Week 4-2: Support Vector Machine

Last time

- Logistic regression
- LDA and QDA
- High dimensional logistic regression

Today

- Confusion matrix and metrics
- ROC curve
- Support Vector Machine

Reference

- James Sharpnack's lecture notes
- Ch 12 of ESL
- Corinna Cortes and Vladimir Vapnik (1995). Support-Vector Networks. Machine Learning, 20:273--297.
- Pragya Sur and Emmanuel Candès (2019). A modern maximum-likelihood theory for high-dimensional logistic regression. PNAS, 116:14516--14525
- Boyd and Vandenberghe. https://web.stanford.edu/~boyd/cvxbook/
- How to plot svm linear margin: https://medium.com/geekculture/svm-classification-with-sklearn-svm-svc-how-to-plot-a-decision-boundary-with-margins-in-2d-space-7232cb3962c0

An interesting phenomenon on logistic regression (Sur and Candès, 2019)

A simulation:

The classical theory assumes $p \ll n$, as $n \to \infty$. What if p is not vanishingly small compared with n?

Say $n = 4,000$ and $p = 800$,

Confusion matrix and metrics

	Pred 1	Pred -1
True 1	True Pos	False Neg
True -1	False Pos	True Neg

$$\mathrm{FPR} = \frac{FP}{FP+TN}$$

$$\mathrm{TPR, Recall} = \frac{TP}{TP+FN}$$

$$\mathrm{Precision} = \frac{TP}{TP+FP}$$

In [21]:
```
plt.style.use('ggplot')
```

In [22]:
```
score_lr = X_te @ lr.coef_[0,:]
fpr_lr, tpr_lr, threshs = metrics.roc_curve(y_te,score_lr)
prec_lr, rec_lr, threshs = metrics.precision_recall_curve(y_te,score_lr)
```

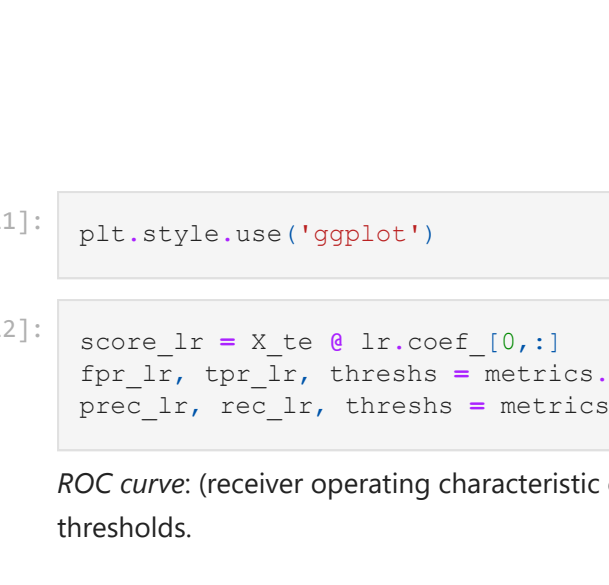
ROC curve: (receiver operating characteristic curve) is a graph showing the performance of a classification model at all classification thresholds.

Lowering the classification threshold classifies more items as positive, thus increasing both False Positives and True Positives.

The area under the ROC curve is known as *AUC* (area under the ROC Curve), which measures the entire two-dimensional area underneath the entire ROC curve.

