Statistical Methods for Machine Learning
Assignment 2: Basic Learning Algorithms

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1 Regression

1.1 Maximum Likelihood solution

Use linear model

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_D x_D$$

and for the D variables we let $\phi_i(\mathbf{x}) = x_i$ for $i = 1, \ldots, D$ and $\phi_0(\mathbf{x}) = 1$.

1.1.1 Selection 1

For our first selection S_1 our design matrix becomes a 200×5 matrix.

$$\mathbf{\Phi}_{S_1} = \begin{bmatrix} 1 & \mathbf{x}_{1,1} & \mathbf{x}_{1,2} & \mathbf{x}_{1,3} & \mathbf{x}_{1,4} \\ & & \vdots & & \\ 1 & \mathbf{x}_{i,1} & \mathbf{x}_{i,2} & \mathbf{x}_{i,3} & \mathbf{x}_{i,4} \\ & & \vdots & & \\ 1 & \mathbf{x}_{N,1} & \mathbf{x}_{N,2} & \mathbf{x}_{N,3} & \mathbf{x}_{N,4} \end{bmatrix}$$

where the notation $\mathbf{x}_{i,j}$ indicates the j'th entry in the i'th vector.

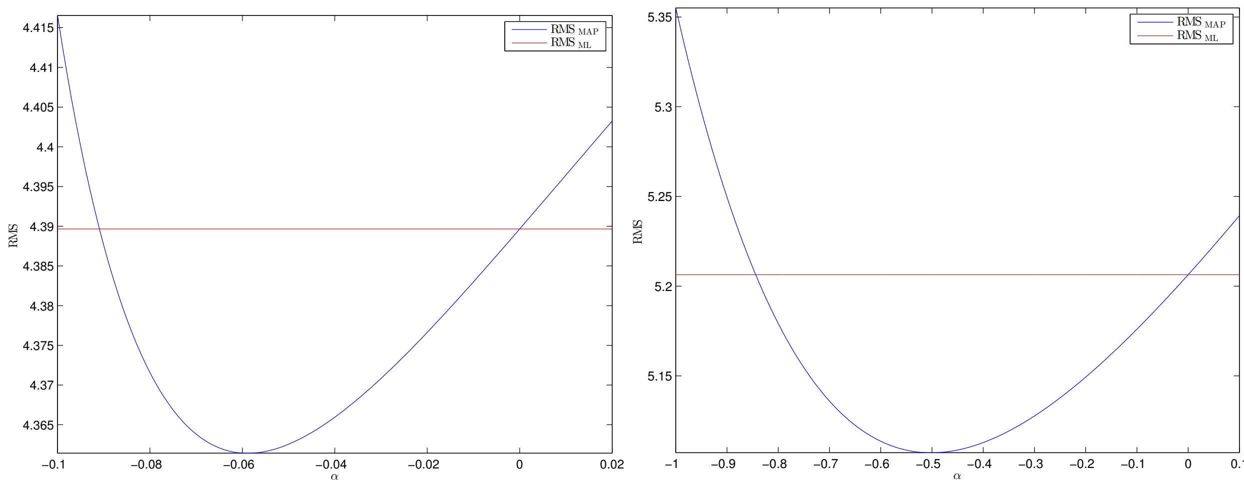
Finding the ML estimate of our parameters for S_1 gives

$$\mathbf{w}_{S_1} = \begin{bmatrix} -43.0947 \\ -0.1299 \\ 0.0352 \\ 0.9335 \\ -0.0433 \end{bmatrix} \quad \text{and} \quad \mathrm{RMS}_{S_1} = 4.3897$$

1.1.2 Selection 2

Our second selection S_2 consists only of the data from the 'Abdomen 2' column, giving a design matrix $\mathbf{\Phi}_{S_2}$ of dimensions 200×2. Training the model on the same training data yields:

$$\mathbf{w}_{S_2} = \begin{bmatrix} -37.4085 \\ 0.6133 \end{bmatrix} \quad \text{and} \quad \mathrm{RMS}_{S_2} = 5.2064$$



(a) (b)

Figure 1: Plot of RMS against varying values of α

1.1.3 Discussion

Just looking at the root mean square values of the two selections, it appears that S_1 performs better than S_2, but not by a lot. This suggests that either the variable ‘Abdomen 2’ is the most descriptive in terms of body, or that the linear model simply is a poor fit no matter how many variables we include. It could be a combination of the two.

