Week 4-1: Classification

Last time

- Lasso - LAR & Coordinate descent
- Variants of the lasso method

Today

- Classification
  - Logistic regression
  - LDA and QDA

Reference

- James Sharpnack's lecture notes
- Ch 4 of ESL

Introduction to classification

We have seen how you can evaluate a supervised learner with a loss function. Classification is the learning task where one tried to predict a binary response variable, this can be thought of as the answer to a yes/no question, as in "Will this stock value go up today?".

This is in contrast to regression which predicts a continuous response variable, answering a question such as "What will be the increase in stock value today?".

Classification has some interesting lessons for other machine learning tasks, and we will try to introduce many of the main concepts in classification.

Recall that the *supervised learning* setting has that the data consists of response variables, y_i and predictor variables x_i for $i = 1, \dots, n$. We will focus on binary classification which we will encode as the binary variable: $y_i \in \{0, 1\}$. We will see that two heuristics can help us understand the basics of evaluating classifiers.

Logistic regression

The logistic regression is a supervised learning algorithm that is widely used for classification. The outcome of the logistic regression is discrete and restricted to a limited number of values.

Consider the logistic regression model with a binary outcome (say, 0 and 1), the model has the form

$$\log \frac{P(C=1|X=x)}{P(C=0|X=x)} = \beta' x,$$

where $\beta = (\beta_0, \beta_1)$, $\beta_0 \in \mathbb{R}$ and $\beta_1 \in \mathbb{R}^p$, and $x = [1, \tilde{x}] \in \mathbb{R}^{p+1}$. The ratio is known as the *odds-ratio*.

By calculation, one can show that

$$P(C=1|X=x) = \frac{e^{\beta' x}}{1 + e^{\beta' x}}$$

We denote the probability $P(C=1|X=x) = p(x;\beta)$, where $\beta = (\beta_0, \beta_1)$; similarly, $P(C=0|X=x) = 1 - p_0(x;\beta)$;

The log-likelihood function can be written as

$$\begin{aligned} \ell(\beta) &= \sum_{i=1}^n \{y_i \log p(x_i;\beta) + (1-y_i)\log(1-p(x_i;\beta))\} \\ &= \sum_{i=1}^n \{y_i \beta' x_i - \log(1 + e^{\beta' x_i})\} \end{aligned}$$

Then by taking derivatives to zero, we have

$$\frac{d\ell(\beta)}{d\beta} = \sum_{i=1}^n x_i (y_i - p(x_i;\beta)) = 0,$$

which are $p+1$ equations that are nonlinear in β. How to solve β? (Newton's algorithm)

Iterating $j = 1, \dots, K$,

$$\beta_j = \beta_{j-1} - s\Big(\frac{d^2\ell(\beta)}{d\beta d\beta'}\Big)^{-1} \frac{d\ell(\beta)}{d\beta}.$$

In [1]:
```python
import pandas as pd
import numpy as np
import matplotlib as mpl
import plotnine as p9
import matplotlib.pyplot as plt
import itertools

import warnings
warnings.simplefilter("ignore")

np.random.seed(2022041801)
```

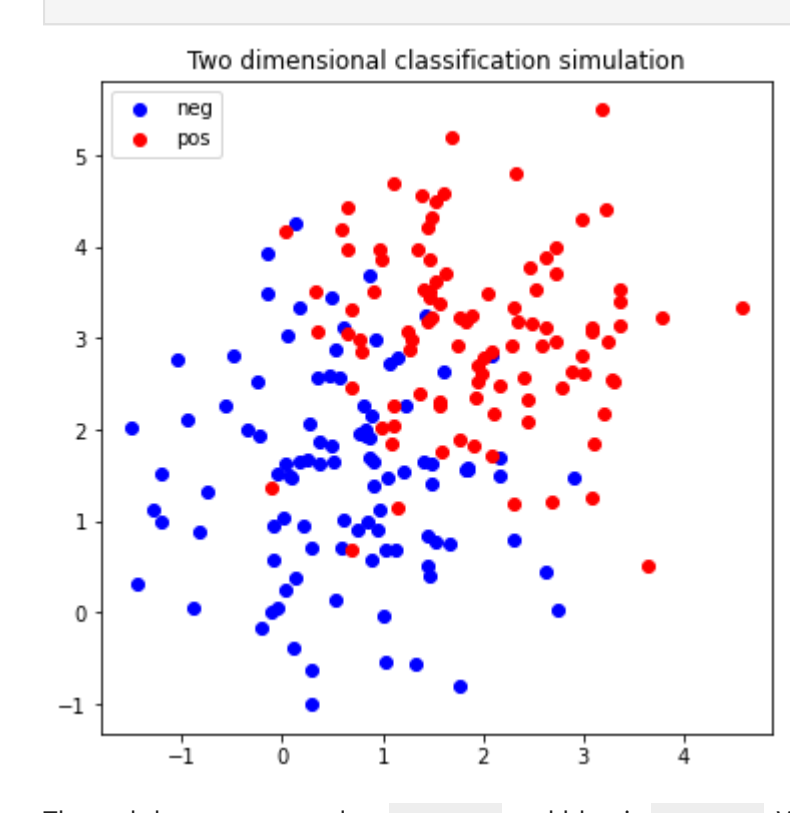
In [2]:
```python
from matplotlib.pyplot import rcParams
rcParams['figure.figsize'] = 6,6
```

