4. Logistic Regression

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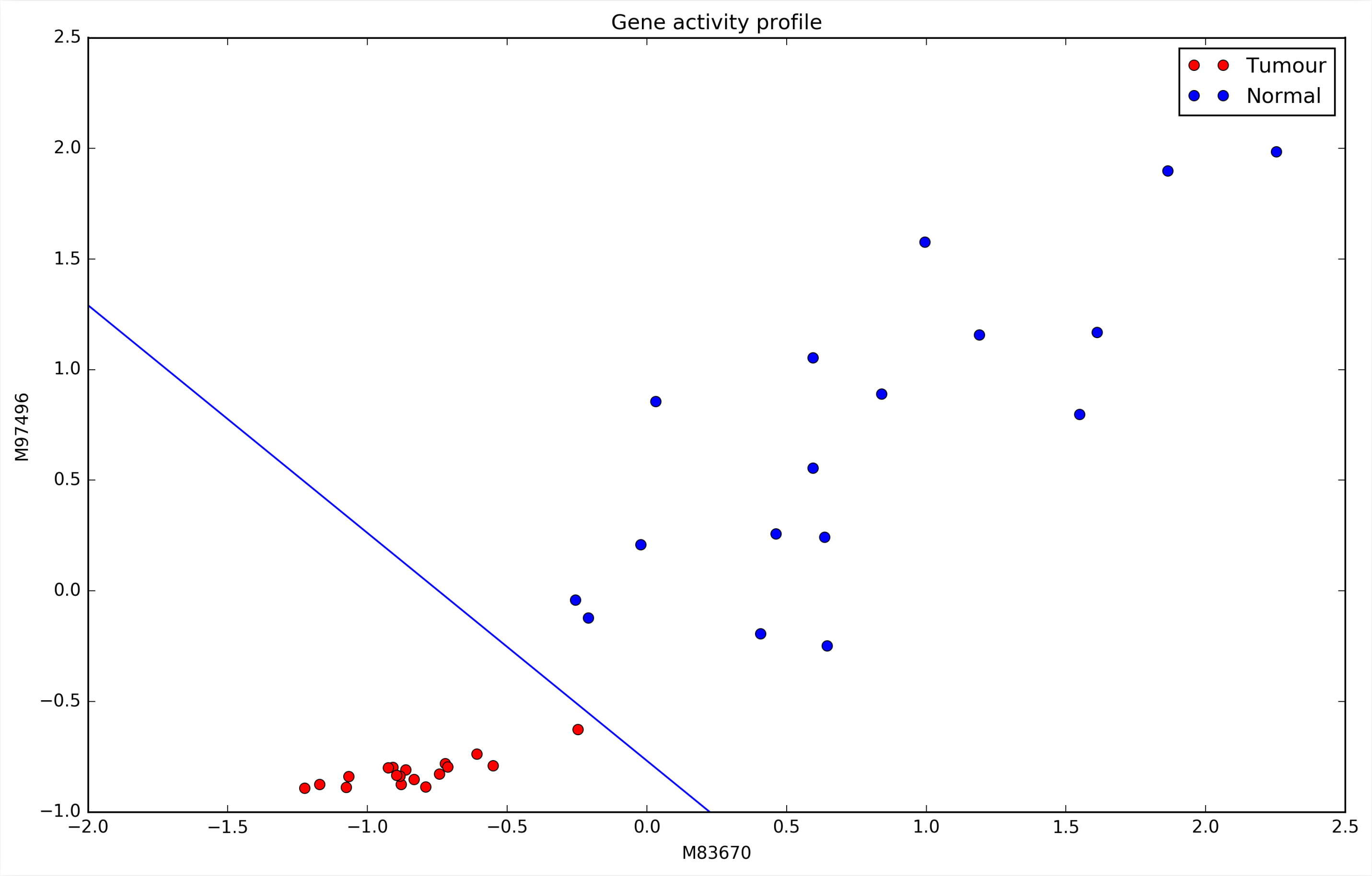
Summary

- Classification, introduction
- Linear separability
- Logistic regression, and playing in higher dimensions

