6.867 Homework 2

Logistic Regression

1.1 Unregularized Logistic Regression

We started by implementing logistic regression with stochastic gradient descent and plotting the norm of the weight vector over time for both the unregularized ($\lambda = 0$) and L2 regularized ($\lambda=1$) objective.

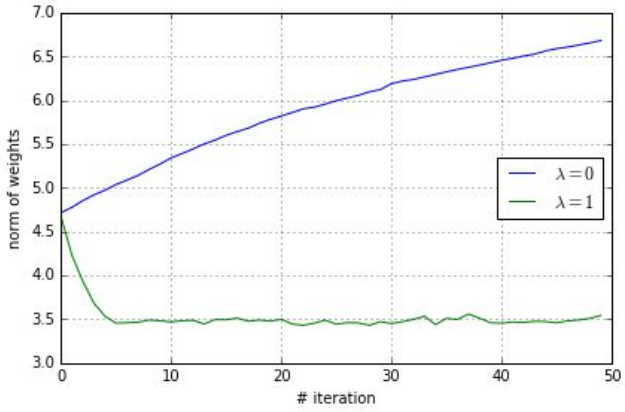


Figure 1. TODO: SOME DESCRIPTION.

As shown in Figure 1, the unregularized weight vector grows indefinitely while the regularized weight vector converges. This can be explained by the fact that larger magnitude weight vectors will result in more confident predictions, moving the prediction closer to 1.0 or 0.0 for positive and negative samples respectively.

Note, however, that a more confident predictor is not necessarily better. In fact, in many cases such as medical applications, a model that is both confident and incorrect is worse than a model that is uncertain on some inputs .

1.2 Hyperparameters for Logistic Regression

We examined each of the four datasets with various regularizers and λ values using the sklearn implementation of logistic regression. In our code, we explicitly adjust the intercept scaling so as not to regularize the bias term.

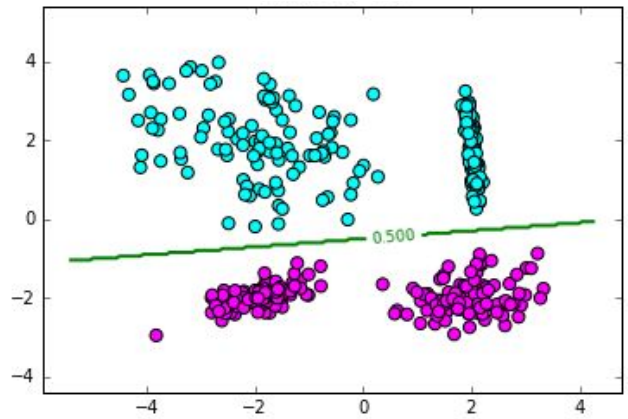


Figure 2. TODO: SOME DESCRIPTION.

The first dataset, shown in figure 2, is linearly separable and every combination of regularizer and λ between 0.0 and 20.0 produced a decision boundary which perfectly separated the two classes on the training, validation, and test set. As the λ constant increases, the norm of the weight vector shrinks.

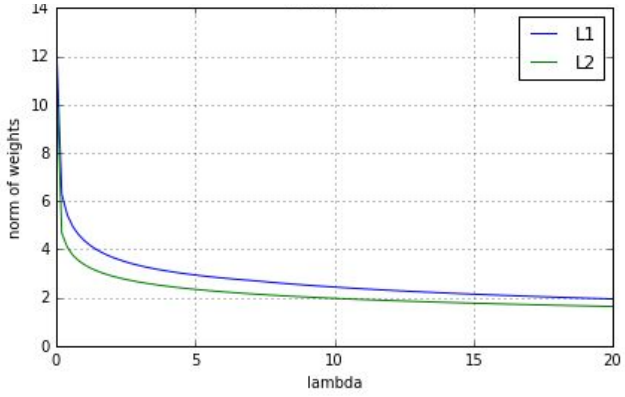


Figure 3. TODO: SOME DESCRIPTION .

On this particular dataset, we can completely ignore the first dimension of the input vector and still separate the two classes. This is reflected by the fact that with a large regularization constant, the L1 regularizer produces a sparse weight vector while the L2 regularizer produces a weight vector where the first dimension is near-zero.