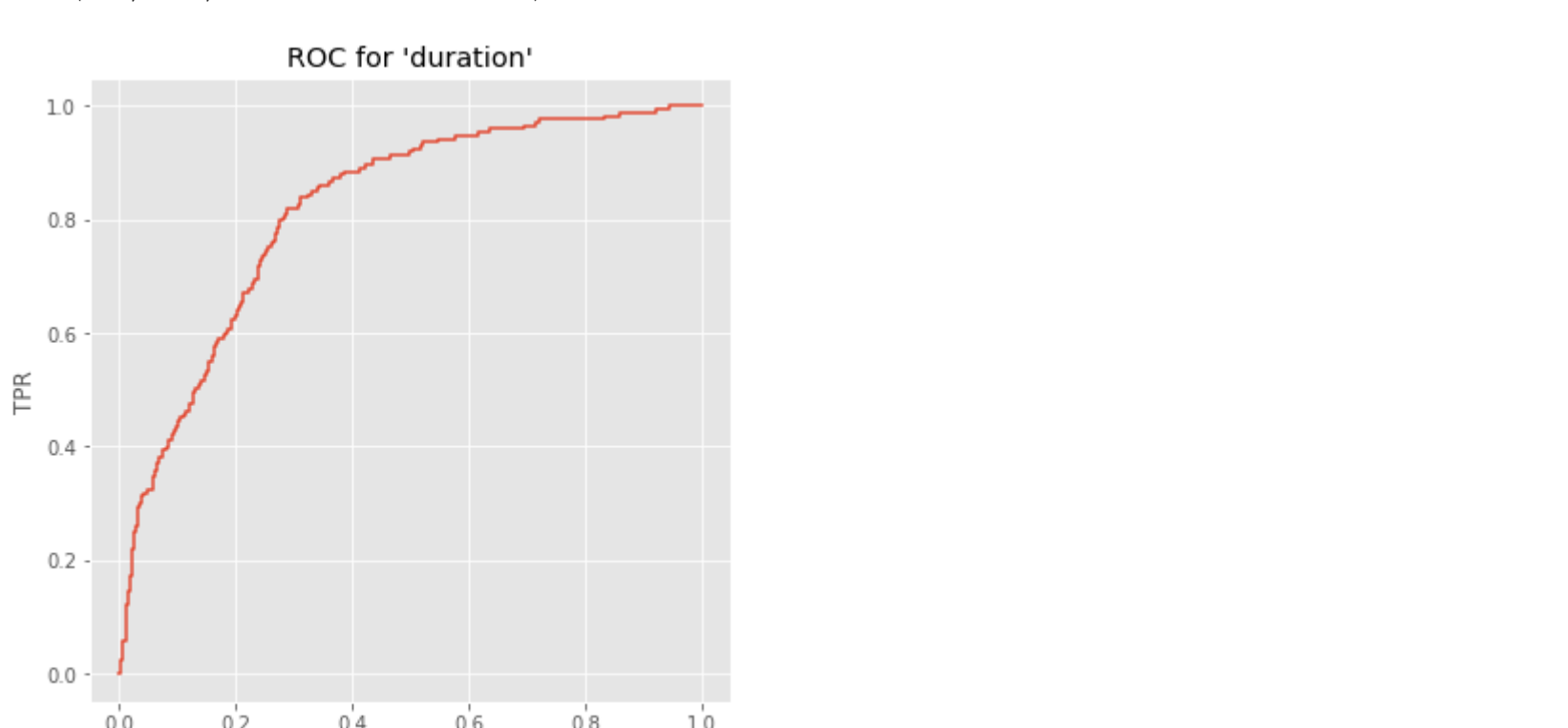
In [23]:
```
plt.figure(figsize=(6,6))
plt.plot(fpr_lr,tpr_lr)
plt.xlabel('FPR')
plt.ylabel('TPR')
plt.title("ROC for 'duration'")
```

Out[23]: `Text(0.5, 1.0, "ROC for 'duration'")`



From Wiki

Support vector classifier


US007478074B2

(12) **United States Patent**
Gates

(10) **Patent No.: US 7,478,074 B2**
(45) **Date of Patent: Jan. 13, 2009**

(54) **SUPPORT VECTOR MACHINE**

(75) Inventor: **Kevin E. Gates**, Taringa (AU)

(73) Assignee: **The University of Queensland**, Queensland (AU)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

(21) Appl. No.: **10/577,189**

(22) PCT Filed: **Oct. 29, 2004**

2003/0093393 A1 5/2003 Mangasarian et al.