Separability

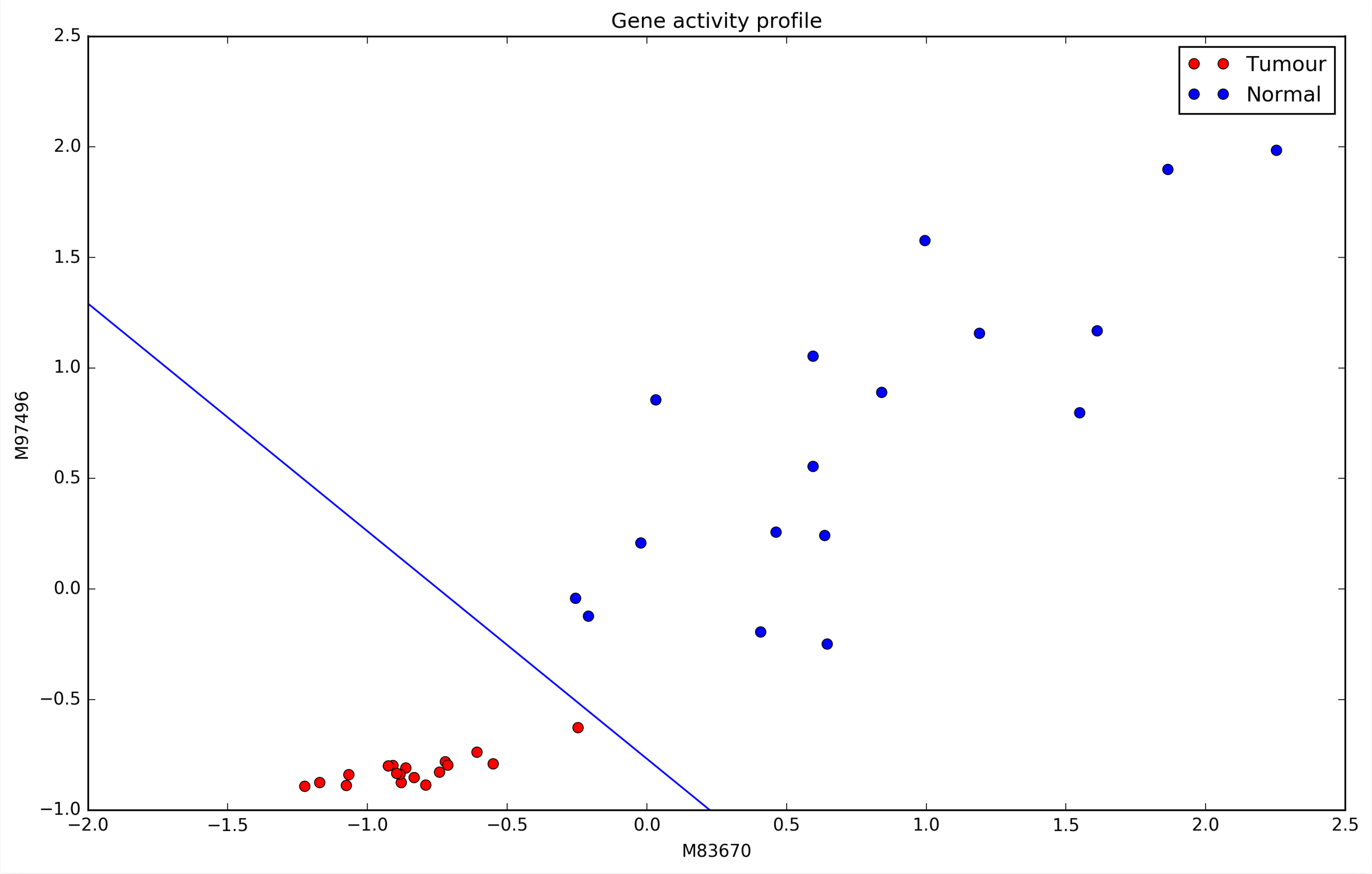
Separability

- Classes are linearly separable if they can be separated by some linear combination of feature values (a hyperplane).