Logistic regression in action

In [3]:
```python
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 [4]:
```python
X_sim,y_sim,X0,X1 = lm_sim()
```

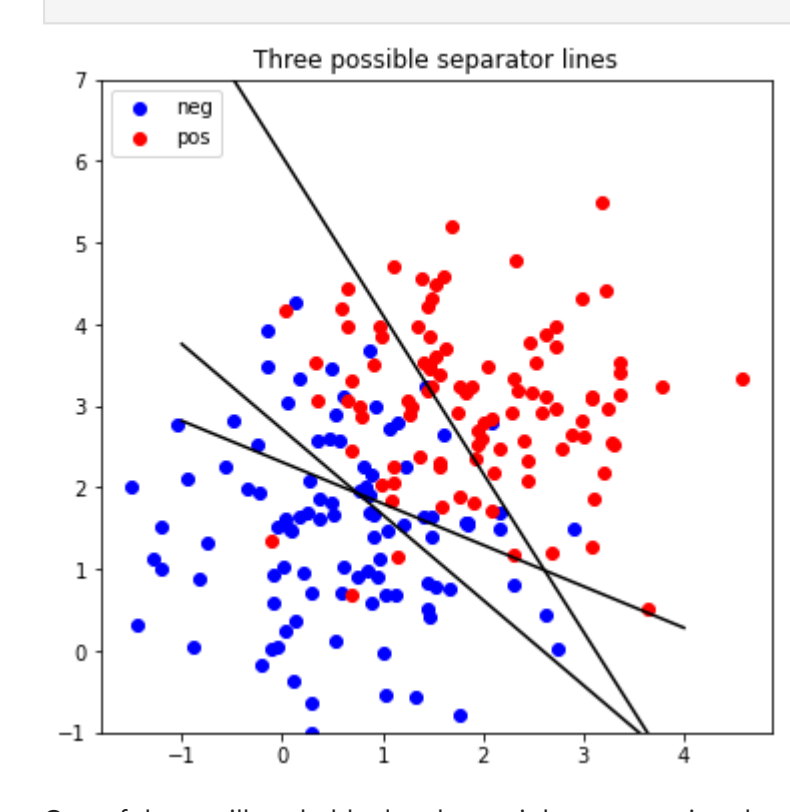
In [5]:
```python
plt.scatter(X0[:,0],X0[:,1],c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],c='r',label='pos')
plt.title("Two dimensional classification simulation")
_ = plt.legend(loc=2)
```



The red dots correspond to `Y = +1` and blue is `Y = -1`. We can see that a classifier that classifies as +1 when the point is in the upper right of the coordinate system should do pretty well. We could propose several β vectors to form linear classifiers and observe their training errors, finally selecting the one that minimized the training error. We have seen that a linear classifier has a separator hyperplane (a line in 2 dimensions). To find out what the prediction the classifier makes for a point one just needs to look at which side of the hyperplane it falls on. Consider a few such lines.

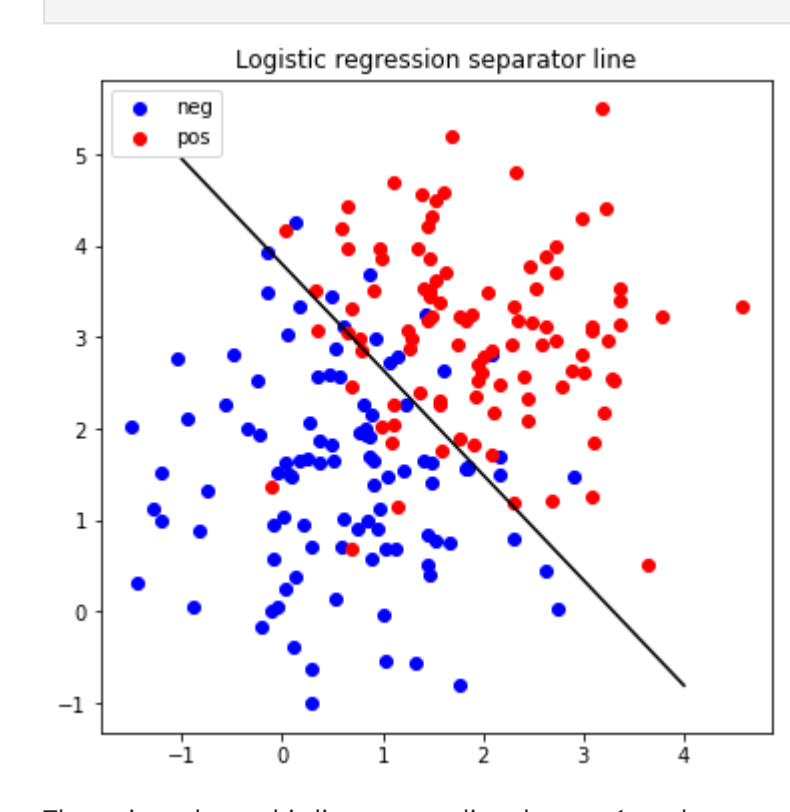
In [6]:
```python
from sklearn import linear_model