The second dataset, however, is not linearly separable and there is no linear decision boundary capable of perfectly discriminating between positive and negative samples.

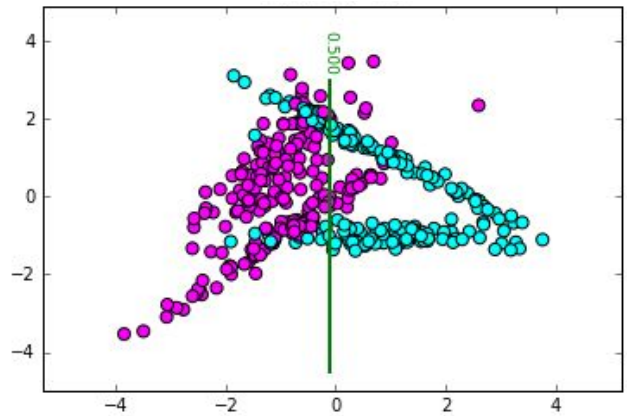


Figure 4. TODO: SOME DESCRIPTION.

As we increased λ, we observed that the norm of the weights behaved exactly like it did for the first dataset. On the other hand, the training and validation accuracy changed significantly as we adjusted λ and the regularizer.

A subset of the regularizer and λ values we examined is shown below in figure 5, where the bolded entry indicates a pair of values which minimizes the validation error.

L	λ	Train Error	Validation Error	Test Error
-	0	0.1700	0.1750	0.1950
L1	**1**	**0.1675**	**0.1750**	**0.1950**
L2	1	0.1675	0.1750	0.1950
L1	2	0.1700	0.1800	0.1900
L2	2	0.1650	0.1750	0.1950

Figure 5. TODO: SOME DESCRIPTION

The third dataset was nearly linearly separable. We determined that L2 regularization with a λ of 0.5 produced the smallest validation error.

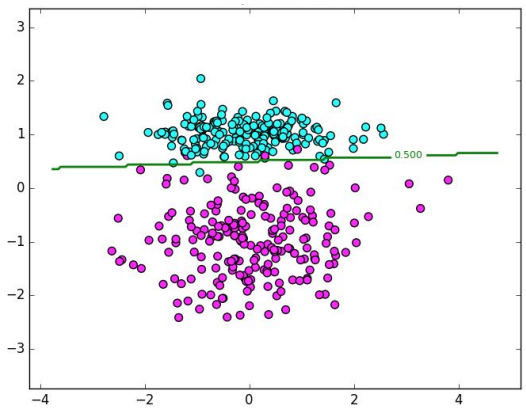


Figure 6. TODO: SOME DESCRIPTION.

L	λ	Train Error	Validation Error	Test Error
-	0	0.0125	0.035	0.050
L1	0.5	0.0200	0.030	0.045
L2	**0.5**	**0.0125**	**0.025**	**0.400**
L1	1	0.0175	0.035	0.045
L2	1	0.0225	0.030	0.030

Figure 7. TODO: SOME DESCRIPTION.

The fourth dataset reminiscent of the XOR problem and is not linearly separable. Any linear decision boundary is guaranteed to be wrong on half (or more) of the inputs.

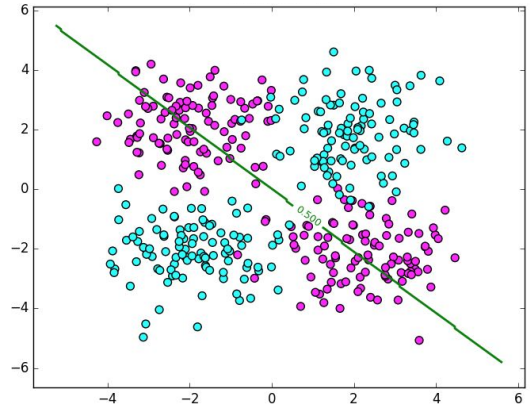


Figure 8. TODO: SOME DESCRIPTION.