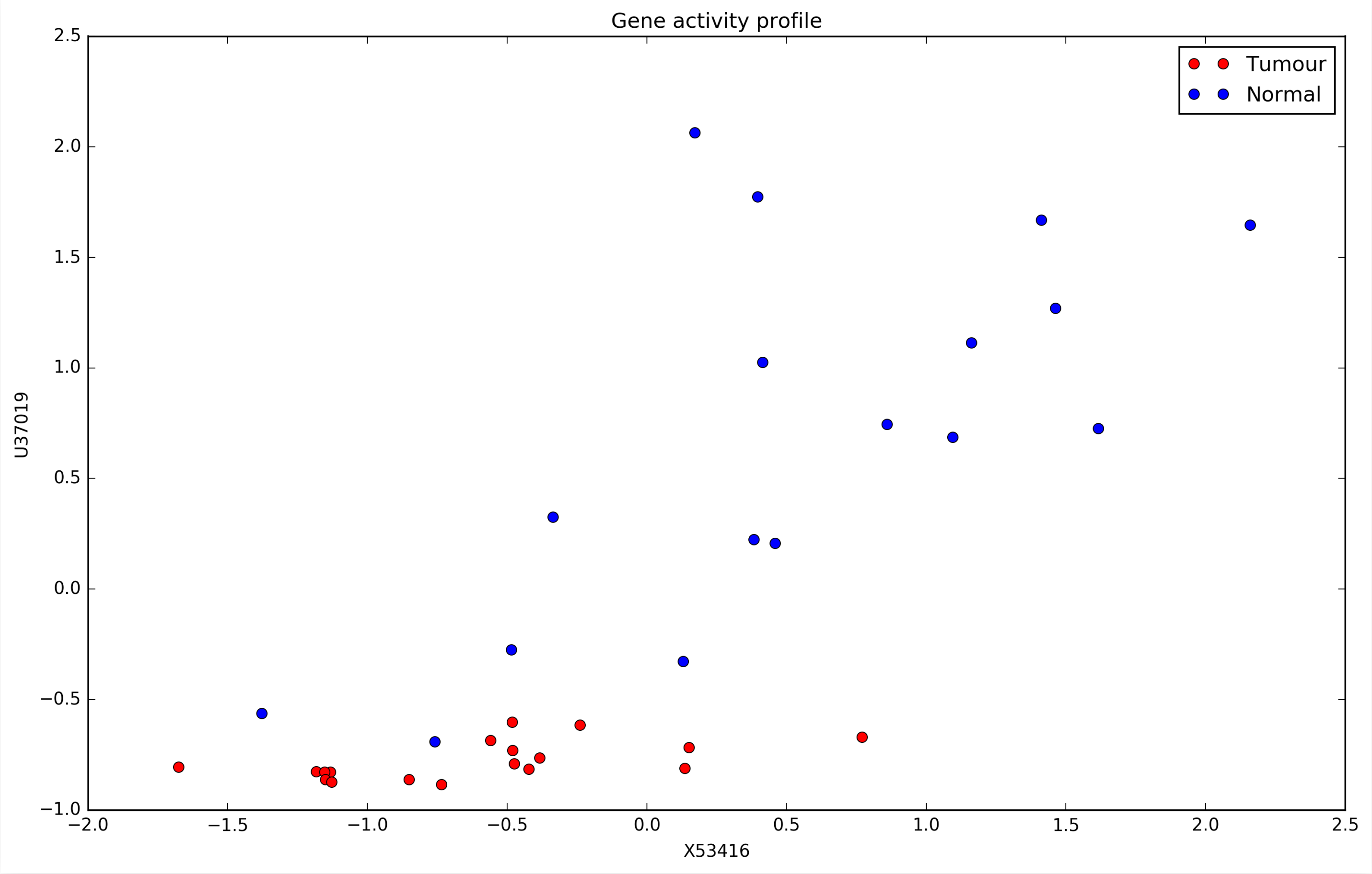
Separability

- This frontier is a linear discriminant.



Separability

- Otherwise, classes in the dataset are not linearly separable



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Separability

Classification

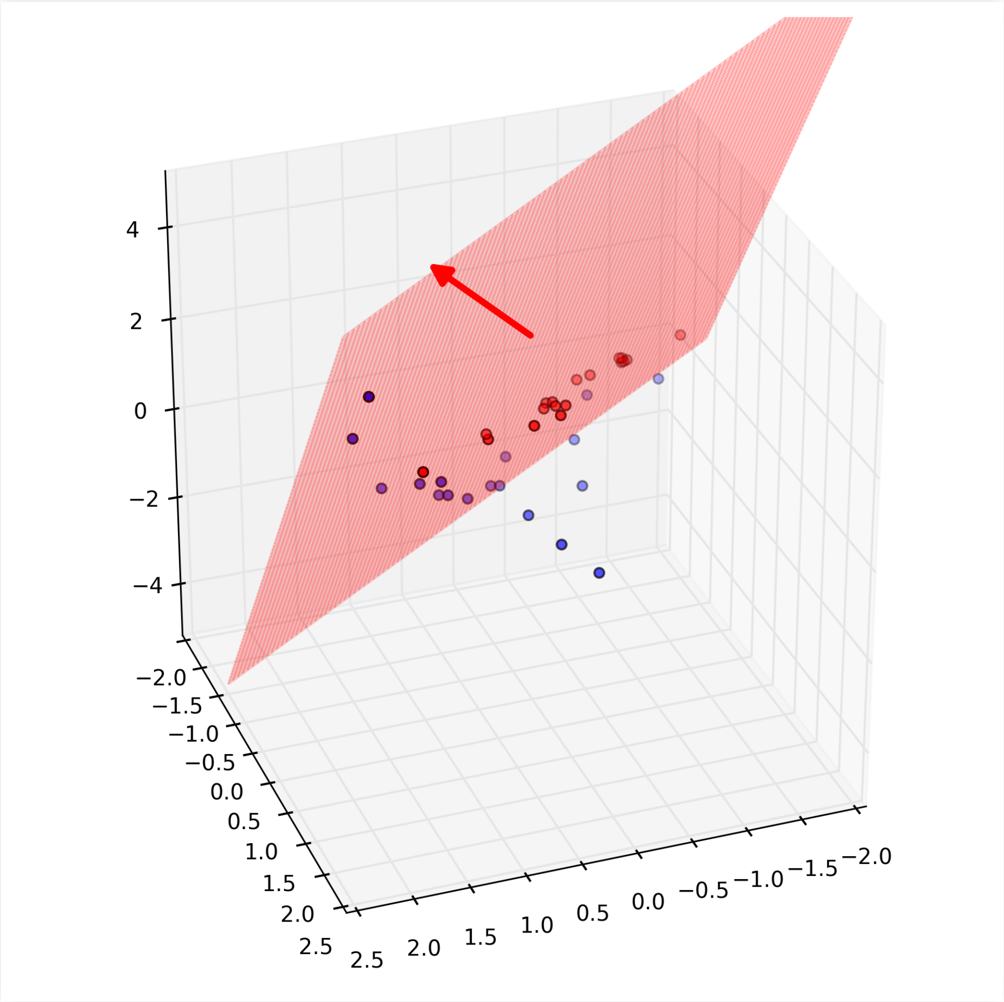
- In regression, we defined a straight line with two parameters:
  $y = \theta_1 x + \theta_2$
- But in classification we need to know which side of the line is which
- More generally, a hyperplane in N dimensions
- This we can do if we define the hyperplane with a perpendicular vector:

$$\vec{w}^T \vec{x} + w_0 = 0$$

- Note: $\vec{x}$ is an N dimensional vector

Separability

$$\vec{w}^T \vec{x} + w_0 = 0$$



Separability

(Linear) Discriminant

- Frontier given by function

$$y(\vec{x}) = \vec{w}^T \vec{x} + w_0$$

  that is positive on one side of the hyperplane and negative on the other.