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

beta1 = lr_sim.coef_[0,0]
beta2 = lr_sim.coef_[0,1]
beta0 = lr_sim.intercept_

mults=0.8
T = np.linspace(-1,4,100)
x2hat = -(beta0 + beta1*T) / beta2
line1 = -(beta0 + np.random.randn(1)*2 +
          (beta1 + np.random.randn(1)*mults) *T) / (beta2 + np.random.randn(1)*mults)
line2 = -(beta0 + np.random.randn(1)*2 +
          (beta1 + np.random.randn(1)*mults) *T) / (beta2 + np.random.randn(1)*mults)
line3 = -(beta0 + np.random.randn(1)*2 +
          (beta1 + np.random.randn(1)*mults) *T) / (beta2 + np.random.randn(1)*mults)
```

In [7]:
```python
plt.scatter(X0[:,0],X0[:,1],c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],c='r',label='pos')
plt.plot(T,line3,c='k')
plt.plot(T,line1,c='k')
plt.plot(T,line2,c='k')
plt.ylim([-1,7])
plt.title("Three possible separator lines")
_ = plt.legend(loc=2)
```



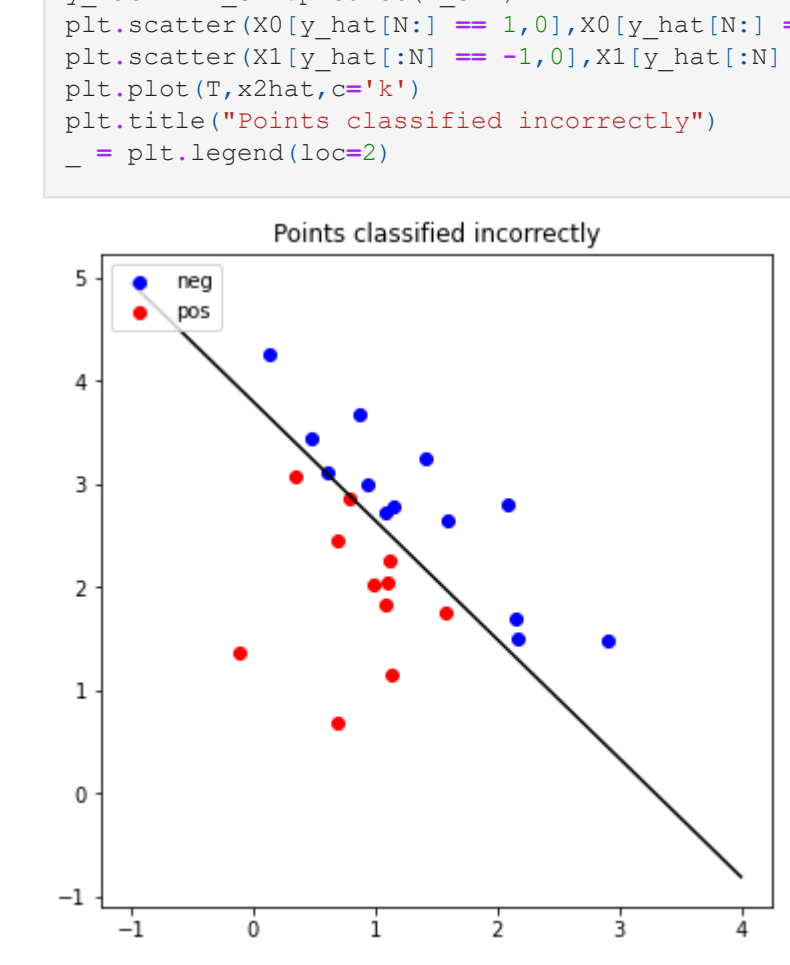
One of these will probably do a better job at separating the training data than the others, but if we wanted to do this over all possible $\beta \in \mathbb{R}^{p+1}$ then we need to solve the program (0-1 min) above.

In [8]:
```python
plt.scatter(X0[:,0],X0[:,1],c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.title("Logistic regression separator line")
_ = plt.legend(loc=2)
```



The points above this line are predicted as a +1, and so we can also isolate those points that we classified incorrectly. The 0-1 loss counts each of these points as a loss of 1.

In [9]:
```python
N = 100
y_hat = lr_sim.predict(X_sim)
plt.scatter(X0[y_hat[N:] == 1,0],X0[y_hat[N:] == 1,1],c='b',label='neg')
plt.scatter(X1[y_hat[:N] == -1,0],X1[y_hat[:N] == -1,1],c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.title("Points classified incorrectly")
_ = plt.legend(loc=2)
```



Linear discriminant analysis

