1 Exercise 1: SVM

In the general case of solving a linear SVM with slack variables without a regularizer, the objective function is:

$$
\begin{aligned}
\underset{\alpha}{\text{minimize}} \quad & -\sum_{i=1}^{n} \alpha_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (x^{(i)} \cdot x^{(j)}) && \text{(1a)} \\
\text{subject to} \quad & 0 \le \alpha_i \le C \quad \forall i\,, && \text{(1b)} \\
& \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 && \text{(1c)}
\end{aligned}
$$

Using the Python CVXOPT package, the general form of the objective function is:

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & \frac{1}{2} x^T P x + q^T x && \text{(2a)} \\
\text{subject to} \quad & Gx \le h && \text{(2b)} \\
& Ax = b && \text{(2c)}
\end{aligned}
$$

The general form for converting our slack variable objective function in Equation 1 to the CVXOPT objective function in Equation 2 is described in Table 1.

CVXOPT	Conversion from Equation 1
x	If there are n points in the training set, an $n \times 1$ vector equal to the values of x in the training data
P	An $n \times n$ matrix which is the kernel matrix between all pairs of training data x weighted by the corresponding value of y from the training data
q	An $n \times 1$ vector of -1s
G	A $2n \times n$ matrix where the top $n \times n$ is the identity matrix and the bottom $n \times n$ is the negative identity matrix
h	A $2n \times 1$ vector with the top $n \times 1$ vector of Cs and the bottom $n \times 1$ vector of 0s
A	An $1 \times n$ vectors with elements $y^{(i)}$ from the training set for all values of i
b	An 1×1 vector of 0s

Table 1: Conversion rule for deriving CVXOPT constraints

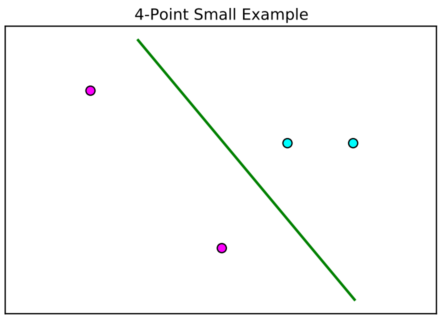
For the small example with $(1, 2), (2, 2)$ as positive examples and $(0, 0), (-2, 3)$ as negative examples, the constraints from CVXOPT as written above are written in Equation 3.

$$P = \begin{bmatrix} 5 & 6 & 0 & -4 \\ 6 & 8 & 0 & -2 \\ 0 & 0 & 0 & 0 \\ -4 & -2 & 0 & 13 \end{bmatrix} \qquad q = \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

$$G = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \qquad h = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 1 & -1 & -1 \end{bmatrix} \qquad b = \begin{bmatrix} 0 \end{bmatrix}$$

The decision boundary generated by the SVM code for the small example is shown in Figure 1a.



(a) Decision boundary for 4 points using CVXOPT and SVM with slack variables

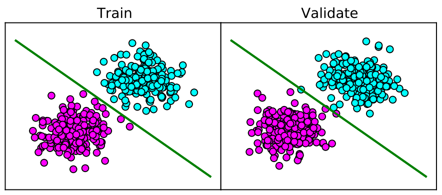
Dataset	Kernel	Training	Validation
smallOverlap	Linear	.24	.24
smallOverlap	Gaussian $\beta = 0.1$	.26	.25
smalloverlap	Gaussian $\beta = 1$	.26	.25
bigoverlap	linear	.305	.255
bigoverlap	Gaussian $\beta = 0.1$	.3	.255
bigoverlap	Gaussian $\beta = 1$	.3	.255
ls	linear	0	0.00375
ls	Gaussian $\beta = 0.1$	0.0625	0.0775
ls	Gaussian $\beta = 1$	0.0625	0.0775
nonsep2	linear	.485	.495
nonsep2	Gaussian $\beta = 0.1$	.48	.4975
nonsep2	Gaussian $\beta = 1$	.48	.4975
stdev1	Gaussian $\beta = 0.5$	0	.005
stdev1	Gaussian $\beta = 1$	0	.005

(b) Error rates for training and validation sets, $c = 1$, linear and Gaussian kernels

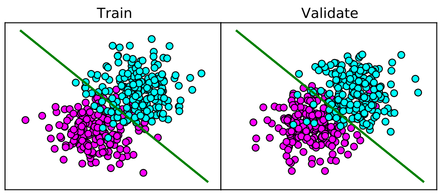
Setting $C = 1$, the error rates for the training and validation sets for different data sets and kernels is shown in Table 1b. If a data set did not come with a training / validation set pair, the dataset was randomly cut in half for each class to use as training and validation. In general, the more separable the data set is, the better the slack-variable SVM without a regularizer does. In the non-separable case, depending on the nature of the inseparability, the solution has a higher error rate.