It could probably be argued that the linear regression model is a poor predictor, but including more variables should improve the results.

1.2 Maximum a posteriori solution

In fig. 1 two plots are found of the root mean square values for varying values of α. In both plots we set $\beta = 1$. The RMS value of the ML solution is plotted as a straight line.

We can observe for both plots that when $\alpha = 0$, we obtain the same RMS error for the MAP estimate as for the ML solution. This is expected and demonstrates that when our prior precision parameters are set to zero, the MAP estimate becomes the ML estimate.

Fig. 1(a) is the plot for S_1, and it can be seen that the RMS_{MAP} error drops below the RMS_{ML} in the interval $[-0.091, 0]$. In fig. 1(b) the plot for S_2 similarly gives us that the RMS_{MAP} error is lower in the interval $[-0.844, 0]$.

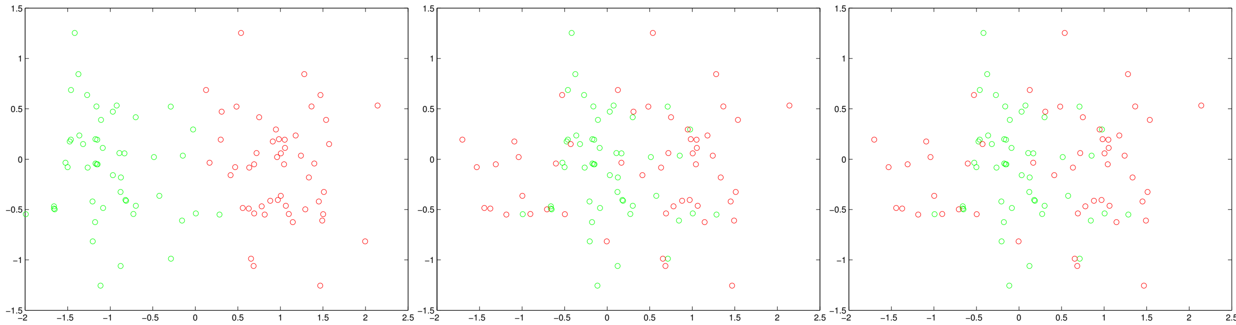
1.3 Theory

Verify result in equation (3.49) for the posterior distribution of the parameters $\mathbf{w}$ in the linear basis function in which $\mathbf{m}_N$ and $\mathbf{S}_N$ are defined

2 Linear Discriminant Analysis

Visualize the training data sets in three 2D plots.

Apply LDA to the training data, report accuracies of the classifier on the training as well as on the test sets. Explain the results. Discuss similarities and differences in performance on three data sets. Could a non-linear method do better?



(a) KNOLLA (b) KNOLLB (c) KNOLLC

Figure 2: Visualisation of the training data for each of the KNOLL problems

Implement LDA algorithm by hand.

3 Nearest Neighbor Classification

3.1 Nearest Neighbor Classification with Euclidian Metric

Implement k-NN. Train for all three KNOLL problems using training data sets. Report accuracy on corresponding sets for $k = 1, 2, 3, \ldots, 9$. Explain results; discuss similarities and differences in performance on the three data sets. Compare results to LDA results.

Hand in: classifier source code, results, short discussion.

3.2 Changing the Metric

To prove that d is a metric, given

$$d(\mathbf{x}, \mathbf{z}) = \|\mathbf{M}\mathbf{x} - \mathbf{M}\mathbf{z}\|, \text{ where } \mathbf{M} = \begin{pmatrix} 100 & 0 \\ 0 & 1 \end{pmatrix}$$

and $\|\cdot\|$ is the standard L_2-norm (in $\mathbb{R}^2$), we need to verify $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ that 1) $d(\mathbf{x}, \mathbf{y}) \geq 0$; 2) $d(\mathbf{x}, \mathbf{y}) = 0 \Leftrightarrow \mathbf{x} = \mathbf{y}$; 3) $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ (symmetry) and 4) $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^2 : d(\mathbf{x}, z) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$.