- So one class is the positive one, the other the negative one.

How do we find the discriminant?

The Wrong Answer

Wrong Answer

Fitting with LMS

- We want to find the best $\vec{w}$ and w_0 for

$$y(\vec{x}) = \vec{w}^T \vec{x} + w_0$$

- This function is negative one one side and positive on the other
- So we can try minimizing the squared error, considering classes 1 and -1:

$$E = \sum_{j=1}^{N} \left(y(\overrightarrow{x_j}) - t_j \right)^2$$

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Fitting with LMS

- Data on gene expression (Uri Alon et. al.,PNAS, 96(12), 1999)

- Carbonic anhydrase IV gene (M83670)
- Guanylate cyclase activator 2A gene (M97496)
- Tumour (1) or Normal (0)

```
-81     10      1
-30     60      1
-1      48      1
4       78      1
...
116     542     0
718     1816    0
332     412     0
```

Wrong Answer

Preprocessing the data

- Need to rescale the values
  - Normalization: $x_{new} = \frac{x - min(X)}{max(X) - min(X)}$
  - Standardization: $x_{new} = \frac{x - \mu(X)}{\sigma(X)}$
- Important: store these parameters and apply to all new points

```
import numpy as np

mat = np.loadtxt('gene_data.txt',delimiter='\t')
Ys = mat[:,[-1]]
Xs = mat[:,:-1]
means = np.mean(Xs,0)
stdevs = np.std(Xs,0)
Xs = (Xs-means)/stdevs
```

Simplifying the expression

- Instead of

$$y(\vec{x}) = \vec{w}^T \vec{x} + w_0$$

- Let's merge the parameters and add a 1 to the feature vectors:

$$\widetilde{w} = (\vec{w}, w_0), \widetilde{x} = (\vec{x}, 1), y(\vec{x}) = \widetilde{w}^T \widetilde{x}$$

- Add the 1s

```
def expand_features(X):
    """append a columns of 1
    """
    X_exp = np.ones((X.shape[0],X.shape[1]+1))
    X_exp[:,:-1] = X
    return X_exp
```

Wrong Answer

Fitting with LMS

- Measure the error
- Note that the class values are 0 and 1, so change to -1 and 1

```
def quad_cost(theta,X,y):
    """return  error value comparing signed distance with y
    """
    coefs = np.zeros((len(theta),1))
    coefs[:,0] = theta
    vals = np.dot(X,coefs)
    return np.mean((vals-(2*y-1))**2)
```