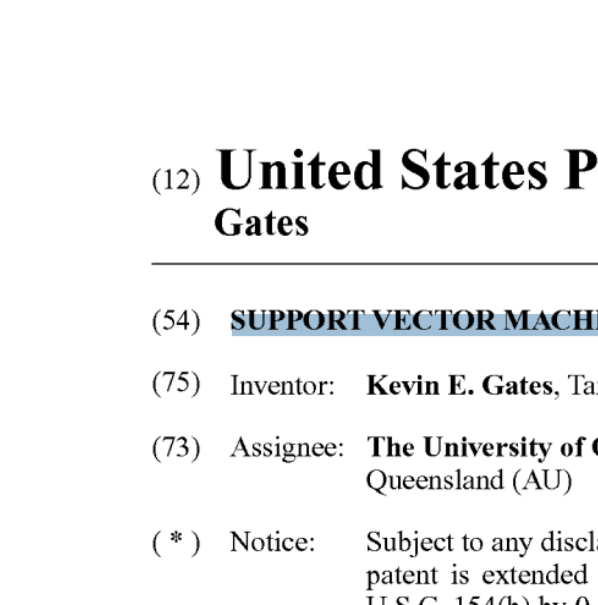
OTHER PUBLICATIONS

Fung et al., "Minimal Kernel Classifiers", 2002.*
Cluster Analysis (CA), "Cluster Analysis", 2001.*
Downs, T. et al, *Exact Simplification of Support Vector Solutions*, Journal of Machine Learning Research, vol. 2, Dec. 2001, pp. 293-297.
Lee, Y.-J. et al, *RSVM: Reduced Support Vector Machines*, First SIAM International Conference on Data Mining, 2001.
Fung, G.M. et al., *Minimal Kernel Classifiers*, Journal of Machine

Linear classifier - Hard and soft margin

See notes

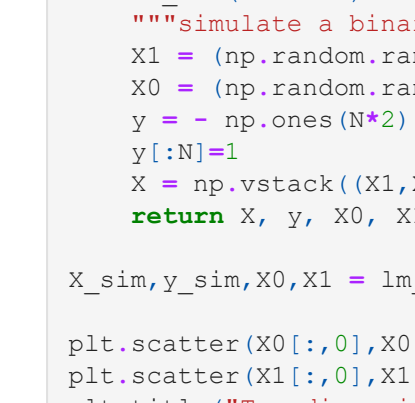
In [14]:
```
import numpy as np
import matplotlib.pyplot as plt
np.random.seed(2022)


def lm_sim(N = 100):
    """simulate a binary response and two predictors"""
    X1 = (np.random.randn(N*2)).reshape((N,2)) + np.array([2,3])
    X0 = (np.random.randn(N*2)).reshape((N,2)) + np.array([-2,-3])
    y = - np.ones(N*2)
    y[:N]=1
    X = np.vstack((X1,X0))
    return X, y, X0, X1

X_sim,y_sim,X0,X1 = lm_sim()

plt.scatter(X0[:,0],X0[:,1],c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],c='r',label='pos')
plt.title("Two dimensional classification simulation")
_ = plt.legend(loc=2)
```



In [15]:
```
from sklearn import svm

clf = svm.SVC(kernel='linear')
clf.fit(X_sim, y_sim)
```

Out[15]: `SVC(kernel='linear')`

In [40]:
```
# revised from https://scikit-learn.org/stable/auto_examples/svm/plot_svm_margin.html

from matplotlib import cm

# get the separating hyperplane
w = clf.coef_[0]
a = -w[0] / w[1]
xx = np.linspace(-5, 5)
yy = a * xx - (clf.intercept_[0]) / w[1]

# plot the parallels to the separating hyperplane that pass through the
# support vectors (margin away from hyperplane in direction
# perpendicular to hyperplane). This is sqrt(1+a^2) away vertically in
# 2-d.
margin = 1 / np.sqrt(np.sum(clf.coef_ ** 2))
yy_down = yy - np.sqrt(1 + a ** 2) * margin
yy_up = yy + np.sqrt(1 + a ** 2) * margin

    # plot the line, the points, and the nearest vectors to the plane
plt.figure(1, figsize=(4, 3))
plt.clf()
plt.plot(xx, yy, "k-")
plt.plot(xx, yy_down, "k--")
plt.plot(xx, yy_up, "k--")

plt.scatter(
    clf.support_vectors_[:, 0],
    clf.support_vectors_[:, 1],
    s=80,
    facecolors="none",
    zorder=10,
    edgecolors="k",
    cmap=cm.get_cmap("RdBu"),
)
plt.scatter(
    X0[:,0], X0[:,1], c='b', zorder=10, cmap=cm.get_cmap("RdBu"), edgecolors="k"
)

plt.scatter(
    X1[:,0], X1[:,1], c='r', zorder=10, cmap=cm.get_cmap("RdBu"), edgecolors="k"
)

plt.axis("tight")
x_min = -4.8
x_max = 4.2
y_min = -6
y_max = 6

YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
Z = clf.decision_function(xy).reshape(XX.shape)

    # Put the result into a contour plot
plt.contourf(XX, YY, Z, cmap=cm.get_cmap("RdBu"), alpha=0.5, linestyles=["-"])

plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)

plt.xticks(())
plt.yticks(())

plt.show()
```



