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Machine Learning Assignment 1
Linear Models & Kernel Methods

Submission deadline: October 26, 2024

1 Problem 1. Ridge Regression (10 points)

In a regression task, we have vectors $\mathbf{x} \in \mathbb{R}^D$, target values $y \in \mathbb{R}$ associated with them, and some model $f(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}$ to predict the target values for arbitrary vectors in $\mathbb{R}^D$.

Suppose we have a training dataset $\{\mathbf{\Phi}, \mathbf{t}\}$, where $\mathbf{\Phi} \in \mathbb{R}^{N \times D}$ is the design matrix in which each row is a feature vector $\phi(\mathbf{x})$ of a training point $\mathbf{x}$, and $\mathbf{t} \in \mathbb{R}^{N \times 1}$ is the vector with target values for the training points. N is the number of points in the training dataset, and D is the dimensionality of the feature space. Suppose that each entry in the last column of $\mathbf{\Phi}$ is equal to 1. Your task is to derive the closed form solution for the optimal parameters of a ridge regression model.

- State the equation of a ridge regression model and identify the model parameters
- State the equation for the loss function (mean squared error) with an ℓ_2 regularization weighted by λ
- State which condition should be met in order to find the model parameters
- Find the ideal model parameters under the proposed loss function.

Note: You can use $\|\cdot\|$ as the Euclidean norm of a vector; $\phi(\mathbf{x}_n)$ and t_n are the n-th rows of $\mathbf{\Phi}$ and $\mathbf{t}$ respectively.

2 Problem 2. Feature Engineering (10 points) and Basic Concepts (10 points)

Suppose you have the following set S of 2D points, $S_n = (x_n^{(1)}, x_n^{(2)})$.

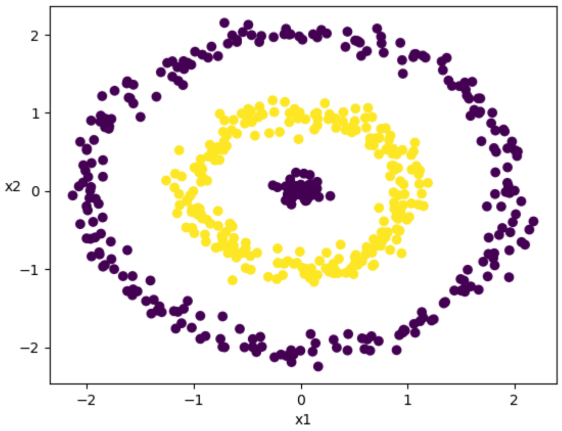

Figure 1: Color denotes the class attribution of a point: blue points belong to the class C_1, yellow points belong to the class C_2.

- Explain in detail 2 classification algorithms that could solve the problem. Discuss advantages and disadvantages of each.
- Propose new features for points in S based on $x^{(1)}$ and $x^{(2)}$. In this new feature space, classes C_1 and C_2 should be linearly separable. Come up with 2 different solutions meeting the stated criteria.

Problem 3. Kernel Functions (10 points)

Consider the following function $f : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$:

$$f(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{x})(\mathbf{x}^T\mathbf{y})(\mathbf{y}^T\mathbf{y})$$

Prove that f is a valid kernel or prove the opposite.

The only rules allowed to use without proof are the following:

- Kernel functions are *linear* and positive.
- Kernel functions can be expressed as an inner product
- A kernel function of 2 inputs can be expressed as another kernel of a transformation of those inputs (into a potentially different space).

Begin by formalizing those rules and apply them to prove or disprove the statement.

Problem 4. SVM (10 points)

Consider the following training data:

Class	x_1	x_2
$+$	1	1
$+$	2	2
$+$	0	2
$-$	1	-1
$-$	-1	0
$-$	0	0

1. Plot the six training points. Are the classes $\{+, -\}$ linearly separable?
2. Construct the weight vector of the maximum margin hyperplane by inspection and identify the support vectors.
3. If you remove one of the support vectors, does the size of the optimal margin decrease, stay the same, or increase?
4. Is your answer to (3) also true for any dataset? Provide a counterexample or give a short proof.