Using a Gaussian kernel at different bandwidths does not change the error rates much unless the data is distributed with a Gaussian distribution, as shown in Table 1b.

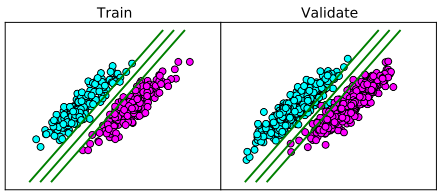
Extending the original Equation 1 to use kernels, the objective function becomes as written in Equation 4. Using the Gaussian kernel compared to the linear kernel is shown in Figures 4c and 4d.



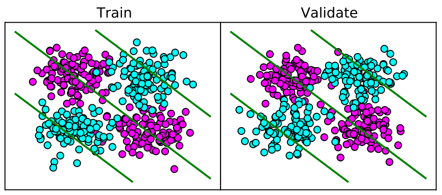
(a) stdev1



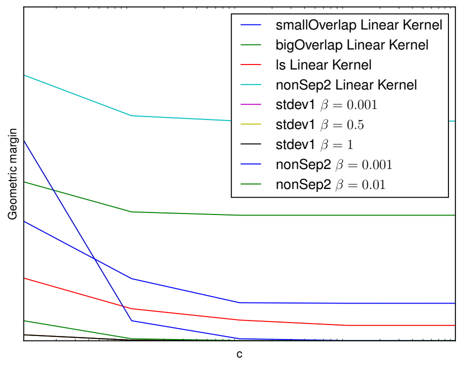
(b) stdev2



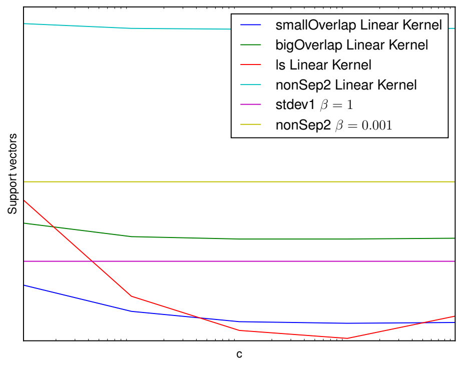
(c) ls



(d) nonSep2



(a) plot of the geometric margin as a function of c for various kernels and datasets



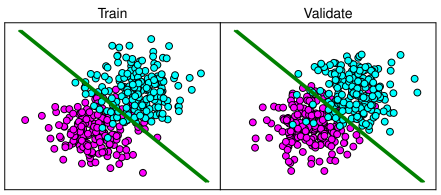
(b) plot of the number of support vectors as a function of c for various kernels and datasets

$$\underset{\alpha}{\text{minimize}} \quad -\sum_{i=1}^{n} \alpha_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} K(x^{(i)}, x^{(j)})) \tag{4a}$$

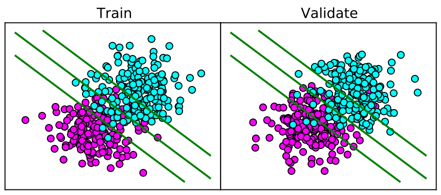
$$\text{subject to} \quad 0 \le \alpha_i \le C \quad \forall i\,, \tag{4b}$$

$$\sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \tag{4c}$$

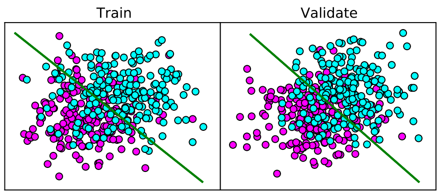
As c increases, the geometric margin decreases, as shown for various values of c, various kernels, and various datasets in figure 3a. this always happens as c increases, because this means there can be more slack in the final SVM, which means the SVM will be more tolerable to incorrect classifications for inseparable data. the number of support vectors first decreases, then increases as c increases, as shown in figure 3b. this means that the classifier is less overfit on the training data and will have smaller errors on the testing data. choosing c for maximizing the margin will yield a value of c equal to zero, which is the same as having a hard-margin SVM that does not perform well on non-separable data. an alternate criteria for choosing c could be the minimum number of support vectors (since the number of support vectors eventually increases with a higher value of c as the classifier gets over-fit to the training data). Changing c has almost no effect on the training error unless the data is highly non-separable.