In [44]:
```
y_pred = clf.predict(X_sim)
y_pred
```

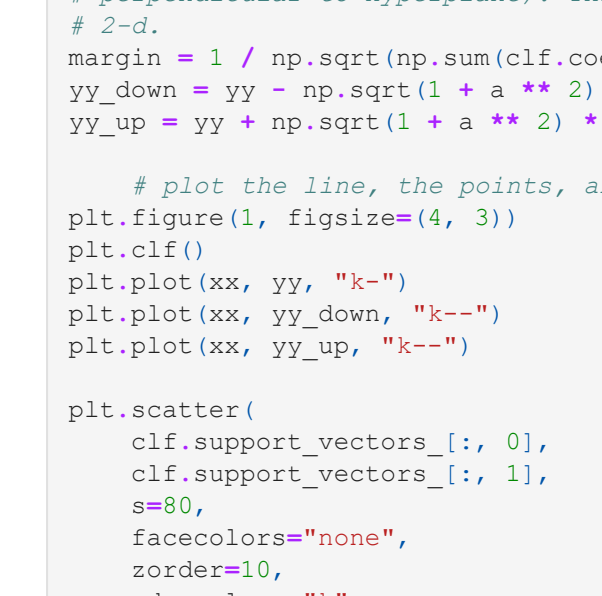
Out[44]:
```
array([ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
       -1., -1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1., -1.,  1., -1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1., -1., -1.,  1., -1., -1.,  1.,  1.,  1.,  1.,
       -1.,  1.,  1.,  1.,  1.,  1.,  1., -1., -1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1., -1.,  1.,  1.,  1.,  1., -1.,  1.,
       -1.,  1.,  1.,  1., -1.,  1.,  1., -1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1., -1.,  1.,  1.,  1.,
        1.,  1.,  1.,  1.,  1.])
```

Example from Week 4-1

In [46]:
```
np.random.seed(200)

def lm_sim(N = 100):
    """simulate a binary response and two predictors"""
    X1 = (np.random.randn(N*2)).reshape((N,2)) + np.array([2,3])
    X0 = (np.random.randn(N*2)).reshape((N,2)) + np.array([.5,1.5])
    y = - np.ones(N*2)
    y[:N]=1
    X = np.vstack((X1,X0))
    return X, y, X0, X1
```

In [47]:
```
X_sim,y_sim,X0,X1 = lm_sim()
```

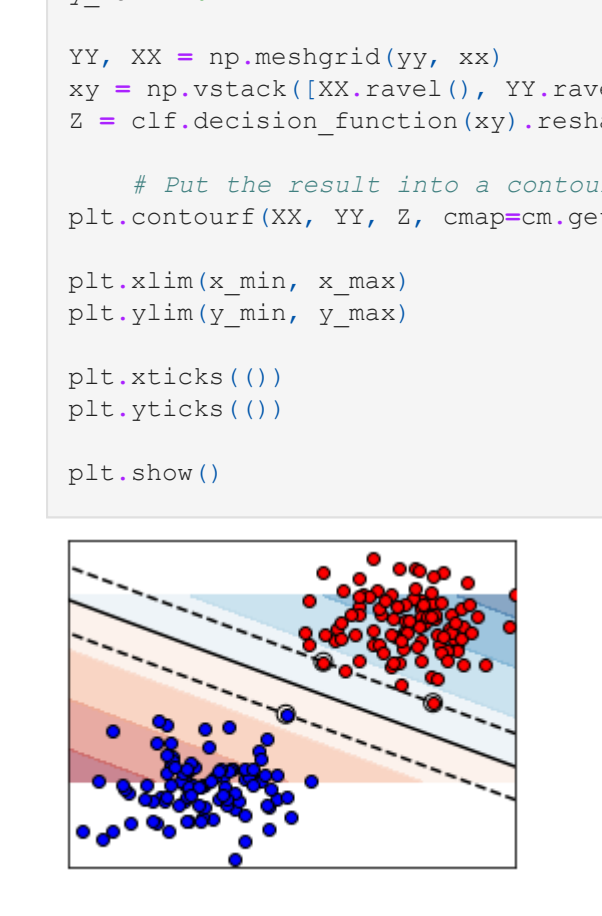
In [48]:
```
plt.scatter(X0[:,0],X0[:,1],c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],c='r',label='pos')
plt.title("Two dimensional classification simulation")
_ = plt.legend(loc=2)
```



In [49]:
```
from sklearn import svm

clfo = svm.SVC(kernel='linear')
clfo.fit(X_sim, y_sim)
```