1 Problem 1. Ridge Regression (10 points)

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a • State the equation of a ridge regression model and identify the model parameters

b • State the equation for the loss function (mean squared error) with an ℓ_2 regularization weighted by λ

c • State which condition should be met in order to find the model parameters

d • Find the ideal model parameters under the proposed loss function.

Note: You can use $\|\cdot\|$ as the Euclidean norm of a vector; $\phi(\mathbf{x}_n)$ and t_n are the n-th rows of $\boldsymbol{\Phi}$ and $\mathbf{t}$ respectively.

$$\phi^{N\times D} = \begin{pmatrix} \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_D(x_1) & 1 \\ \vdots & \vdots & & & 1 \\ & & & & 1 \\ & & & & 1 \\ \phi_0(x_N) & \phi_1(x_N) & \cdots & \phi_D(x_N) & 1 \\ & & & & 1 \end{pmatrix} \qquad t^{N\times 1} = \begin{pmatrix} t_1 \\ \vdots \\ t_N \end{pmatrix}$$

$$x^{D\times 1} = \begin{pmatrix} x_1 \\ \vdots \\ x_D \end{pmatrix}$$

$$w^{D\times 1} = \begin{pmatrix} w_1 \\ \vdots \\ w_D \end{pmatrix}$$

a) Ridge regression model

$\hat{y}$: predicted target values

Φ : design matrix

w : model parameters

$$\hat{y} = \Phi w$$

b) $E(w) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{2} \left(w^T \phi(x_n) - t_n \right)^2$ MSE

MSE loss function with ℓ_2 reg. term.:

$$L(w) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{2} \left(w^T \phi(x_n) - t_n \right)^2 + \frac{\lambda}{2} \|w\|_2^2$$

c) Condition to find the model parameters:

$$\frac{\partial L(w)}{\partial w} = 0$$

d) optimal parameters

$$L(w) = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{2}\left(w^T\phi(x_n) - t_n\right)^2 + \frac{\lambda}{2}\|w\|_2^2$$

$$\frac{\partial L}{\partial w} = \frac{1}{N}\sum_{n=1}^{N}\left(\frac{1}{2}\cdot 2\left(w^T\phi(x_n) - t_n\right)\cdot\phi_j(x_n)\right) + \lambda w$$

$$= \frac{1}{N}\sum_{n=1}^{N}\left(w^T\phi(x_n) - t_n\right)\phi_j(x_n)) + \lambda w$$

$$= \frac{1}{N}\left(w^T\sum_{n=1}^{N}\phi(x_n)\phi^T(x_n) - \sum_{n=1}^{N} t_n\phi^T(x_n)\right) + \lambda w$$

$$= \frac{1}{N}\left(w^T\Phi^T\Phi - T^T\Phi\right) + \lambda w \overset{!}{=} 0$$

$$w^T \Phi^T \Phi + \lambda w = \tau^T \Phi$$

$$\Phi^T \Phi w + \lambda w = \Phi^T \tau$$

$$(\Phi^T \Phi + \lambda I) w = \Phi^T \tau$$

$$w_{min} = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T \tau$$

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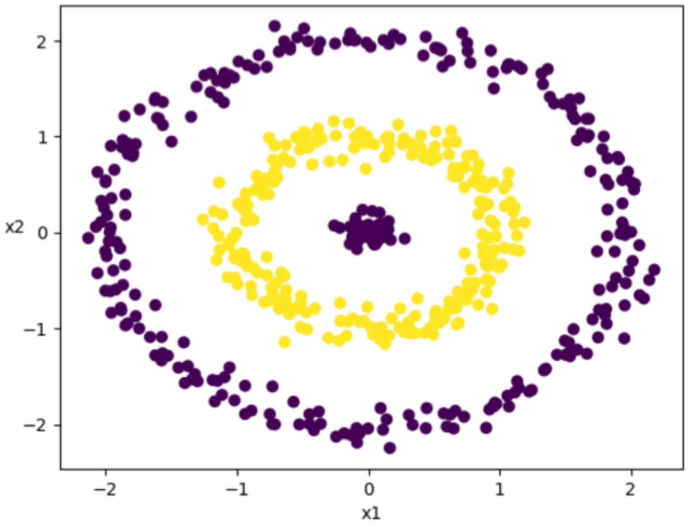

$z = x_1^2 + x_2^2$

Figure 1: Color denotes the class attribution of a point: blue points belong to the class C_1, yellow points belong to the class C_2.

a
- Explain in detail 2 classification algorithms that could solve the problem. Discuss advantages and disadvantages of each.

b
- Propose new features for points in S based on $x^{(1)}$ and $x^{(2)}$. In this new feature space, classes C_1 and C_2 should be linearly separable. Come up with 2 different solutions meeting the stated criteria.

a) non parametric KKN classifier:

this algorithm consider the closest k data points to determine by majority to which class the current data point has to be assigned.