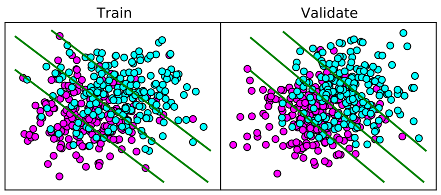
(a) stdev2 using a Gaussian Kernel



(b) stdev2 using a Linear Kernel, $c = 0.1$



(c) stdev4 using a Gaussian Kernel



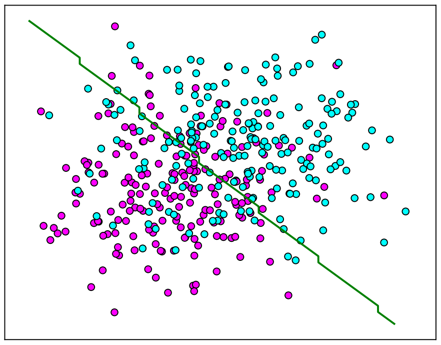
(d) stdev4 using a Linear Kernel, $c = 0.1$

2 Exercise 2: logistic regression

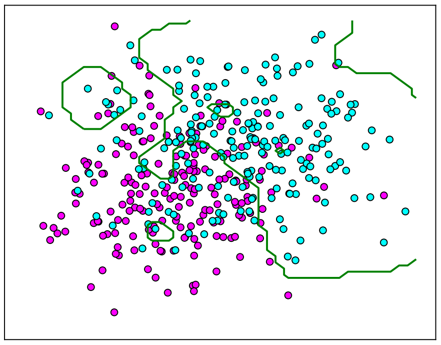
The kernelized form of the regression objective and the associated prediction function I used for logistic regression having all data with $y^{(i)} \in -1, 1$ is written in Equation 5. K is the kernel function, which in the linear case is $x^{(i')} \cdot x^{(i)}$. For accurate results, it was important to set the tolerance of the solver to $1e^{-12}$.

$$\text{NLL}(\alpha, w_0) = \sum_i \log\left(1 + e^{-y^{(i)}\left(\sum_{i'} \alpha_{i'} K(x^{(i')}, x^{(i)}) + w_0\right)}\right) \tag{5a}$$

$$y(x_t) = \text{sgn}\left(w_0 + \sum_i \alpha_i K(x^{(i)}, x_t)\right) \tag{5b}$$

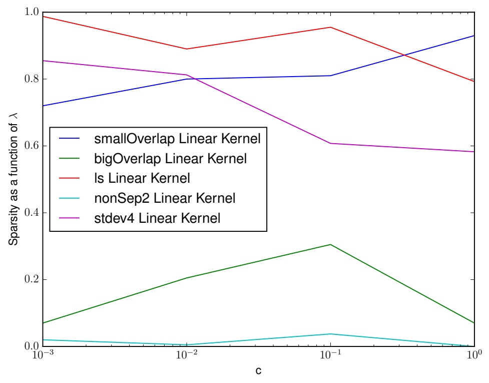


(a) Decision boundary on non-separable data for linear kernel. Error = .265

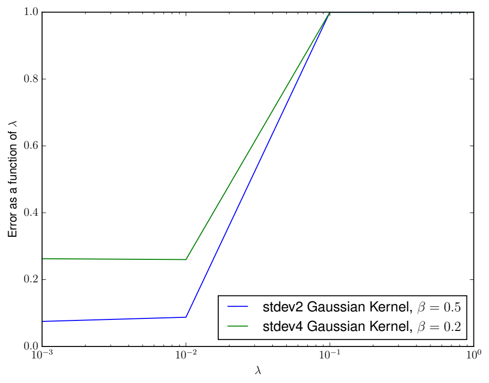


(b) Decision boundary on non-separable data for Gaussian kernel. Error = .2625

When comparing Gaussian kernels and linear kernels on the same dataset, Gaussian kernels perform much better on non-separable datasets. The decision boundaries on the same dataset (stdev4, which is highly non-separable) using a linear and a Gaussian kernel (with $\beta =$ chosen using the minimum training set error while holding $\lambda = 0$) is shown in Figures 5a and 5b. In this case the optimal value of β was 0.2 The corresponding error rates on the test set are .265 for the linear kernel and .2625 for the Gaussian kernel. When computing the Gaussian kernel, the maximum number of iterations of the minimization function was set to reduce computation time.