3.2.1 Revised proof — basic observations

We need only to observe that $\mathbf{M}$ is a projection $m : \mathbb{R}^2 \to \mathbb{R}^2$, i.e. onto $\mathbb{R}^2$ itself, given by $m(\mathbf{x}) = \mathbf{M}\mathbf{x}$. This immediately gives us all the properties we need, because L_2 is itself a (complete) metric on $\mathbb{R}^2$.

For instance, if we let $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^2$ and $\mathbf{x'}, \mathbf{y'}, \mathbf{z'}$ be the result of applying m on $\mathbf{x}, \mathbf{y}, \mathbf{z}$ respectively, we can prove the triangle inequality:

$$\begin{aligned} d(\mathbf{x}, \mathbf{z}) &= \|\mathbf{M}\mathbf{x} - \mathbf{M}\mathbf{z}\| \\ &= \|\mathbf{M}\mathbf{x} - \mathbf{M}\mathbf{y} + \mathbf{M}\mathbf{y} - \mathbf{M}\mathbf{z}\| \\ &= \|(\mathbf{x'} - \mathbf{y'}) + (\mathbf{y'} - \mathbf{z'})\| \\ &\leq \|\mathbf{x'} - \mathbf{y'}\| + \|\mathbf{y'} - \mathbf{z'}\| \quad \text{(by property of } L_2 \text{ norm)} \\ &= d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}) \end{aligned} \tag{1}$$

3.2.2 Original proof — the long way

Let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$. As it is easier to consider the square of the L_2 norm, we will do so:

$$
\begin{aligned}
d(\mathbf{x}, \mathbf{y})^2 &= \left\| \begin{pmatrix} 100 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} 100 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \right\|^2 \\
&= \left\| \begin{pmatrix} 100(x_1 - y_1) \\ x_2 - y_2 \end{pmatrix} \right\|^2 \\
&= \begin{pmatrix} 100(x_1 - y_1) \\ x_2 - y_2 \end{pmatrix}^T \begin{pmatrix} 100(x_1 - y_1) \\ x_2 - y_2 \end{pmatrix} \\
&= (100(x_1 - y_1))^2 + (x_2 - y_2)^2. \qquad (2)
\end{aligned}
$$

From (2) we observe that $(x_1 - y_1)^2 \geq 0$ and similarly $(x_2 - y_2)^2 \geq 0$ for all values in $\mathbb{R}$, so our first criteria for a metric is fulfilled. We also observe that if $d(\mathbf{x}, \mathbf{y}) = 0$ it implies $x_1 - y_1 = 0$ and $x_2 - y_2 = 0$, which means that $x_1 = y_1$ and $x_2 = y_2$, thus d fulfills our second requirement for a metric.

Our requirement of symmetry requires a little more investigation. Proceeding from (2), we find

$$
\begin{aligned}
(100(x_1 - y_1))^2 + (x_2 - y_2)^2 &= 100^2(x_1^2 - 2x_1y_1 + y_1^2) + (x_2^2 - 2x_2y_2 + y_2^2) \\
&= 100^2(y_1^2 - 2y_1x_1 + x_1^2) + (y_2^2 - 2y_2x_2 + x_2^2) \\
&= (100(y_1 - x_1))^2 + (y_2 - x_2)^2 \\
&= d(\mathbf{y}, \mathbf{x})^2, \qquad (3)
\end{aligned}
$$

where (3) gives us $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ and therefore fulfills the symmetry requirement.

Our last requirement is the triangle inequality, i.e. $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}), \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^2$.

Let $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^2$.

$$
\begin{aligned}
d(\mathbf{x}, \mathbf{z}) &= \|\mathbf{Mx} - \mathbf{Mz}\| \qquad (4) \\
&= \|\mathbf{Mz} - \mathbf{My} + \mathbf{My} - \mathbf{Mz}\| \qquad (5) \\
&\leq \|\mathbf{Mz} - \mathbf{My}\| + \|\mathbf{My} - \mathbf{Mz}\| \qquad (6) \\
&= d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}) \qquad (7)
\end{aligned}
$$

3.2.3 Results

Use d as metric in k-NN classifier and apply to KNOLLC. Explain results.