Consider estimating $P(C=1|X)$ for binary clusters. Suppose $f_1(x)$ is the class-conditional density of X in $C=1$, let π be the prior probability of this class, by applying Bayes rule, we have

$$P(C=1|X=x) = \frac{f_1(x)\pi}{f_0(x)(1-\pi) + f_1(x)\pi},$$

where $f_0(\cdot)$ the conditional density of X in $C=0$.

Assuming $f_k \sim N(\mu_k, \Sigma_k)$ and $\Sigma_k = \Sigma$ for $k = 0, 1$, then the log-ratio between the two classes are

$$\begin{aligned} \log\frac{P(C=1|X)}{P(C=0|X)} &= \log\frac{f_1(x)}{f_0(x)} + \log\frac{\pi}{1-\pi} && (1) \\ &= \log\frac{\pi}{1-\pi} - \frac{1}{2}(\mu_1+\mu_0)'\Sigma^{-1}(\mu_1+\mu_0) + x'\Sigma^{-1}(\mu_1-\mu_0), && (2) \end{aligned}$$

which is *linear in x*.

In practice, we do not know the parameters of the Gaussian distributions, we estimate them from the training data:

- $\hat{\pi} = n_1/n$, where n_1 is the number observation in Class 1;
- $\hat{\mu}_k = \sum_{i \in N_k} x_i/n_k$, where N_k is the set containing the observations in Class 1;
- $\hat{\Sigma} = \sum_{k=0}^1 \sum_{i \in N_k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)'/(n - n_k)$

The LDA rule in favor of Class 1 if the log-ratio is larger than 1, i.e.,

$$x'\Sigma^{-1}(\mu_1 - \mu_0) > \frac{1}{2}(\mu_1+\mu_0)'\Sigma^{-1}(\mu_1+\mu_0) - \log\frac{\pi}{1-\pi}.$$

Quadratic Discriminant Analysis (QDA)

Similar to LDA, but allow Σ_k to differ. Then

- $\hat{\Sigma}_k = \sum_{i \in N_k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)'/(n - n_k)$

Regularized Discriminant Analysis

Friedman (1989) proposed a compromise between LDA and QDA, which allows one to shrink the separate covariance of QDA toward a common covariance as in LDA

$$\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma}$$

In [10]:
```python
import matplotlib as mpl
from matplotlib import colors