Wrong Answer

Fitting with LMS

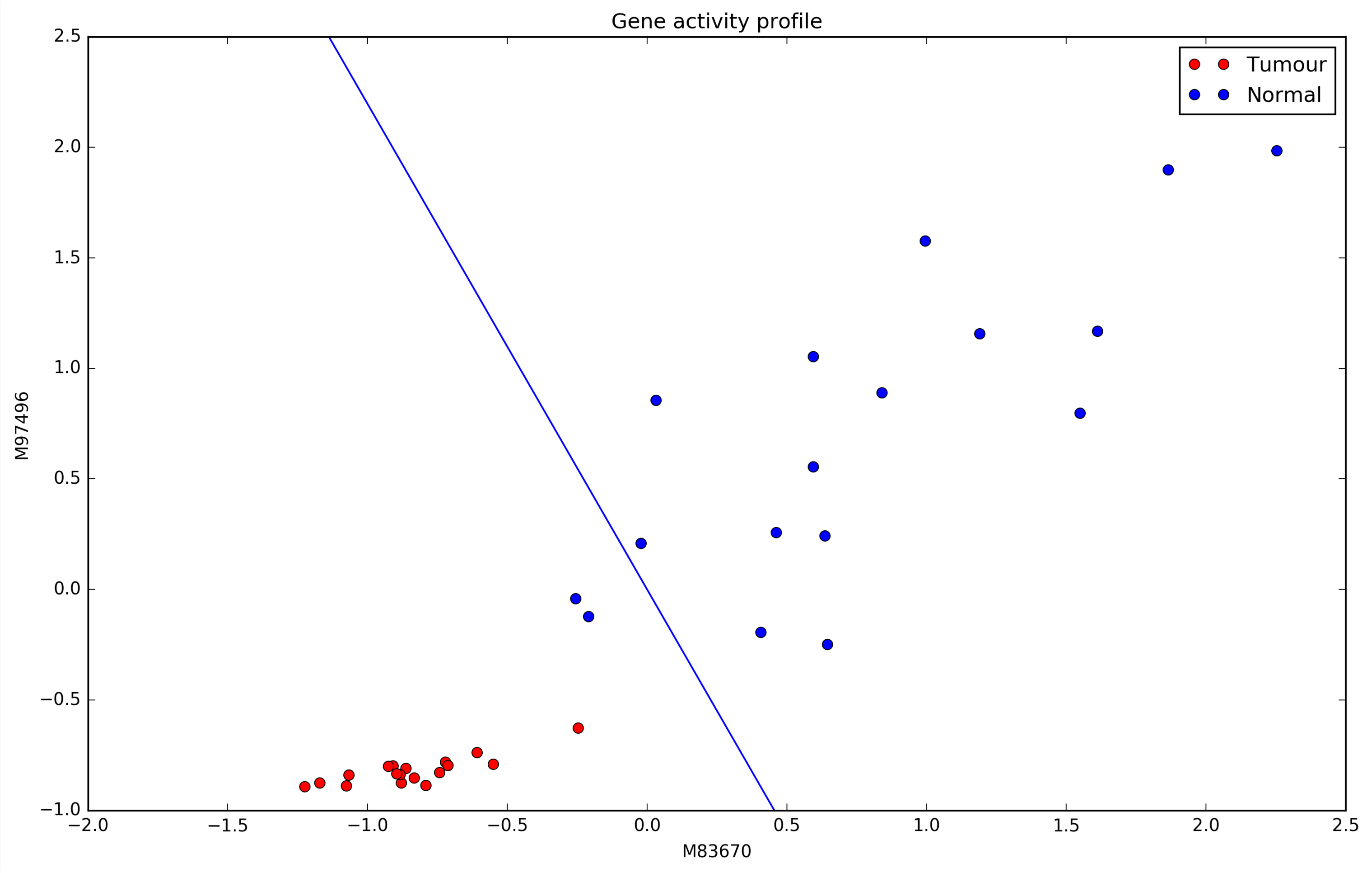
- Minimize the error

```
from scipy.optimize import minimize
import matplotlib.pyplot as plt

X_exp = expand_features(Xs)
coefs = np.ones(X_exp.shape[1])
opt = minimize(quad_cost,coefs,(X_exp,Ys),tol=0.00001)
coefs = opt.x
# plot the chart
```

Wrong Answer

Not a good result...



Wrong Answer

Fitting with LMS

- Not a good result...
- Minimizing the squared error makes points away from the discriminant weigh more
- This is good in regression but bad in classification, as it pulls the discriminant towards distant points

Regression

- Fit the data as closely as possible to predict continuous values

Classification

- Find discriminant between discrete classes

Logistic Regression

Logistic Regression

- Assume there is a function:

$$g(\vec{x}, \widetilde{w}) = P(C_1|\vec{x})$$

- We want our hyperplane to be at

$$P(C_1|\vec{x}) = P(C_0|\vec{x}) = 1 - P(C_1|\vec{x})$$

- Regression on probabilities, but we'll use it as a classifier.
  - Vector $\vec{x}$ is an N dimensional vector of features
  - Based on those features we choose the class with larger estimated probability
- Assumed: $g(\vec{x}, \widetilde{w}) = P(C_1|\vec{x})$
- Plane: $P(C_1|\vec{x}) = P(C_0|\vec{x}) = 1 - P(C_1|\vec{x})$

$$\ln \frac{P(C_1|\vec{x})}{1 - P(C_1|\vec{x})} = 0 = \ln \frac{g(\vec{x}, \widetilde{w})}{1 - g(\vec{x}, \widetilde{w})}$$