Out[49]: `SVC(kernel='linear')`

In [79]:
```
from matplotlib import cm

# get the separating hyperplane
w = clfo.coef_[0]
a = -w[0] / w[1]
xx = np.linspace(-3, 5)
yy = a * xx - (clfo.intercept_[0]) / w[1]

# plot the parallels to the separating hyperplane that pass through the
# support vectors (margin away from hyperplane in direction
# perpendicular to hyperplane). This is sqrt(1+a^2) away vertically in
# 2-d.
margin = 1 / np.sqrt(np.sum(clfo.coef_ ** 2))
yy_down = yy - np.sqrt(1 + a ** 2) * margin
yy_up = yy + np.sqrt(1 + a ** 2) * margin

    # plot the line, the points, and the nearest vectors to the plane
plt.figure(1, figsize=(6, 6))
plt.clf()
plt.plot(xx, yy, "k-")
plt.plot(xx, yy_down, "k--")
plt.plot(xx, yy_up, "k--")

plt.scatter(
    clfo.support_vectors_[:, 0],
    clfo.support_vectors_[:, 1],
    s=80,
    facecolors="none",
    zorder=10,
    edgecolors="k",
    cmap=cm.get_cmap("RdBu"),
)
plt.scatter(
    X0[:,0], X0[:,1], c='b', zorder=10, cmap=cm.get_cmap("RdBu"), edgecolors="k"
)

plt.scatter(
    X1[:,0], X1[:,1], c='r', zorder=10, cmap=cm.get_cmap("RdBu"), edgecolors="k"
)

plt.axis("tight")
x_min = -4
x_max = 7
y_min = -1
y_max = 8

YY, XX = np.meshgrid(yy, xx)
xy = np.vstack([XX.ravel(), YY.ravel()]).T
Z = clf.decision_function(xy).reshape(XX.shape)

    # Put the result into a contour plot
plt.contourf(XX, YY, Z, cmap=cm.get_cmap("RdBu"), alpha=0.5, linestyles=["-"])

plt.xlim(x_min, x_max)
plt.ylim(y_min, y_max)

plt.xticks(())
plt.yticks(())

plt.show()
```



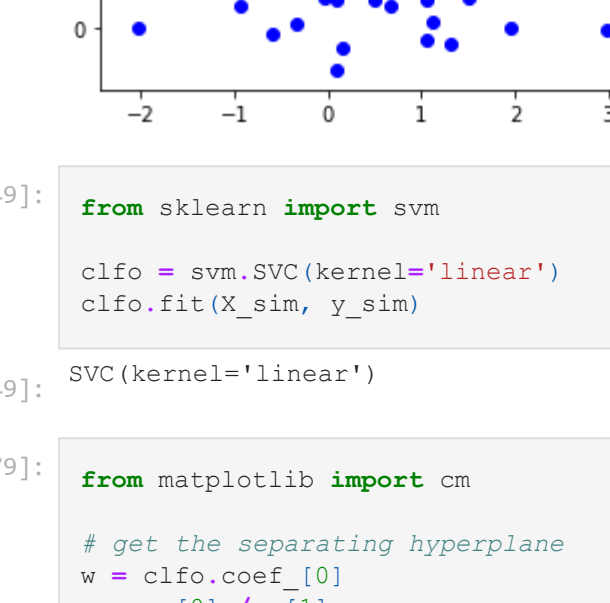
In [72]:
```
clfo.intercept_
```

Out[72]: `array([-4.07596093])`

In [74]:
```
yy
```

Out[74]:
```
array([ 9.82628914,  9.58314552,  9.3400019 ,  9.09685828,  8.85371466,
        8.61057104,  8.36742741,  8.12428379,  7.88114017,  7.63799655,
        7.39485293,  7.15170931,  6.90856569,  6.66542207,  6.42227845,
        6.17913482,  5.9359912 ,  5.69284758,  5.44970396,  5.20656034,
        4.96341672,  4.7202731 ,  4.47712948,  4.23398586,  3.99084224,
        3.74769861,  3.50455499,  3.26141137,  3.01826775,  2.77512413,
        2.53198051,  2.28883689,  2.04569327,  1.80254965,  1.55940602,
        1.3162624 ,  1.07311878,  0.82997516,  0.58683154,  0.34368792,
        0.1005443 , -0.14259932, -0.38574294, -0.62888657, -0.87203019,
       -1.11517381, -1.35831743, -1.60146105, -1.84460467, -2.08774829])
```