(a) Sparsity as a function of λ for the linear kernel



(b) Error as a function of λ and β for Gaussian kernels

Define sparsity as the percentage of points in the training data that are used as support vectors (with alpha values greater than $1e^{-5}$. Using L1 regularization with parameter λ on the α values to ensure sparsity, the relationship between λ and sparsity is shown in Figure 6a for various datasets for the linear kernel. In general, the sparsity follows a U-pattern, sometimes in two places, as λ increases. The optimal value of λ is the one that in the separable case makes the sparsity the lowest for the smallest value of λ. As λ gets too large, the error on the training and testing sets increases too much, so it is better to choose a smaller value of λ that allows for low training / testing error. In the non-separable case, the sparsity either follows a U-shape or decreases as λ increases.

The performance of the Gaussian kernel depends on choosing the optimal β. In general, the optimal β is the near the standard deviation of the distribution of the data. The effect of λ on performance once the optimal β is chosen is shown in Figure 6b. In general, the affect of λ on the error is a U-shape, and the optimal λ should be chosen to minimize the validation set error after the value of β has already been chosen.

Comparing SVMs to logistic regression in terms of sparsity, logistic regression tends to be more sparse than SVM, and the support vectors chosen in SVM dictate the boundary more strongly.

3 Exercise 3: Multiclass LR and SVM

3.1 Multiclass Logistic Regression

The form of the objective for kernelized multiclass logistic regression is the same as for the two-class case shown in Equation 5, except that the y values are $1 \times K$ vectors where K is the total number of classes. All the entries in y are 0 except for the entry that corresponds to the class that y belongs to, which is 1. So if $x^{(i)}$ were in class 3 out of a total of 5 classes, $y^{(i)}$ would take on the value $[0, 0, 1, 0, 0]$. The resulting prediction function was then modified as shown in Equation 6. So for each class c there is a separate set of α and w_0 values, and the class that is predicted is the class who's α and w_0 values maximize the objective function.

$$y = \underset{c}{\operatorname{argmax}} \left(w_0 + \sum_i \alpha_i^c K(x^{(i)}, x_t) \right) \tag{6a}$$

There were numerous problems in implementing logistic regression for multiclass, especially on running the Kaggle dataset. There were many features and many data points, so it was especially important not to have any operations involving for loops, doing everything with the optimized versions of Python's numpy / scipy library. Another trick I used was to use the logexpsum function from the scipy library to calculate the error in the objective function as needed. At all places possible, I used built-in functions in scipy and numpy to do any calculations rather than write it by hand. For most experiments with logistic regression, the regularization term was L1 regularization to keep the α values sparse. It was also important to always initialize the starting value of the minimization function to zeros rather than using numpy's built-in 'empty' function for creating arrays. This is because using the 'empty' function reuses empty places in memory (most likely taken by the coefficients from the previous run of the minimization), therefore causing the function to be stuck in a local minimum.

Experimenting on small subsets of Kaggle data with linear and Gaussian kernels, it was immediately clear that with a Gaussian kernel and a relatively small number of data points (approximately 10) and a Gaussian kernel, there can immediately be an error rate of 0.0 on the validation set. Therefore, for all larger experiments, only the Gaussian kernel was used when doing multiclass logistic regression.

In about 20-30 minutes of run time, I used all 54 features and 40 training samples from each class for a training and validation set, randomly selected without replacement. I used the training set to choose the optimal value of β while holding $\lambda = 0$, then I used the validation set to choose the optimum value of λ, and finally tested on the rest of the un-chosen values of the dataset. After a few runs, the results were that the best β value was $\beta = 2$ and the best λ was $\lambda = 0.001$ for an error rate of .83 on the entire dataset.

3.2 Multiclass SVM

For multiclass SVM, it was also critical not to use any for loops or unnecessary mathematical operations. Using the one-versus-rest approach in which K separate SVMs of the form written in Equation 1 are trained and optimized where the kth SVM is trained from class C_k as positive examples and the rest of the classes as negative examples. The predictor is then of the form written in Equation 7.

$$y = \underset{c}{\mathrm{argmax}} y_k(x) \tag{7a}$$

Because my implementation was a little bit too slow for testing in a reasonable amount of time, the 'sklearn' Python package was used to perform SVM on the entire Kaggle Forest dataset. One major drawback of using this package the super-fast package did not implement Gaussian kernels, so the results given here are using linear kernels. Using hinge loss and L2 regularization, the optimal value for λ was 0.01 and the test error was .261 on the entire dataset. Using squared loss and L1 regularization, the optimal λ was $1e^{-7}$ and the test error was .143.