L	λ	Train Error	Validation Error	Test Error
-	0	0.4850	0.5075	0.5025
L1	**1**	**0.4825**	**0.5025**	**0.5000**
L2	1	0.4850	0.5075	0.5025
L1	3	0.4825	0.5050	0.5000
L2	3	0.4850	0.5075	0.5025

Figure 9. TODO: SOME DESCRIPTION.

Support Vector Machine

We tested our support vector machine on a toy dataset consisting of (2, 2), (2, 3), (0, -1), and (-3, -2) with two positive and two negative examples. Our implementation produced the below objective function and constraints.

$$\min_\alpha \frac{1}{2} \begin{bmatrix}\alpha_0\\ \alpha_1\\ \alpha_2\\ \alpha_3\end{bmatrix}^T \begin{bmatrix}8 & 0.1 & 2.0 & 0.1\\ 0.1 & 0.13 & 3.0 & 0.12\\ 2.0 & 3.0 & 1.0 & 2.0\\ 0.1 & 0.12 & 2.0 & 0.13\end{bmatrix} \begin{bmatrix}\alpha_0\\ \alpha_1\\ \alpha_2\\ \alpha_3\end{bmatrix} - \begin{bmatrix}\alpha_0\\ \alpha_1\\ \alpha_2\\ \alpha_3\end{bmatrix}$$

$$s.t.\ 0 < \alpha_i < C,\ \sum_i alpha_i = 0$$

By solving this quadratic programming problem, we get the following decision boundary which only depends on two support vectors, (2,2) and (0, -1).

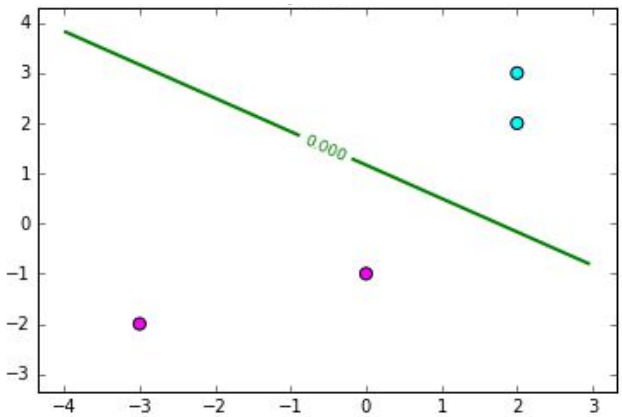


Figure 10. TODO: SOME DESCRIPTION.

Dataset 1

For the first dataset, we noted the various C values in the set {0.01, 0.1, 1, 10, 100} did not have a significant impact on the linear decision boundary; in fact, just like when applying logistic regression, every C value produced a boundary which perfectly separated the two classes.

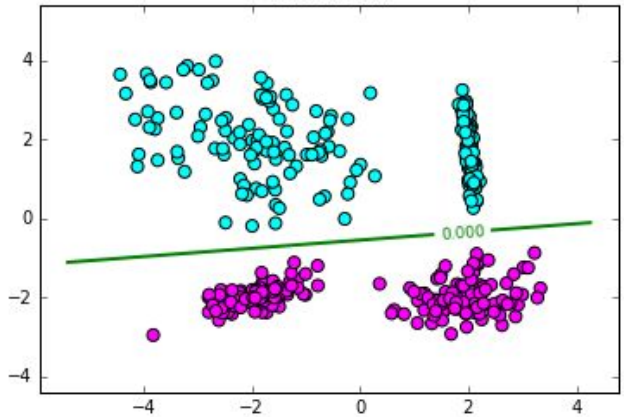


Figure 11. TODO: SOME DESCRIPTION.

When using the radial basis function kernel, we were able to achieve a reasonable decision boundary for all values of C in the above set. By increasing the bandwidth, we were able to produce decision boundaries that ranged from a nearly straight line (on the local scale) to a circular boundary which completely encircled one of the classes.