from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
```

In [11]:
```python
lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
y_hat_lda = lda.fit(X_sim, y_sim).predict(X_sim)
```

In [12]:
```python
y_hat_lda - y_hat
```

Out[12]:
```
array([0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 2., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       2., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
       0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.])
```

LDA vs logistic regression?

Note that the log-odds of the LDA model is linear to x:

$$\begin{aligned} \log\frac{P(C=1|X)}{P(C=0|X)} &= \log\frac{f_1(x)}{f_0(x)} + \log\frac{\pi}{1-\pi} && (3) \\ &= \log\frac{\pi}{1-\pi} - \frac{1}{2}(\mu_1+\mu_0)'\Sigma^{-1}(\mu_1+\mu_0) + x'\Sigma^{-1}(\mu_1-\mu_0) && (4) \\ &= \alpha_0 + \alpha_1' x && (5) \end{aligned}$$

The log-odds of the logistic regression is

$$\log\frac{P(C=1|X=x)}{P(C=0|X=x)} = \beta_0 + \beta_1' x$$

Indeed, the two models seem are the same!

Note that the difference between the two models is the linear coefficients that are estimated. The logistic regression model is more general, as it makes less assumptions. Why?

Q: how to implement LDA and logistic regression for multiclass classification?

Regularized logistic regression

Simliar to the lasso, we can add the ℓ_1 penalty for logistic regression for variable selection and shrinkage coefficents, i.e., $$ \max_{\beta0, *\beta} \Big{ \sum*{i=1}^n \Big(y_i (\beta_0 + \beta'x_i) - \log (1+e^{\beta_0 + \beta'x_i)} \Big)

    - \lambda \|\beta\|_1

\Big} $$ Note that usually we do not penalize β_0.

In python, the package impliment ℓ_1, ℓ_2, and elastic net penalty functions.

In [13]:
```python
from sklearn import LogisticRegression
```

In [14]:
```python
bank = pd.read_csv('../data/bank.csv',sep=';',na_values=['unknown',999,'nonexistent'])
bank.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4521 entries, 0 to 4520
Data columns (total 17 columns):
 #   Column     Non-Null Count  Dtype
---  ------     --------------  -----
 0   age        4521 non-null   int64
 1   job        4483 non-null   object
 2   marital    4521 non-null   object
 3   education  4334 non-null   object
 4   default    4521 non-null   object
 5   balance    4519 non-null   float64
 6   housing    4521 non-null   object
 7   loan       4521 non-null   object
 8   contact    3197 non-null   object
 9   day        4521 non-null   int64
 10  month      4521 non-null   object
 11  duration   4521 non-null   int64
 12  campaign   4521 non-null   int64
 13  pdays      4521 non-null   int64
 14  previous   4521 non-null   int64
 15  poutcome   816 non-null    object
 16  y          4521 non-null   object
dtypes: float64(1), int64(6), object(10)
memory usage: 600.6+ KB
```

In [15]:
```python
bank_tr, bank_te = model_selection.train_test_split(bank,test_size=.33)
```

In [16]:
```python
bank_tr['y'].describe()
```

Out[16]:
```
count     4521
unique       2
top         no
freq      4000
Name: y, dtype: object
```

In [17]:
```python
def train_bank_to_xy(bank):
    """standardize and impute training"""
    bank_sel = bank[['age','balance','duration','y']].values
    X,y = bank_sel[:,:-1], bank_sel[:,-1]
    scaler = preprocessing.StandardScaler().fit(X)
    imputer = impute.SimpleImputer(fill_value=0).fit(X)
    trans_prep = lambda Z: imputer.transform(scaler.transform(Z))
    X = trans_prep(X)
    y = 2*(y == 'yes')-1
    return (X, y), trans_prep

