1 Exercise 1: SVM

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

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

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

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

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

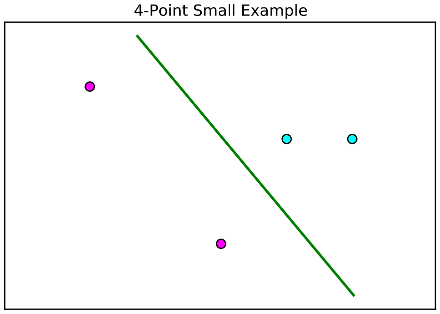
For the small example with $(1, 2), (2, 2)$ as positive examples and $(0, 0), (-2, 3)$ as negative examples, the constraints from CVXOPT as written above are written in Equation 3.

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

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

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

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

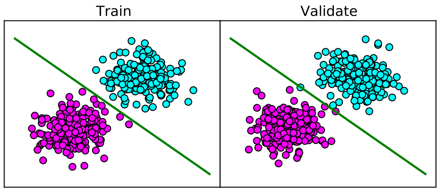
Dataset	Kernel	Training	Validation
smallOverlap	Linear	.24	.24
smallOverlap	Gaussian $\beta = 0.1$	.26	.25
smalloverlap	Gaussian $\beta = 1$	.26	.25
bigoverlap	linear	.305	.255
bigoverlap	Gaussian $\beta = 0.1$	.3	.255
bigoverlap	Gaussian $\beta = 1$	.3	.255
ls	linear	0	0.00375
ls	Gaussian $\beta = 0.1$	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

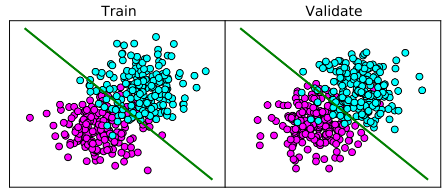
Setting $C = 1$, the error rates for the training and validation sets for different data sets and kernels is shown in Table 1b. If a data set did not come with a training / validation set pair, the dataset was randomly cut in half for each class to use as training and validation. In general, the more 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.

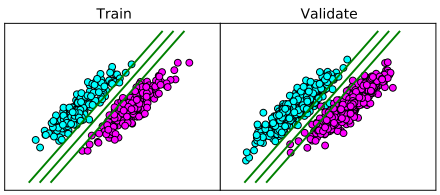
As c increases, the geometric margin decreases, as shown for various values of c, various kernels, and various datasets in figure 3a. this always happens as c increases, because this means there can be more slack in the final svm, which means the svm will be more tolerable to incorrect classifications 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.