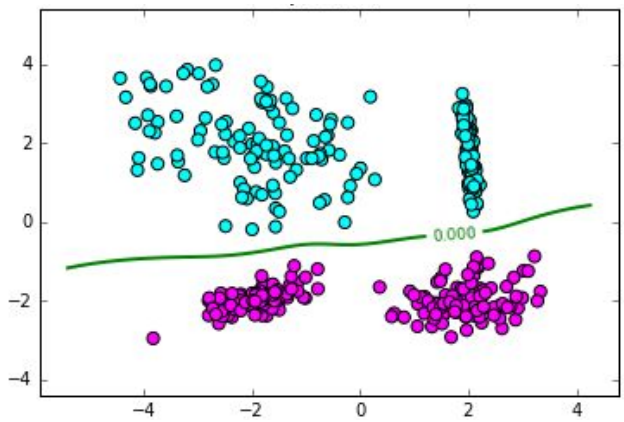


Figure 12. TODO: SOME DESCRIPTION.

We observed that for this particular dataset, increasing C led a decrease in both the geometric margin and number of support vectors. This can be explained by the fact that the C value controls the tradeoff between a wider margin and the number of mistakes. By increasing C, the support vector machine penalizes mistakes more heavily.

Dataset 2

The second dataset helped provide a better understanding of the relationship between the C value and the decision boundary. We started by establishing a baseline using the linear support vector machine, achieving error rates of 0.165 on the validation set and 0.19 on the test set.

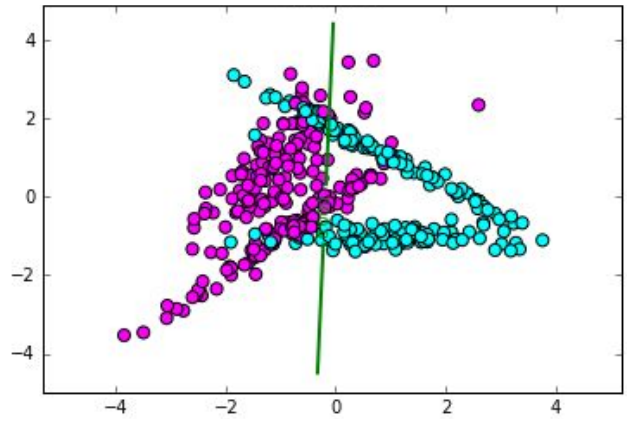


Figure 13. TODO: SOME DESCRIPTION.

For small values of C such as C = 0.01, we observed that the decision boundary was nearly linear, achieving similar accuracy rates. As we increased the C value to C = 10.0, we observed a decision boundary with validation error 0.099 and test error 0.045, significantly outperforming the linear support vector machine.

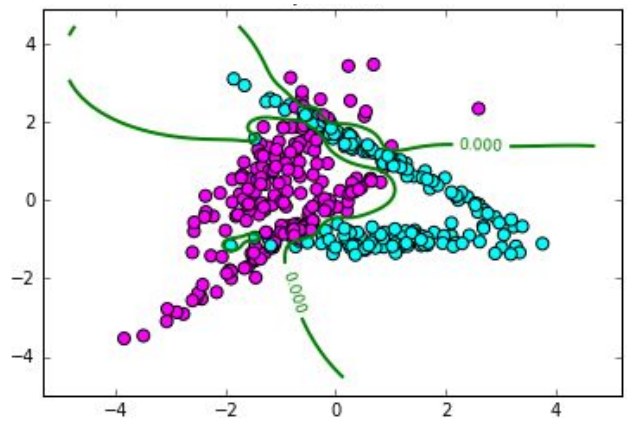


Figure 14. TODO: SOME DESCRIPTION.

Although our goal for this dataset was not to find the optimal decision boundary, we noted that choosing C values by maximizing the geometric margin on the training set is not as effective as using the validation set.

Dataset 3

The third dataset was slightly unusual as for certain combinations of C and bandwidth values, the Gaussian kernel was less effective than the linear kernel.

A visual inspection of the dataset gives some intuition about why this may be the case: the two classes are naturally separated by a linear boundary. Even if C is set to a small value to give the slack variables more room to maneuver, it is still at risk of overfitting to the data points which lie on the wrong side of the decision boundary.