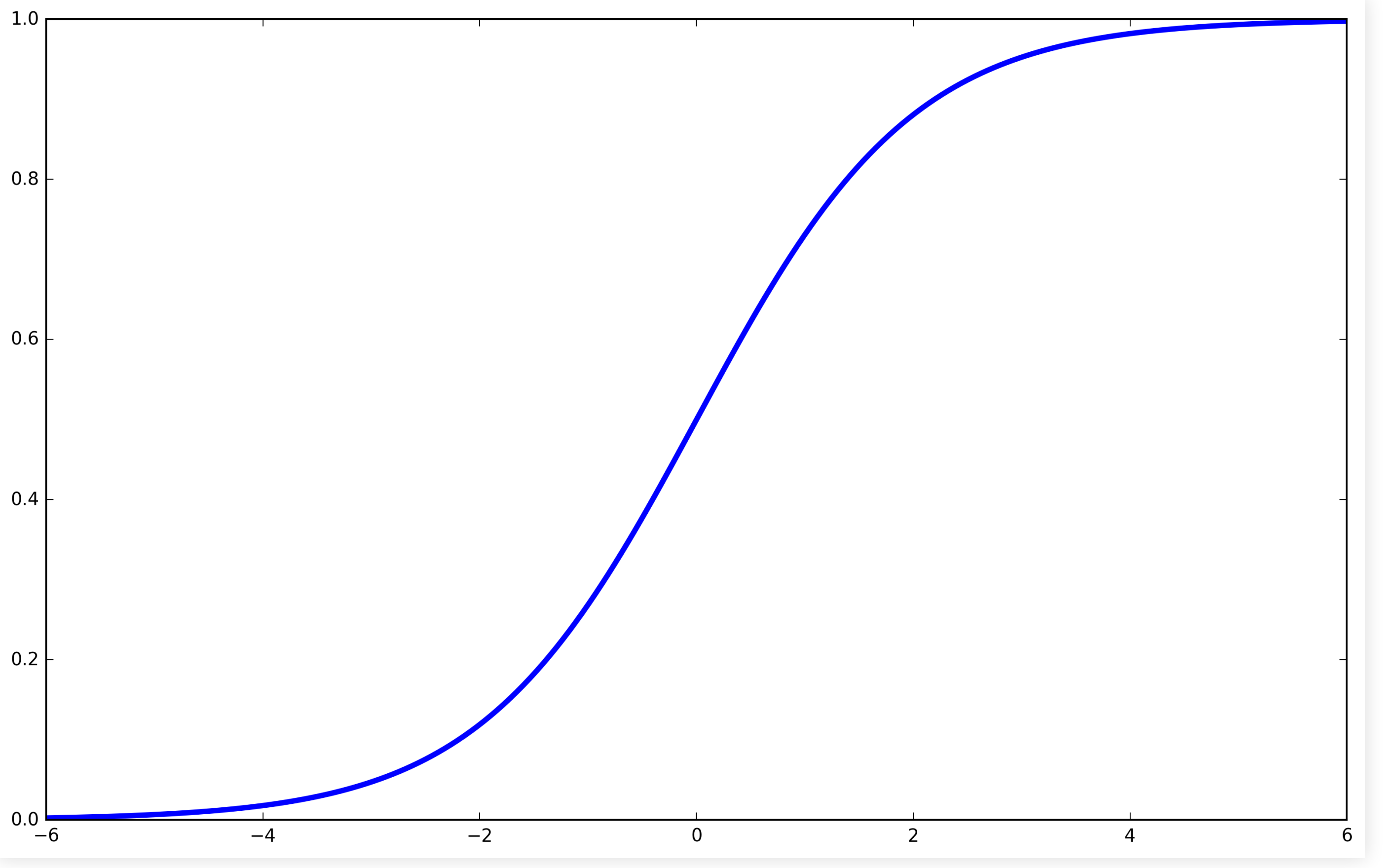
Logistic Regression

- Assumed: $g(\vec{x}, \widetilde{w}) = P(C_1|\vec{x})$
- Plane: $P(C_1|\vec{x}) = P(C_0|\vec{x}) = 1 - P(C_1|\vec{x})$

$$\ln \frac{g(\vec{x}, \widetilde{w})}{1 - g(\vec{x}, \widetilde{w})} = \vec{w}^T \vec{x} + w_0$$

$$ln \frac{g(\vec{x}, \widetilde{w})}{1 - g(\vec{x}, \widetilde{w})} = \vec{w}^T \vec{x} + w_0 \Leftrightarrow g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-(\vec{w}^T \vec{x} + w_0)}}$$

Logistic Function: $f(x) = \frac{1}{1+e^{-k(x-x_0)}}$

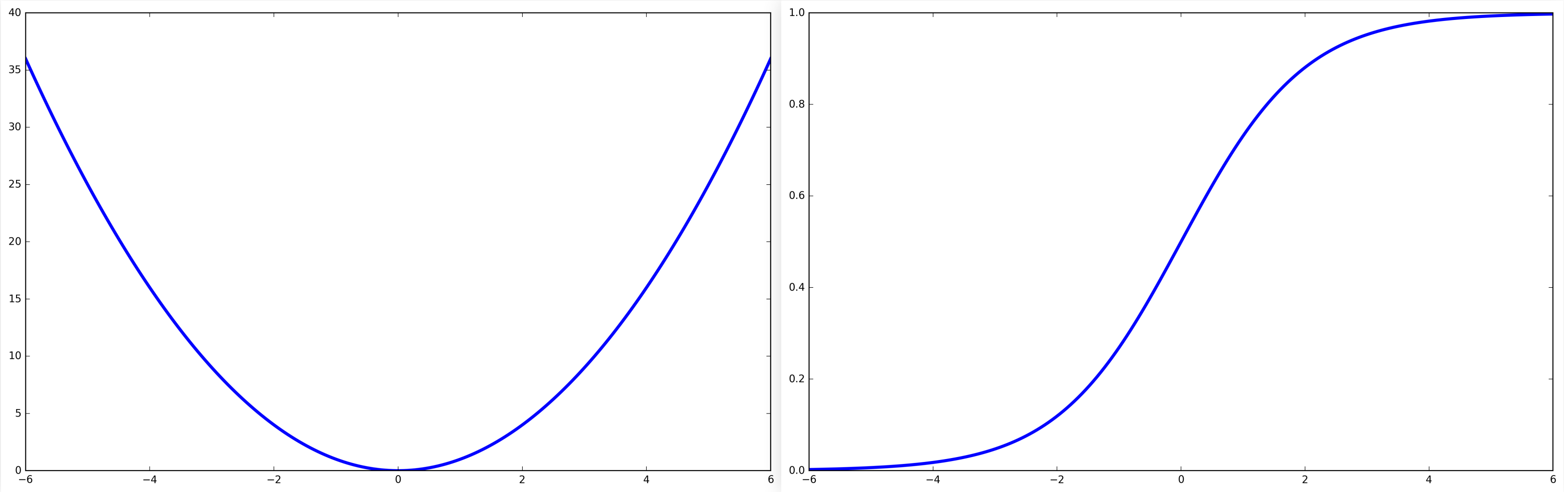


Logistic Regression

Logistic Function

- Unlike quadratic curve, logistic function levels with distance

$$g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-(\vec{w}^T \vec{x} + w_0)}}$$