In [81]:
```
# svm prediction error
y_pred_svm = clfo.predict(X_sim)

N = 100
plt.scatter(X0[y_pred_svm[N:] == 1,0],X0[y_pred_svm[N:] == 1,1],c='b',label='neg')
plt.scatter(X1[y_pred_svm[:N] == -1,0],X1[y_pred_svm[:N] == -1,1],c='r',label='pos')
plt.plot(xx,yy,c='k')
plt.title("Points classified incorrectly (SVM)")
_ = plt.legend(loc=2)
```

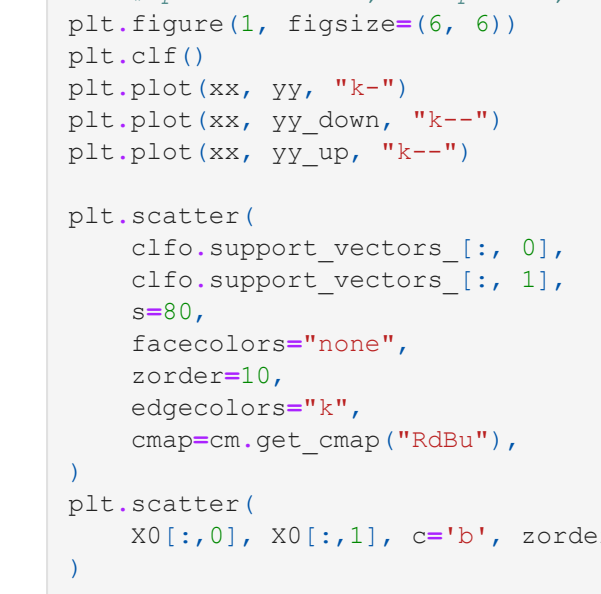


In [88]:
```
np.count_nonzero(y_pred_svm - y_sim)
```

Out[88]: `25`

Comparing to the logistic regression and LDA

In [86]:
```
from sklearn import linear_model

lr_sim = linear_model.LogisticRegression()
lr_sim.fit(X_sim,y_sim)

N = 100
beta1 = lr_sim.coef_[0,0]
beta2 = lr_sim.coef_[0,1]
beta0 = lr_sim.intercept_
xx = np.linspace(-3,5, 100)
x2hat = -(beta0 + beta1*xx) / beta2
lr_pred = lr_sim.predict(X_sim)
plt.scatter(X0[lr_pred[N:] == 1,0],X0[lr_pred[N:] == 1,1],c='b',label='neg')
plt.scatter(X1[lr_pred[:N] == -1,0],X1[lr_pred[:N] == -1,1],c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.title("Points classified incorrectly (LR)")
_ = plt.legend(loc=2)
```



In [87]:
```
np.count_nonzero(lr_pred - y_sim)
```

Out[87]: `25`

In [89]:
```
# LDA model

from sklearn.discriminant_analysis import LinearDiscriminantAnalysis

lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
y_lda = lda.fit(X_sim, y_sim).predict(X_sim)

np.count_nonzero(y_lda - y_sim)
```

Out[89]: `28`

SVM with Kernels

In [102...
```
# using the radial basis kernel

clfk = svm.SVC(kernel="rbf")
clfk.fit(X_sim, y_sim)
```

Out[102...: `SVC()`

In [115...
```
nonlinear_svm = clfk.predict(X_sim)
np.count_nonzero(nonlinear_svm - y_sim)
```

Out[115...: `24`

From Ch 12 of ESL

Loss function

0-1 loss

We can rewrite the 0-1 loss for a linear classifier as

$$\ell_{0/1}(\beta, x_i, y_i) = 1\{y_i \beta^\top x_i < 0\}. \qquad \text{(0-1 loss)}$$

Loss function for logistic regression

Logistic regression uses a loss function that mimics some of the behavior of the 0-1 loss, but is not discontinuous. So, it is a *surrogate loss*, which will make our life easier.

The logistic loss is a function of $y_i \beta^\top x_i$, which is

$$\ell_L(\beta, x_i, y_i) = \log(1 + \exp(-y_i \beta^\top x_i)). \qquad \text{(logistic)}$$

Loss function for SVM

SVM uses a hinge loss

$$\ell_H(\beta, x_i, y_i) = (1 - y_i \beta^\top x_i)_+ \qquad \text{(hinge)}$$

(why?) or $(1 - y_i f(x_i)))_+$ in general. where $a_+ = a 1\{a > 0\}$ is the positive part of the real number a.