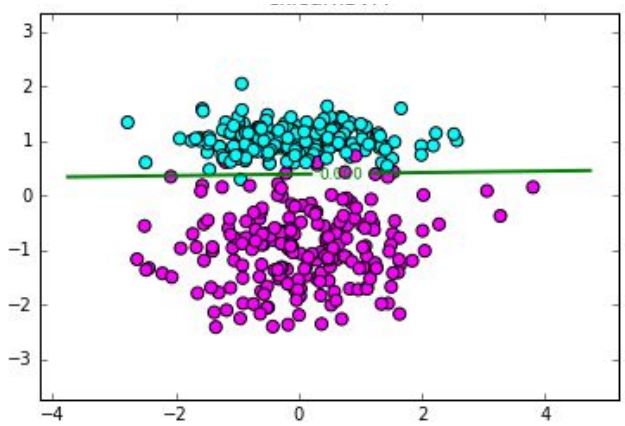


Figure 15. C=1.0, 0.035 validation error, 0.050 test error

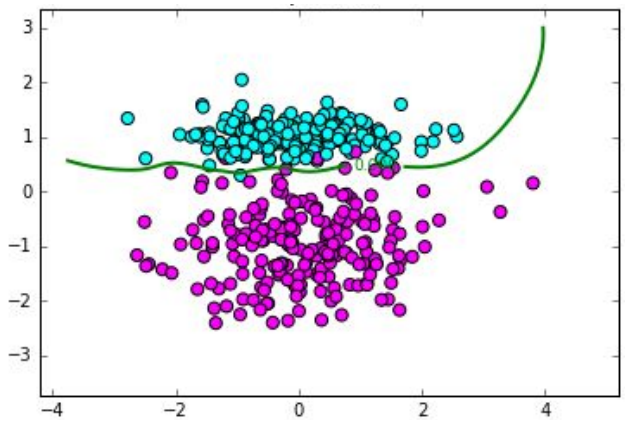


Figure 16. C=0.01, 0.045 validation error, 0.030 test error

Dataset 4

Unlike the third dataset, the fourth dataset requires a nonlinear kernel to produce a reasonable classifier. The linear support vector machine produces a model that is no better than to random guessing due to the linearly inseparable nature of the dataset.

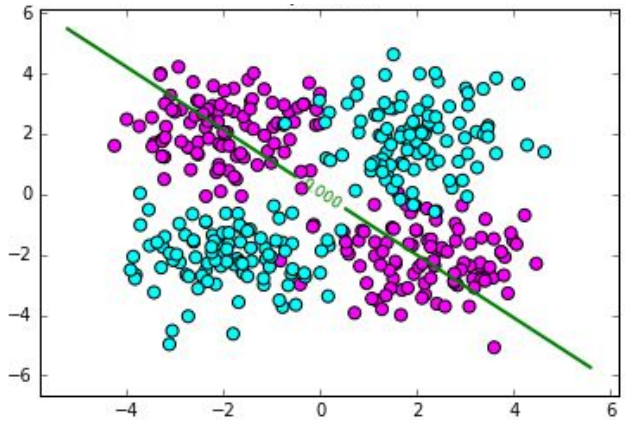


Figure 17. C=1.0, 0.52 validation error, 0.51 test error

By introducing the Gaussian RBF kernel, the model improves dramatically, correctly classifying over 95% of the test data.

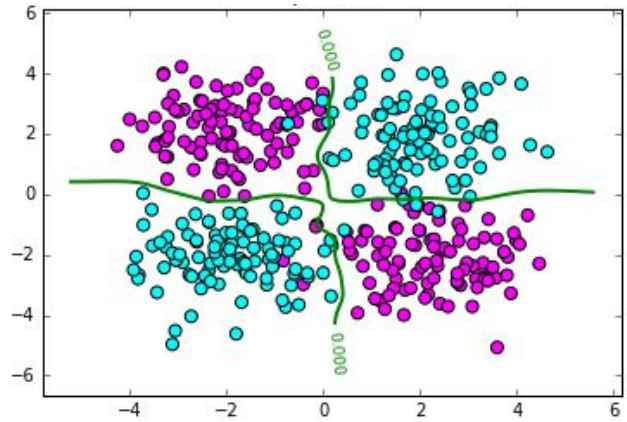


Figure 18. C=1.0, 0.05 validation error, 0.045 test error

Hyperparameters

Based on our observations, we believe that in most cases, as C increases, the number of support vectors increases while the geometric margin decreases. This is not true in all cases, but in most cases, heavily penalizing the slack variables should result in a larger weight vector and therefore produce a smaller geometric margin.