def test_bank_to_xy(bank, trans_prep):
    """standardize and impute test"""
    bank_sel = bank[['age','balance','duration','y']].values
    X,y = bank_sel[:,:-1], bank_sel[:,-1]
    X = trans_prep(X)
    y = 2*(y == 'yes')-1
    return (X, y)
```

In [18]:
```python
(X_tr, y_tr), trans_prep  = train_bank_to_xy(bank_tr)
X_te, y_te = test_bank_to_xy(bank_te, trans_prep)
```

In [19]:
```python
lamb = 1.
lr = linear_model.LogisticRegression(penalty='l2', C = 1/lamb)
lr.fit(X_tr,y_tr)
```

Out[19]:
```
LogisticRegression()
```

We can then predict on the test set and see what the resulting 0-1 test error is.

In [20]:
```python
yhat = lr.predict(X_te)
(yhat != y_te).mean()
```

Out[20]:
```
0.11327077747989277
```

Confusion matrix and metrics

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

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

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

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

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

In [22]:
```python
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)
```

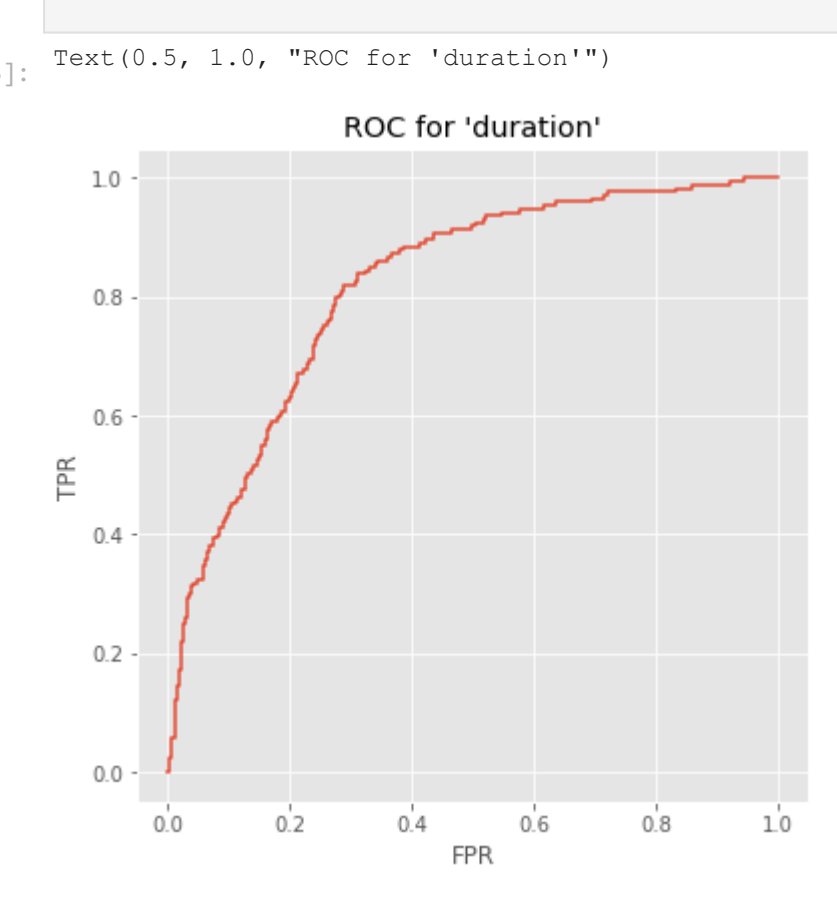
ROC curve: (receiver operating characteristic curve) is a graph showing the performance of a classification model at all classification thresholds.

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]:
```python
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

What is the 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. In this way, it is a surrogate loss, that acts as a surrogate for the 0-1 loss. It turns out that it is one of a few nice options for surrogate losses. Notice that we can rewrite the 0-1 loss for a linear classifier as

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

Throughout we will denote our losses as functions of β to reflect the fact that we are only considering linear classifiers. The logistic loss and the hinge loss are also functions of $y_i \beta^\top x_i$, they are

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

There are other loss functions, we will earn them soon, e.g., the hinge loss used by support vector machine (SVM)

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

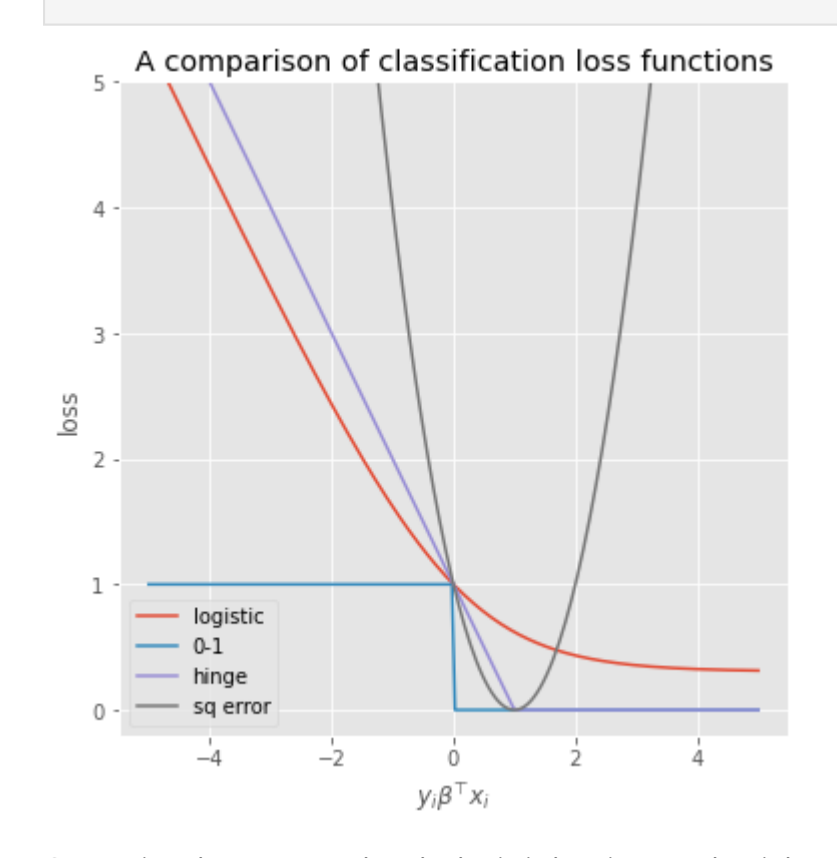
where $a_+ = a1\{a > 0\}$ is the positive part of the real number a.