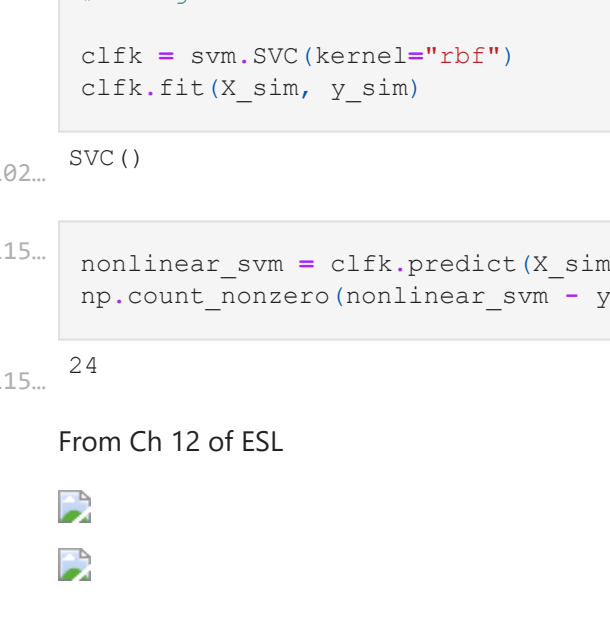
Squared Hinge loss

If we are free to select training loss functions, then why not square error loss? For example, we could choose

$$\ell_S(\beta, x_i, y_i) = (y_i - \beta^\top x_i))^2 = (1 - y_i \beta^\top x_i))^2. \qquad \text{(squared hinge error)}$$

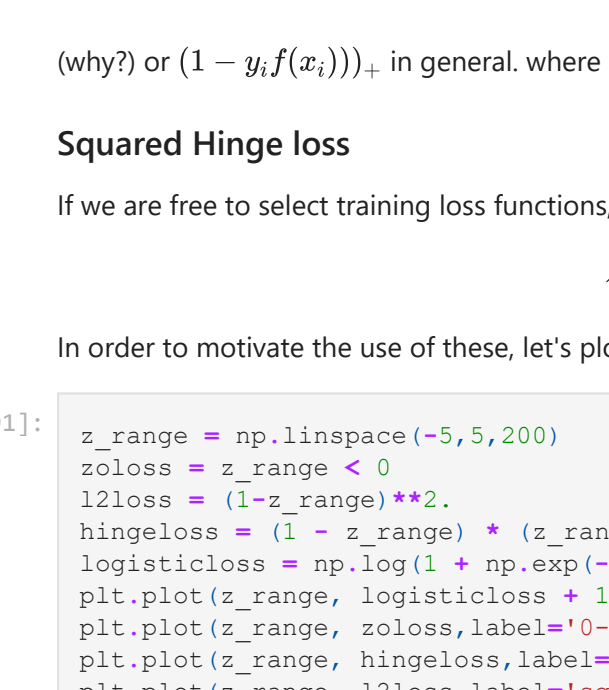
In order to motivate the use of these, let's plot the losses as a function of $y_i \beta^\top x_i$.

In [91]:
```
z_range = np.linspace(-5,5,200)
zoloss = z_range < 0
l2loss = (1-z_range)**2.
hingeloss = (1 - z_range) * (z_range < 1)
logisticloss = np.log(1 + np.exp(-z_range))
plt.plot(z_range, logisticloss + 1 - np.log(2.),label='logistic')
plt.plot(z_range, zoloss,label='0-1')
plt.plot(z_range, hingeloss,label='hinge')
plt.plot(z_range, l2loss,label='sq hinge')
plt.ylim([-.2,5])
plt.xlabel(r'$y_i \beta^\top x_i$')
plt.ylabel('loss')
plt.title('A comparison of classification loss functions')
_ = plt.legend()
```