In addition, we conclude that maximizing the geometric margin is not an appropriate method for selecting C as it is easy to overfit to the training data, especially when using a RBF kernel. It is always better to use a validation set to tune hyperparameters; if the dataset is too small to be split into training, testing, and validation sets, leave-one-out cross-validation is another good alternative.

Pegasos

To try and get better performance on large datasets, we implemented the Pegasos algorithm for training support vector machines. Unlike our quadratic programming SVM implementation, the Pegasos implementation does not use C to penalize slack variables; instead, this implementation uses the λ regularization constant which is inversely proportional to C.

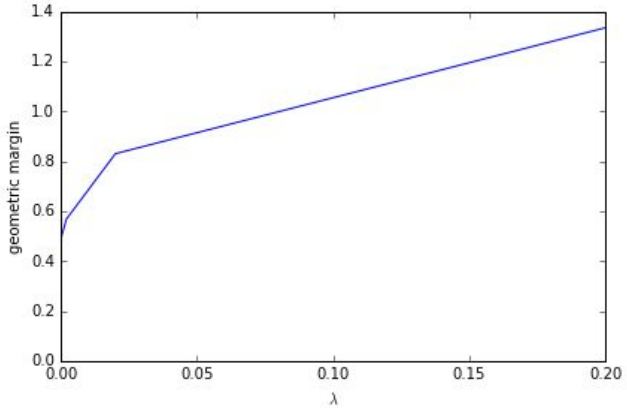


Figure 19. As λ increases, so does the margin.

We observed that as we increased the regularization constant, our model produced smaller weights which resulted in a larger geometric margin. This is consistent with both our understanding of the objective function and our assertion that λ and C are inversely proportional.

Kernels

We extended our Pegasos implementation to accept kernel functions using the below objective function. Unfortunately, this formulation does not have the same sparsity properties as the dual SVM.

$$\min_w \frac{\lambda}{2}\|w\|^2 + \frac{1}{n}\sum_i max\{0, 1 - y_i(w^T\phi(x_i))\}$$

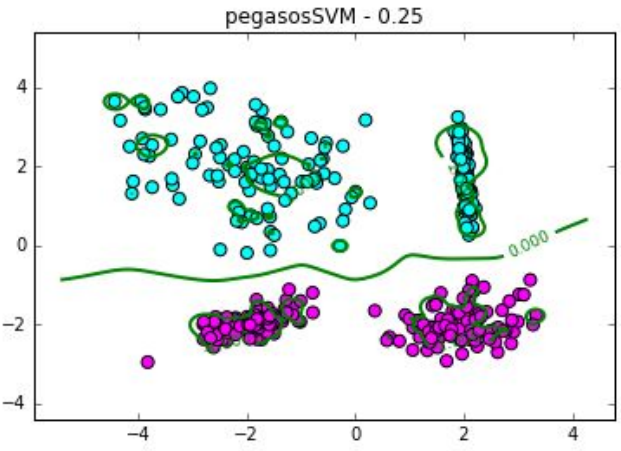
Although this formulation appears to require explicitly computing the feature vector mapping using φ, the training algorithm only requires the kernel operator. Based on this formulation of the objective function, we should use the following prediction rule.