- This solves the problem of points farther away pulling the discriminant

Logistic Regression

- How to find find $\widetilde{w}$ by maximum likelihood
- Given: $g(\vec{x}, \widetilde{w}) = P(t_n = 1|\vec{x})$ and $t_n \in \{0, 1\}$

$$\mathcal{L}(\widetilde{w}|X) = \prod_{n=1}^{N} \left[g_n^{t_n} (1 - g_n)^{1-t_n} \right]$$

$$l(\widetilde{w}|X) = \sum_{n=1}^{N} [t_n \ln g_n + (1 - t_n) \ln(1 - g_n)]$$

- Maximize likelihood is to minimize the error in predicting probabilities (logistic loss or cross entropy):

$$E(\widetilde{w}) = -\frac{1}{N} \sum_{n=1}^{N} [t_n \ln g_n + (1 - t_n) \ln(1 - g_n)]$$

$$g_n = \frac{1}{1 + e^{-(\vec{w}^T \vec{x_n} + w_0)}}$$

Example 1: linearly separable

Example 1

- Load and standardize the data (as before)
- Write logistic function (Note: you won't be doing this)

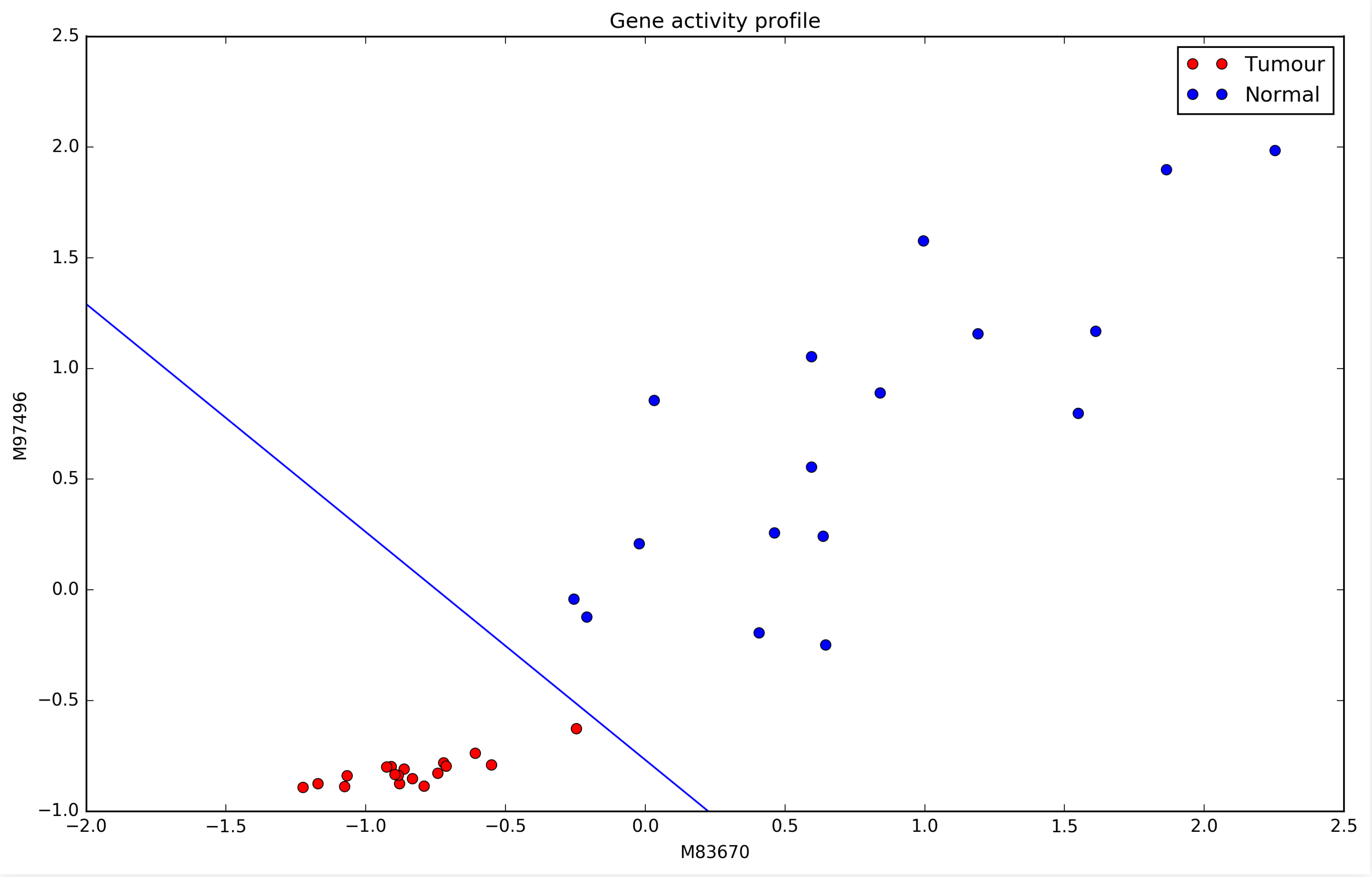
```
def logistic(X):
    """return logistic function of vector X"""
    den = 1.0 + np.e ** (-1.0 * X)
    return 1.0 / den
```