KKN steps:

① set the number of k neighbors

② calculate distance of current point from all other points of the dataset

③ find the k nearest neighbors of the point

④ identify the class of the point by looking at the majority of the k nearest neighbors

advantages:

- no need to train the model
- non parametric, can easily adapt to non linearity
- no assumptions about data distribution

disadvantages:

- need to compute al distances / difficult to define a metric for closeness
- sensitive to outliers
- does not discover structure
- problematic in high dimensional space

Logistic regression

Logistic regression is a linear model used for binary classification. It works by modeling the relationship between the input features and the probability of a point to belong to a specific class.

This model uses a sigmoid function to convert the linear output into a probability (from 0 to 1). During training the algorithm adjust the weights w and the bias b to minimize the log loss function, which penalizes the incorrect predictions.

$$P(y=1|x) = \frac{1}{1+e^{-(w^T x + b)}}$$

advantages:

- training quick and less computing power needed
- probabilistic output useful for confidence level

disadvantages

- not suitable for this case: the classes are not linearly separable unless we introduce non linearity with the features

- sensitive to outliers
- no closed form to compute w and b

b) "Circle" feature introduction

$$z = \sqrt{(x^{(1)})^2 + (x^{(2)})^2}$$

this will introduce a circle/ring based feature and open to non linearity in the model. The decision boundary will follow a circle shape classifing better the points.

New polynomial feature

$$z_1 = (x^{(1)})^2 + (x^{(2)})^2 \qquad z_2 = x^{(1)} \cdot x^{(2)}$$

z_1 introduces the squared radial distance from the origin that combined with z_2 can imitate the ring behaviour of the distribution of the data

$g(x) = (\|x\|^2, x)$

Problem 3. Kernel Functions (10 points)

Consider the following function $f : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$:

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Prove that f is a valid kernel or prove the opposite.

The only rules allowed to use without proof are the following:

a) • Kernel functions are *linear* and positive.

b) • Kernel functions can be expressed as an inner product

c) • A kernel function of 2 inputs can be expressed as another kernel of a transformation of those inputs (into a potentially different space).

Begin by formalizing those rules and apply them to prove or disprove the statement.

a) $k(x,y) = ck_1(x,y)$ $\quad c > 0$

$k(x,y) = k_1(x,y) + k_2(x,y)$

b) $k(x,y) = \phi(x)^T \phi(y)$ $\quad \phi(x), \phi(y)$ transformed feature vectors

c) $k'(x,y) = k(g(x), g(y))$ $\quad g$ transformation function to a new space

To prove that f is a valid kernel we need to show that f is symmetric, positive semi-definite and that it can be expressed as an inner product.

① Symmetric

$$f(x,y) \overset{?}{=} f(y,x)$$

$$(x^Tx)(x^Ty)(y^Ty) \overset{?}{=} (y^Ty)(y^Tx)(x^Tx)$$

yes, since $y^Tx = x^Ty$

② positive semi-definite

for any vector $c \in \mathbb{R}$ $c^TKc \geq 0$ must be satisfied. k is the kernel matrix

let's take $x_1 = \begin{bmatrix}1\\0\end{bmatrix}$ $x_2 = \begin{bmatrix}0\\1\end{bmatrix}$

$$f(x_1,x_2) = (1+0)(0+0)(0+1) = 0 = f(x_2,x_1)$$

$$f(x_2,x_2) = 1\cdot1\cdot1 = 1$$

$$f(x_1,x_1) = 1\cdot1\cdot1 = 1$$

$$k = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} \qquad c = \begin{bmatrix}1\\-2\end{bmatrix}$$

$$c^T \quad k \quad c \quad \overset{?}{\geq} 0$$

$$\begin{bmatrix} 1 & -2 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix} =$$

$$= \begin{bmatrix} -2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -2 \end{bmatrix} = -2 - 2 = \boxed{-4} < 0 \; ! \; ↯$$

$\Rightarrow$ f is not a valid Kernel.