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

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

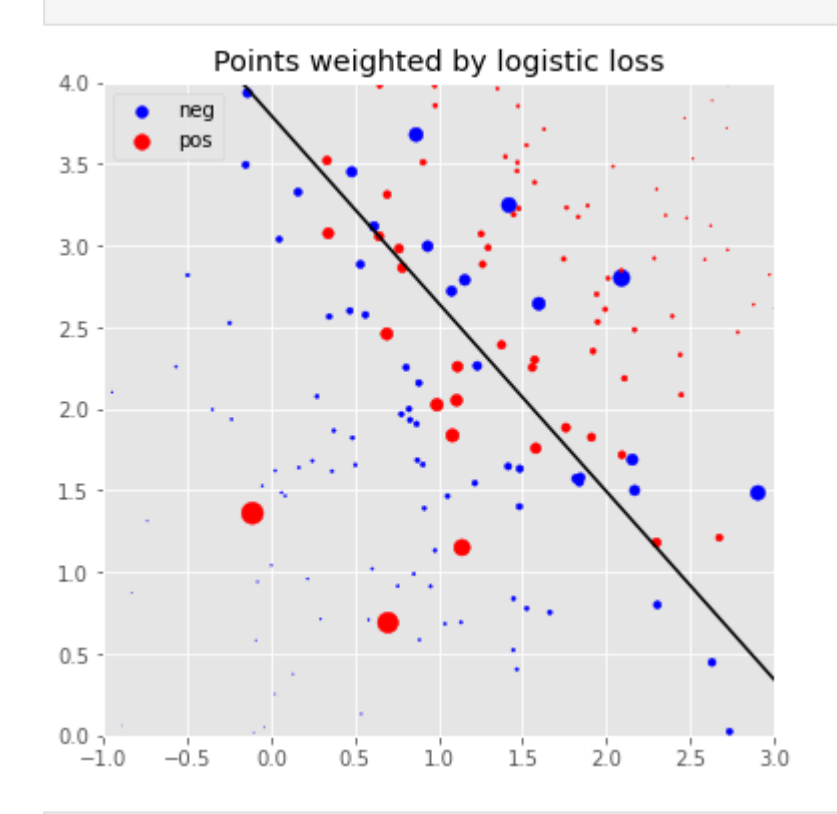
In order to motivate the use of these, let's plot the losses as a function of $y_i \beta^\top x_i$.

In [24]:
```python
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 error')
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()
```

