X}}^T C \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T C \tilde{Y}$$

Thus we get the maximum likelihood estimation of $\mathbf{w} = [b, \quad \beta^T]^T$

$$\begin{aligned} \hat{\beta} &= (\tilde{\mathbf{X}}^T C \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T C \tilde{Y} \\ \hat{b} &= \bar{y} - \beta^T \bar{\mathbf{x}} \end{aligned}$$

- b) When the noise has different variance σ_i for each i , the maximum likelihood function becomes

$$\begin{aligned} \ell(\mathbf{w}) &= \sum_{i=1}^n c_i \log \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp \left(-\frac{(y_i - \mathbf{w}^T \tilde{\mathbf{x}}_i)^2}{2\sigma_i^2} \right) \\ &= \sum_{i=1}^n c_i \log \frac{1}{\sqrt{2\pi\sigma_i^2}} - \sum_{i=1}^n \frac{c_i}{2\sigma_i^2} (y_i - \mathbf{w}^T \tilde{\mathbf{x}}_i)^2 \end{aligned}$$

So we can simply let $c'_i = \frac{c_i}{2\sigma_i^2}$, turning the problem into the same weighted optimization problem as that we solved in a).

Denote

$$C' = \text{diag}(\frac{c_1}{2\sigma_1^2}, \dots, \frac{c_n}{2\sigma_n^2})$$

The maximum likelihood estimate will be

$$\begin{aligned}\hat{\beta} &= (\tilde{\mathbf{X}}^T C' \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}} C' \tilde{\mathbf{Y}} \\ \hat{b} &= \bar{y} - \beta^T \bar{\mathbf{x}}\end{aligned}$$

where

$$\bar{\mathbf{x}} = \frac{\sum_{i=1}^n \frac{c_i}{2\sigma_i^2} \mathbf{x}_i}{\sum_{i=1}^n \frac{c_i}{2\sigma_i^2}}, \quad \bar{y} = \frac{\sum_{i=1}^n \frac{c_i}{2\sigma_i^2} y_i}{\sum_{i=1}^n \frac{c_i}{2\sigma_i^2}}$$

Other notations are the same as those in problem a).

5) a) *Proof.* Given the constraints $t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1 - \xi_i$, $\xi_i \geq 0$, we can write it into

$$\begin{aligned}\xi_i &\geq 1 - t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b) \\ \xi_i &\geq 0\end{aligned}$$

Thus we can obtain

$$\xi \geq \max(0, 1 - t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b))$$

So the optimal solution of ξ_i should be

$$\xi_i = \max(0, 1 - t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b))$$

Therefore minimizing

$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i$$

is equivalent to minimizing

$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \max(0, 1 - t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b))$$

□

b) *Proof.* if $\xi_i^* > 0$, we can obtain

$$t^{(i)}((\mathbf{w}^*)^T \mathbf{x}^{(i)} + b^*) = 1 - \xi_i^*$$

Thus the distance from the training data $\mathbf{x}^{(i)}$ to the margin hyperplane

$$t^{(i)}((\mathbf{w}^*)^T \mathbf{x}^{(i)} + b^*) = 1$$

will be

$$distance = \frac{|t^{(i)}((\mathbf{w}^*)^T \mathbf{x}^{(i)} + b^*) - 1|}{\|\mathbf{w}^*\|} = \frac{1}{\|\mathbf{w}^*\|} \xi_i^*$$

Therefore, the distance is proportional to ξ_i^* .

□

c) When $C \rightarrow \infty$, to conduct the minimization, we will have

$$t^{(i)}((\mathbf{w})^T \mathbf{x}^{(i)} + b) < 0, \forall i$$

Thus the minimization problem becomes

$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{w}\|^2$$

which is equivalent to the hard-margin SVM optimization problem.

- d) (i) For soft-margin SVM, the best C is 0.30, and the test accuracy is 77.61%
(ii) In order to train a hard-margin SVM, we set C as $1e8$, getting a accuracy at 64.55%. From the result we can find that soft-margin SVM performs better than the hard-margin one. I guess is may cause by the reason that data points are so close that we can't find a hard-margin SVM to separate them very well.

Following is the implementation:

```
1 training_label = label(1:500, :);
2 training_data = diabetesscale(1:500, :);
3 test_label = label(501:768, :);
4 test_data = diabetesscale(501:768, :);
5
6 constant = linspace(0.1, 2, 20);
7 losses = [];
8
9 for i = 1 : 20
10     rng(42);
11     model = fitsvm(training_data, training_label, 'KernelFunction',
12                   'linear', 'KernelScale', 1, 'BoxConstraint', constant(i), '
13                   CrossVal', 'on', 'KFold', 5);
14     loss = kfoldLoss(model);
15     losses = [losses loss];
16 end
17 [value, idx] = min(losses);
18 best_c = constant(idx);
19 best_c_model = fitsvm(training_data, training_label, '
20                       KernelFunction', 'linear', 'KernelScale', 1, 'BoxConstraint',
21                       best_c);
22 pred = predict(best_c_model, test_data);
23 fprintf('Best C: %.2f\n', best_c);
24 fprintf('Soft-Margin SVM Test Accuracy: %.2f%%\n', sum(pred==
25               test_label) / 268 * 100);
26
27 hard_margin_model = fitsvm(training_data, training_label, '
28                             KernelFunction', 'linear', 'KernelScale', 1, 'BoxConstraint', 1
29                             e8);
30 pred = predict(hard_margin_model, test_data);
31 fprintf('Hard-Margin SVM Test Accuracy: %.2f%%\n', sum(pred==
32               test_label) / 268 * 100);
```