③ express f as a innerproduct:

there is no way to define f as a inner product $\phi(x)^T \phi(y)$

$$f(x,y) = ||x||^2 \, \phi(x)^T \phi(y) \, ||y||^2$$

$||x||^2$ and $||y||^2$ introduce non linearity.

Furthermore:

- it doesnt exist any linear combination of valid kernel able to create f since it is a non linear combination of inner products.

- we could express f with $g(x) = (\|x\|^2, x)$ s.t.

$$f(x, y) = k'(g(x), g(y))$$

but k' with g doesn't preserve its linearity ex4 ass 1

Task 1 Plot the six training points

0.1 Task 1: Plot the six training points

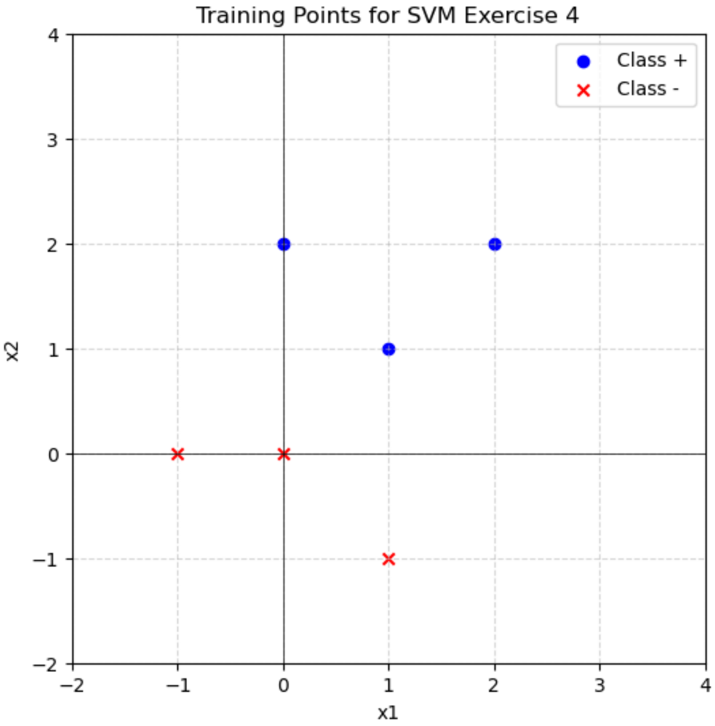

Figure 1:

Task 1 Are the classes linearly separable?

By observing the plot it looks like the two classes are linearly separable

Task 2: Construct the weight vector of the maximum margin hyperplane by inspection and identify the support vectors.

$$\mathbf{w}^T\phi + w_0 = 0$$

where
$\mathbf{w}$ is the weight vector (normal to the Hyperplane)
w_0 is the bias term
ϕ is a point in the feature space
Hyperplane's equation

$$\mathbf{w}^T\phi + w_0 = 0$$

where:
$\mathbf{w}$ is the weight vector (normal to the Hyperplane)
w_0 is the bias term
ϕ is a point in the feature space

$$|y(\phi)| = |\mathbf{w}^T\phi + w_0| \geq 1,$$

i.e.
Normalized equation

$$|y(\phi)| = |\mathbf{w}^T\phi + w_0| \geq 1,$$

i.e.

$$\begin{aligned} &\text{class + (blue):} \quad \text{if} \quad \mathbf{w}^T\phi + w_0 \geq 1 \\ &\text{class - (red):} \quad \text{if} \quad \mathbf{w}^T\phi + w_0 \leq -1 \end{aligned}$$

Let ϕ^- be the closest point on the "minus" margin, thus $\phi^- = (0, 0)$

$$\mathbf{w}^T\phi + w_0 = -1$$
$$\mathbf{w}^T(0, 0) + w_0 = -1$$
$$\Rightarrow w_0 = -1$$