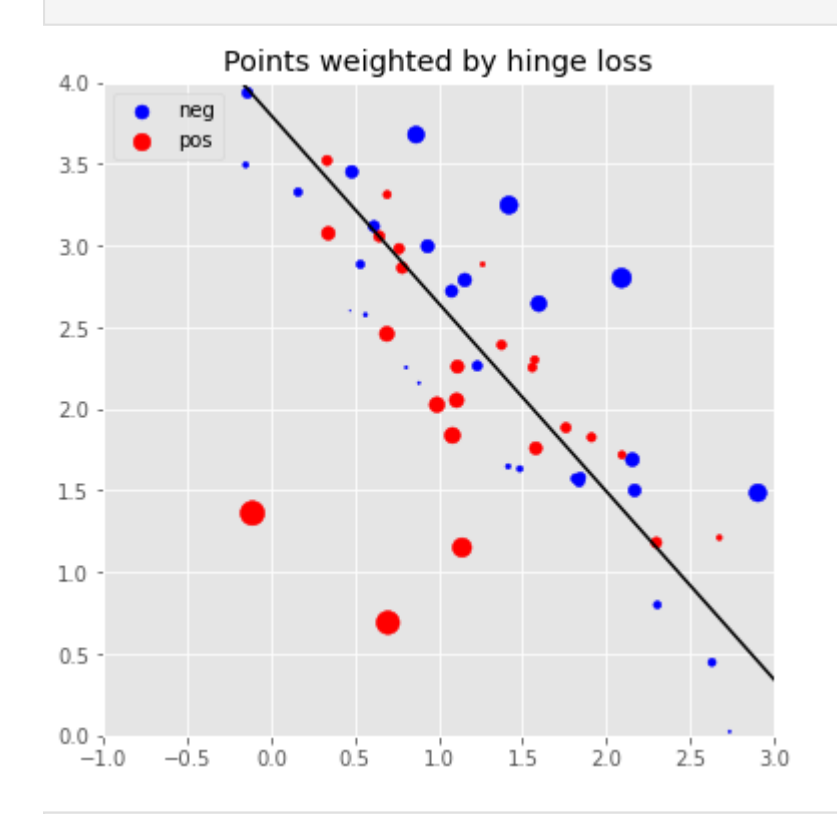


Comparing these we see that the logistic loss is smooth---it has continuous first and second derivatives---and it is decreasing as $y_i \beta^\top x_i$ is increasing. The hinge loss is interesting, it is continuous, but it has a discontinuous first derivative. This changes the nature of optimization 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.

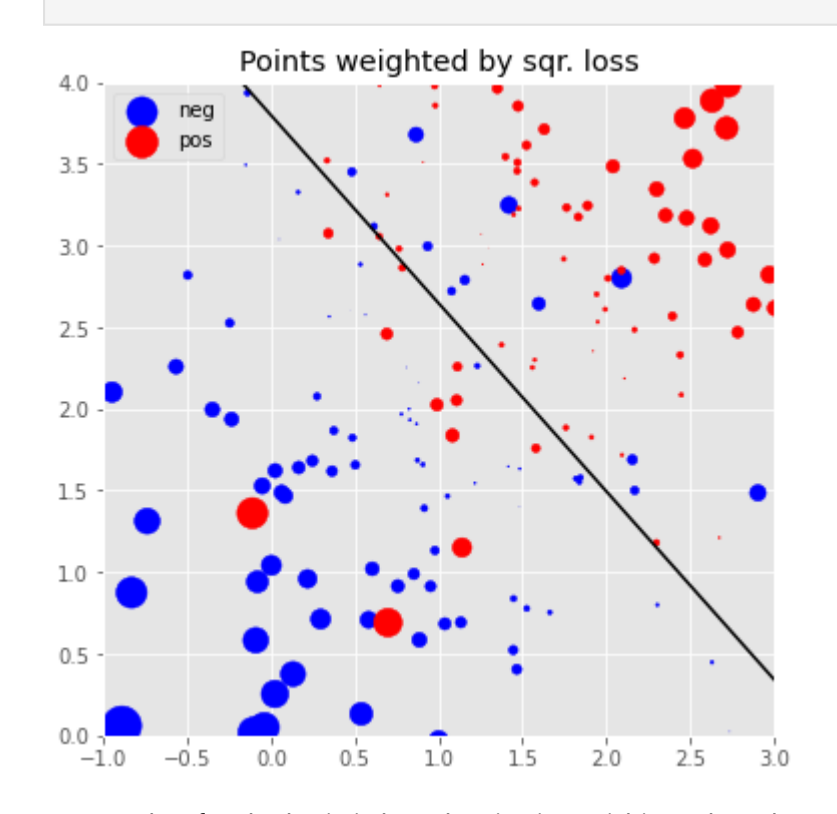
In [25]:
```python
z_log = y_sim*lr_sim.decision_function(X_sim)
logisticloss = np.log(1 + np.exp(-z_log))
plt.scatter(X0[:,0],X0[:,1],s=logisticloss[N:]*30.,c='b',label='neg')
plt.scatter(X1[:,0],X1[:,1],s=logisticloss[:N]*30.,c='r',label='pos')
plt.plot(T,x2hat,c='k')
plt.xlim([-1,3])
plt.ylim([0,4])
plt.title("Points weighted by logistic loss")
_ = plt.legend(loc=2)
```



In [26]:
```python
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([-1,3])
plt.ylim([0,4])
plt.title("Points weighted by hinge loss")
_ = plt.legend(loc=2)
```



In [27]:
```python
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([-1,3])
plt.ylim([0,4])
plt.title("Points weighted by sqr. 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 error loss has increased weight for those far from the hyperplane, even if they are correctly classified. Hence, square error loss is not a good surrogate for 0-1 loss.