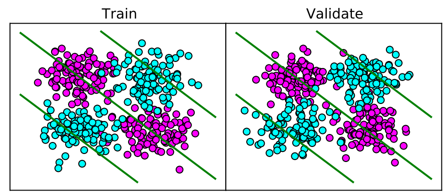
(a) stdev1



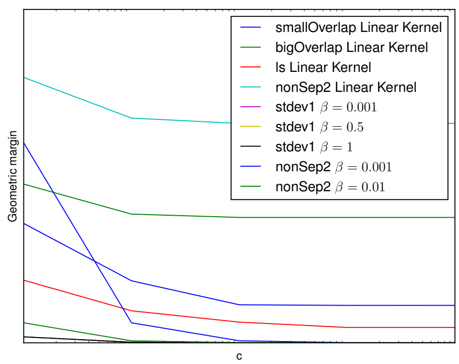
(b) stdev2



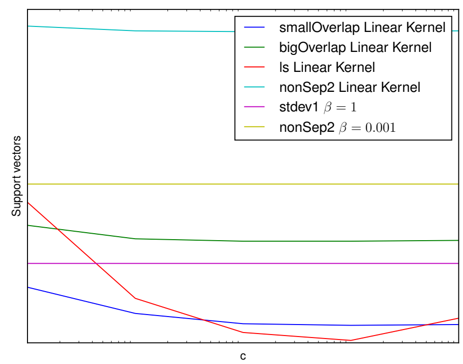
(c) ls



(d) nonSep2



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



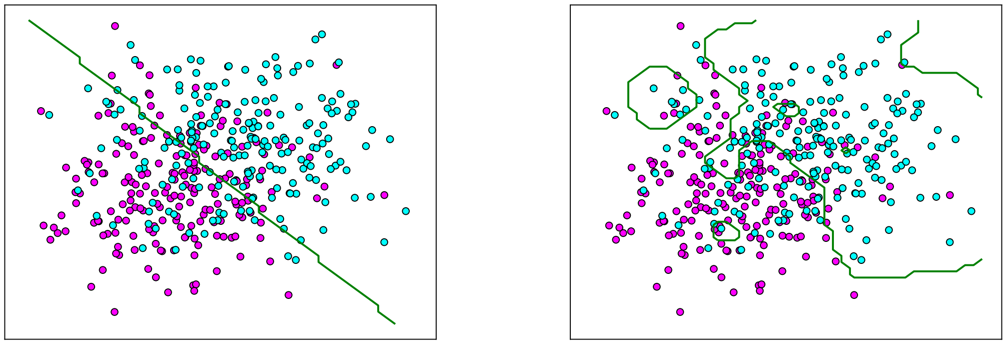
(b) plot of the number of support vectors as a function of c for various kernels and datasets

2 Exercise 2: logistic regression

The kernelized form of the regression objective for logistic regression having all data with $y^{(i)} \in -1, 1$ is written in Equation 4. 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 $1e^{-12}$.

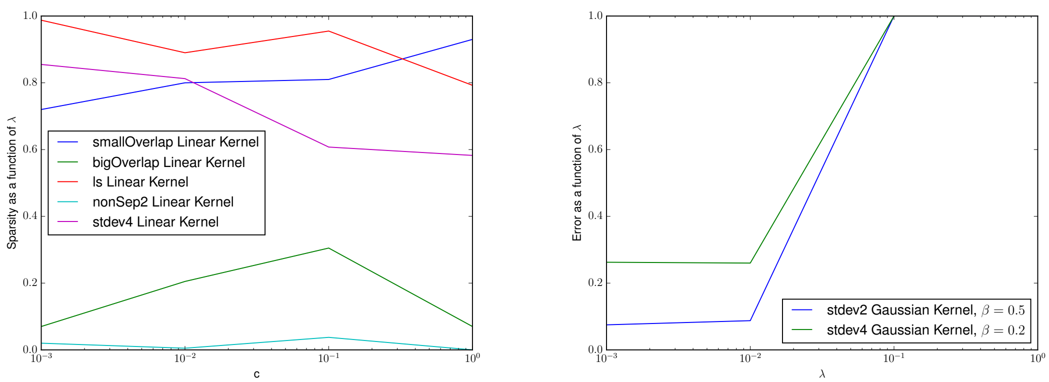
$$\text{NLL}(\alpha, w_0) = \sum_i \log \left(1 + e^{-y^{(i)} \left(\sum_{i'} \alpha_{i'} K(x^{(i')}, x^{(i)}) + w_0 \right)} \right) \tag{4a}$$

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 4a and 4b. 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) Decision boundary on non-separable data for linear kernel. Error = .265

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



(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 5a 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 5b. 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: * https://piazza.com/class/hzdfawvtilo7hf?cid=434 * l2 regularization, linear case * http://blog.datumbox.com/machin
learning-tutorial-the-multinomial-logistic-regression-softmax-regression/

* maybe need to save coefficients or predictions or something?

3.1 - lr: * 2 features, 100 pts, 2 classes, l = 0.01 -¿ error = .485 * might need to randomly select subsets of data points

* bigoverlap - error is .26 on test, ,.305 on training with l = 0.1 * smalloverlap - error is .26 on test, .27 on training with l = 0.1

* tips for getting numerics to work better: * normalize data beforehand (then don't forget to re-normalize later) *

3.2 - multiclass svm: * used http://scikit-learn.org/stable/modules/generated/sklearn.svm.linearsvc.html * can do this so fast it doesn't even make sense to try to do this by myself. * tried an array of l values with l1 loss (multiclasssvm.py), best l with random partitioning of data into 3 sets. rigorous stopping criteria * hinge loss, l2 regularization: * validation error: .187 * test error: .261 * l: 0.01 * squared loss, l1 regularization: * validation error: .143 * test error: .143 * l: 7e-7