Let ϕ^+ be the closest point on the "plus" margin, thus $\phi^+ = (1, 1)$

$$\mathbf{w}^T\phi + w_0 = 1$$
$$\mathbf{w}^T(1, 1) + w_0 = 1$$
$$\Rightarrow w_1 + w_2 + w_0 = 1$$

with $w_0 = -1$ and equal weights $\Rightarrow w_1 = 1$ and $w_2 = 1$

Then,$\phi^+ = \phi^- + \lambda\mathbf{w}$ for a scalar λ. Find $\lambda(1,1) = (0,0) + \lambda(1,1) \Rightarrow \lambda = 1$

Margin

$$M = ||w|| = 1\sqrt{(1)^2 + (1)^2} = \sqrt{2}$$

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Support Vectors

$$\phi^+ = \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix} \qquad \phi^- = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

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Weight vector of the maximum margin

$$w = \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix} \qquad w_0 = -1$$

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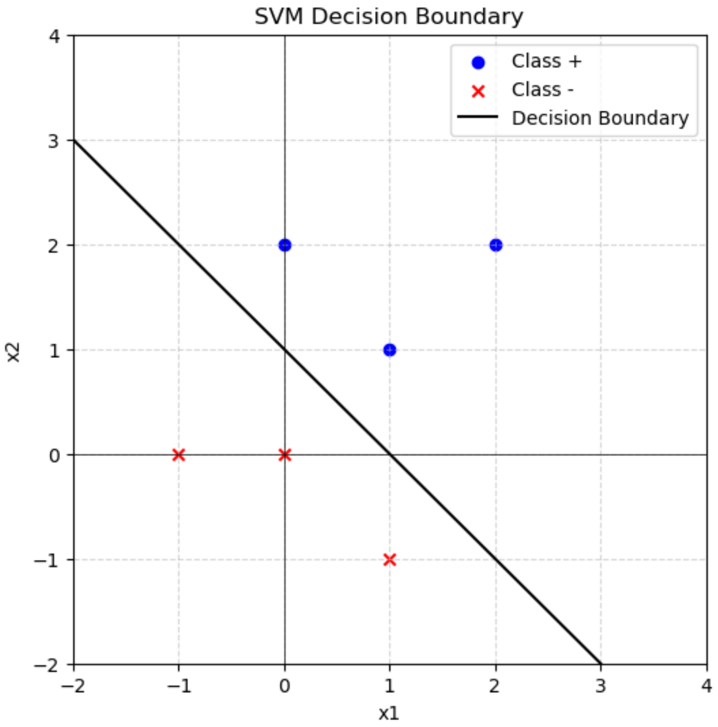

Figure 2:

Task 3 If you remove one of the support vectors, does the size of the optimal margin decrease, stay the same, or increase?

If I remove one support vector, the size of the optimal margin stays the same since there are in both classes other points that have the same distance from the hyperplane like our current support vectors. For example points $(0, 2)$ for class $+$ and $(1, -1)$ for class $-$.

Task 3: If you remove one of the support vectors, does the size of the optimal margin decrease, stay the same, or increase?

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Task 4 Is your answer to (3) also true for any dataset? Provide a counterexample or give a short proof.

No, my answer isn't true for any dataset.

Let's take the dataset from the task before and modify it such that there are no more the points (0,2) and (1,1). The Support Vectors are still the same as before

$$\phi^{+} = \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix} \qquad \phi^{-} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

Thus the weight vector and the optimal margin remain the same.

The new Data Set is:

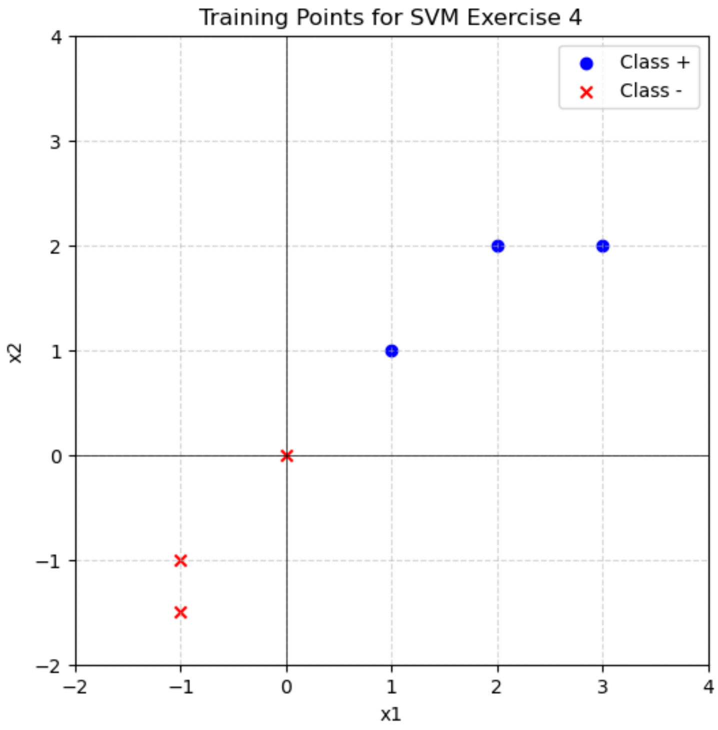

Figure 3:

Now we remove the Support Vectors:

$$\phi^{+} = \begin{bmatrix} \mathbf{1} \\ \mathbf{1} \end{bmatrix} \qquad \phi^{-} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

from the dataset and we recompute the maximum margin hyperplane.

By inspection we can observe that the closest point of the two classes are now (-1,-1) and (2,2)

Let ϕ^- be the closest point on the "minus" margin, thus $\phi^- = (-1, -1)$

$$\mathbf{w}^T\phi + w_0 = -1$$
$$\mathbf{w}^T(-1, -1) + w_0 = -1$$
$$\Rightarrow -w_1 - w_2 + w_0 = -1$$

Let ϕ^+ be the closest point on the "plus" margin, thus $\phi^+ = (2, 2)$

$$\mathbf{w}^T\phi + w_0 = 1$$
$$\mathbf{w}^T(2, 2) + w_0 = 1$$
$$\Rightarrow 2w_1 + 2w_2 + w_0 = 1$$

With two equations:

$$-w_1 - w_2 + w_0 = -1 \quad (1)$$

$$2w_1 + 2w_2 + w_0 = 1 \quad (2)$$

Solve: From (1):

$$w_0 = w_1 + w_2 - 1.$$

Substitute in (2):

$$2w_1 + 2w_2 + (w_1 + w_2 - 1) = 1$$

$$3w_1 + 3w_2 = 2$$

Assuming equal weights $w_1 = w_2$, substitute:

$$3w_1 + 3w_1 = 2 \Rightarrow 6w_1 = 2 \Rightarrow w_1 = \frac{1}{3}, w_2 = \frac{1}{3}$$

$$w_0 = \frac{1}{3} + \frac{1}{3} - 1 = -\frac{1}{3}$$

Recalculate Margin

Then,

$$\lambda = \frac{2}{w^T w}$$

Find λ

$$\lambda = \frac{2}{\begin{bmatrix} \frac{\mathbf{1}}{\mathbf{3}} & \frac{\mathbf{1}}{\mathbf{3}} \end{bmatrix} \begin{bmatrix} \frac{\mathbf{1}}{\mathbf{3}} \\ \frac{\mathbf{1}}{\mathbf{3}} \end{bmatrix}} \qquad \Rightarrow \lambda = \frac{2}{\frac{1}{9} + \frac{1}{9}} = \frac{2}{\frac{2}{9}} = 9.$$

Margin

$$M = ||\lambda \mathbf{w}|| = 9\sqrt{\left(\frac{1}{3}\right)^2 + \left(\frac{1}{3}\right)^2} = 9 * \frac{\sqrt{2}}{3} = 3\sqrt{2} \approx 4.24.$$

Support Vectors

$$\phi^+ = \begin{bmatrix} \mathbf{2} \\ \mathbf{2} \end{bmatrix} \qquad \phi^- = \begin{bmatrix} -\mathbf{1} \\ -\mathbf{1} \end{bmatrix}$$

Weight Vector of the Maximum Margin

$$\mathbf{w} = \begin{bmatrix} \frac{\mathbf{1}}{\mathbf{3}} \\ \frac{\mathbf{1}}{\mathbf{3}} \end{bmatrix} \qquad w_0 = -\frac{1}{3}$$

Conclusion: If before the margin was $\sqrt{2}$, now removing the old support vectors the margin has increased to 4.24 because there aren't any data points with the same distance between them as the ones before.