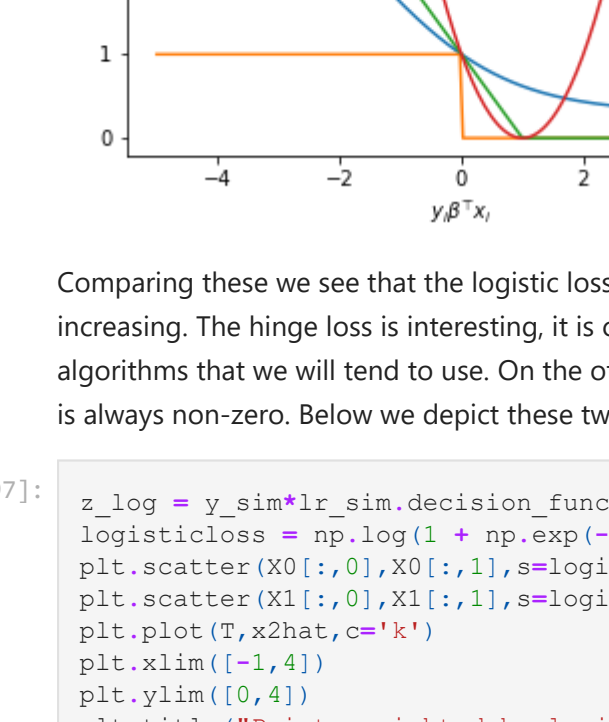


Comparing these we see that the logistic loss is smooth---it has continuous first and second derivatives---and it is decreasing as $y_i \beta^\top x_i$ is increasing. The hinge loss is interesting, it is continuous, but it has a discontinuous first derivative. This changes the nature of optimization algorithms that we will tend to use. On the other hand the hinge loss is zero for large enough $y_i \beta^\top x_i$, as opposed to the logistic loss which is always non-zero. Below we depict these two losses by weighting each point by the loss for the fitted classifier.

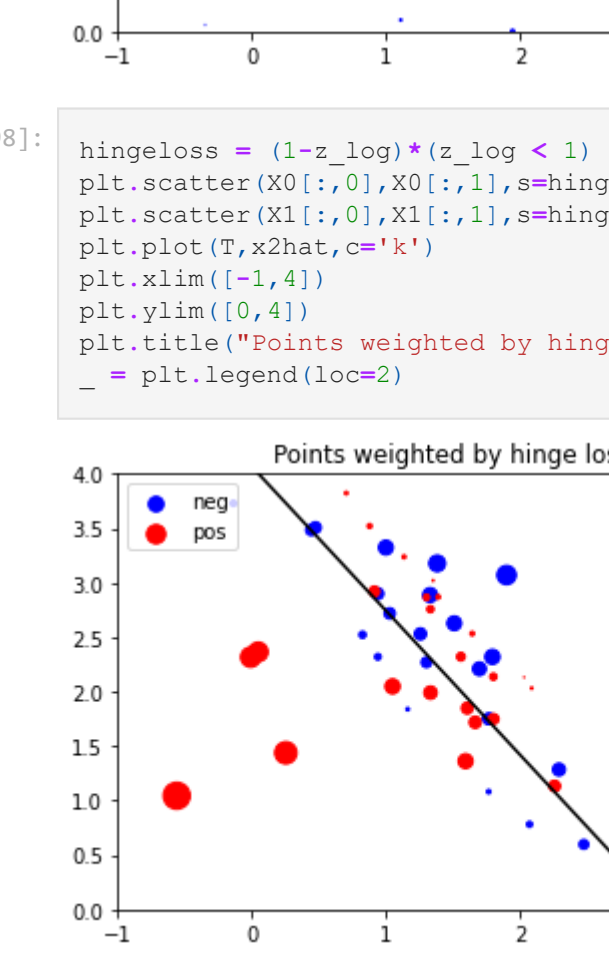
In [97]:
```
z_log = y_sim*lr_sim.decision_function(X_sim)
logisticloss = np.log(1 + np.exp(-z_log))
plt.scatter(X0[:,0],X0[:,1],s=logisticloss[N:]*30.,c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],s=logisticloss[:N]*30.,c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.xlim([-1,4])
plt.ylim([0,4])
plt.title("Points weighted by logistic loss")
_ = plt.legend(loc=2)
```



In [98]:
```
hingeloss = (1-z_log)*(z_log < 1)
plt.scatter(X0[:,0],X0[:,1],s=hingeloss[N:]*30.,c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],s=hingeloss[:N]*30.,c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.xlim([-1,4])
plt.ylim([0,4])
plt.title("Points weighted by hinge loss")
_ = plt.legend(loc=2)
```



In [99]:
```
l2loss = (1-z_log)**2.
plt.scatter(X0[:,0],X0[:,1],s=l2loss[N:]*10.,c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],s=l2loss[:N]*10.,c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.xlim([-1,4])
plt.ylim([0,4])
plt.title("Points weighted by sqr. hinge loss")
_ = plt.legend(loc=2)
```



We see that for the logistic loss the size is vanishing when the points are on the wrong side of the separator hyperplane. The hinge loss is zero if we are sufficiently far from the hyperplane. The square hinge error loss has increased weight for those far from the hyperplane, even if they are correctly classified. Hence, **square hinge error loss is not a good surrogate for 0-1 loss.**