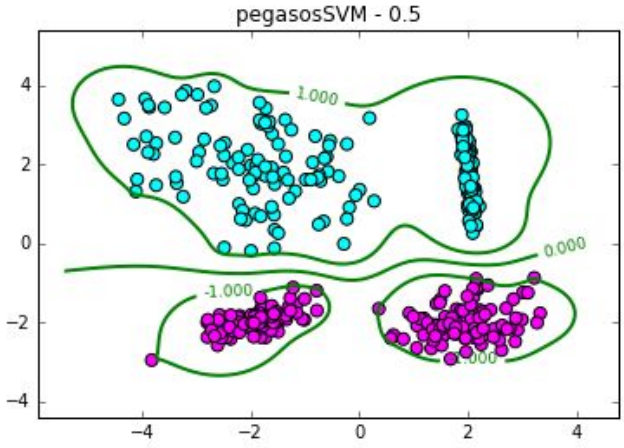
$$sign(\sum_i \alpha_i K(x, x_i))$$

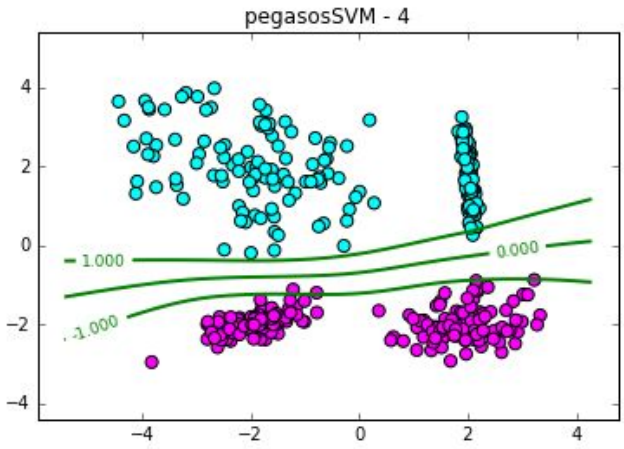
Bandwidth

The relationship between the bandwidth of the Gaussian kernel (γ) and the resulting decision boundary is consistent between the QP and Pegasos algorithms. Smaller bandwidths produced uneven boundaries while larger bandwidths produced smooth boundaries.

As we increased the bandwidth from 2^-2 to 2^2, we observed that the number of support vectors initially decreases before increasing after after γ=1.

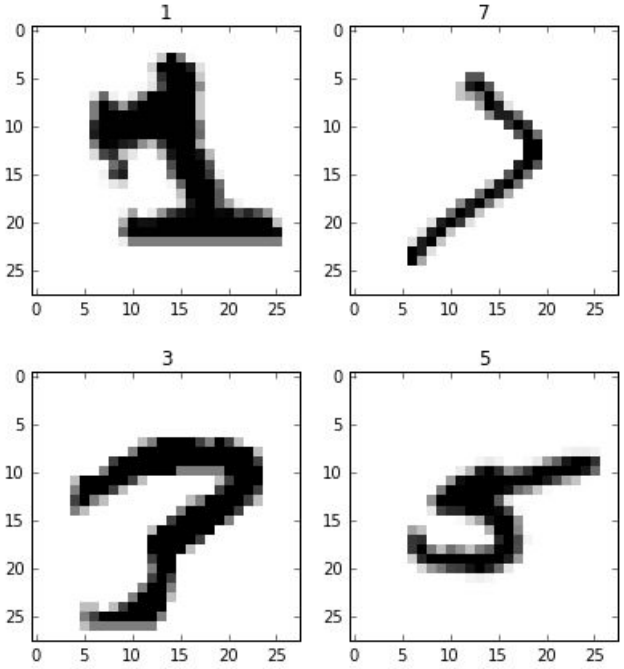


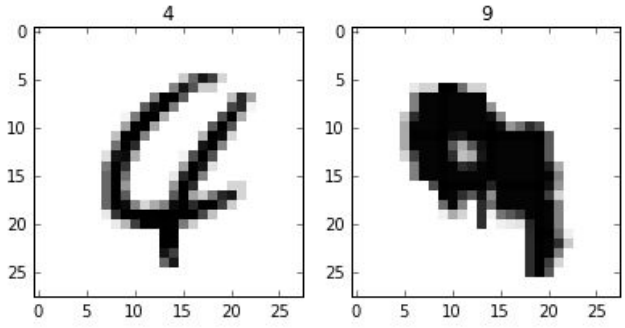




MNIST

Examples that are misclassified by the linear support vector machine.





With a large enough bandwidth, the radial basis function kernel outperformed the linear support vector machine.