- And the logistic cost function to minimize

```
def log_cost(theta,X,y):
    """return  logistic error value
       X is matrix, one example per row and 1 in last column
       y is a vector of classes 0 or 1
    """
    coefs = np.zeros((len(theta),1))
    coefs[:,0] = theta
    sig_vals = logistic(np.dot(X,coefs))
    log_1 = np.log(sig_vals)*y
    log_0 = np.log((1-sig_vals))*(1-y)
    return -np.mean(log_0+log_1)
```

Example 1

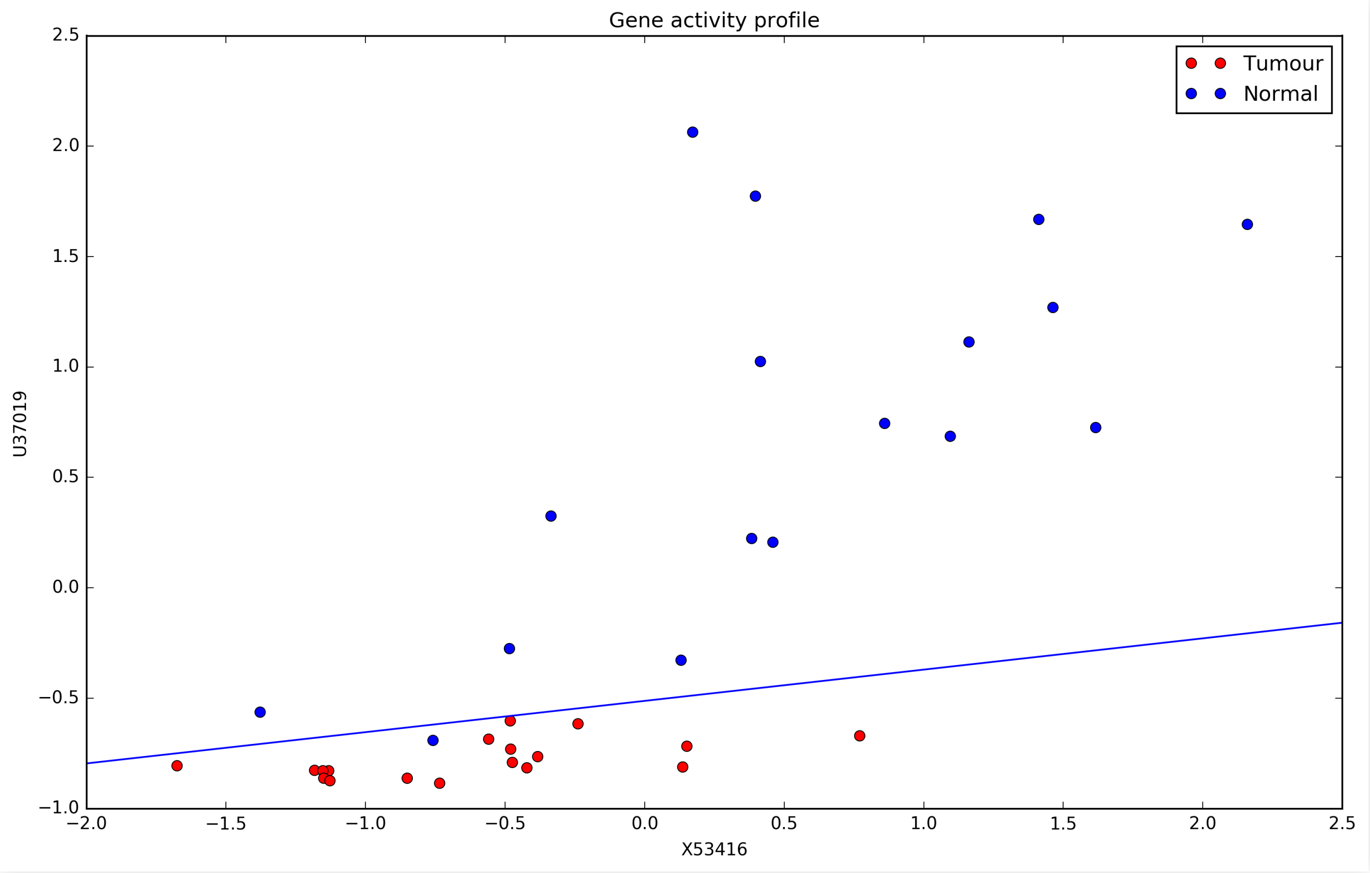
- Minimizing this function, we get a better result:



Nonlinear Separability

This set is not linearly separable

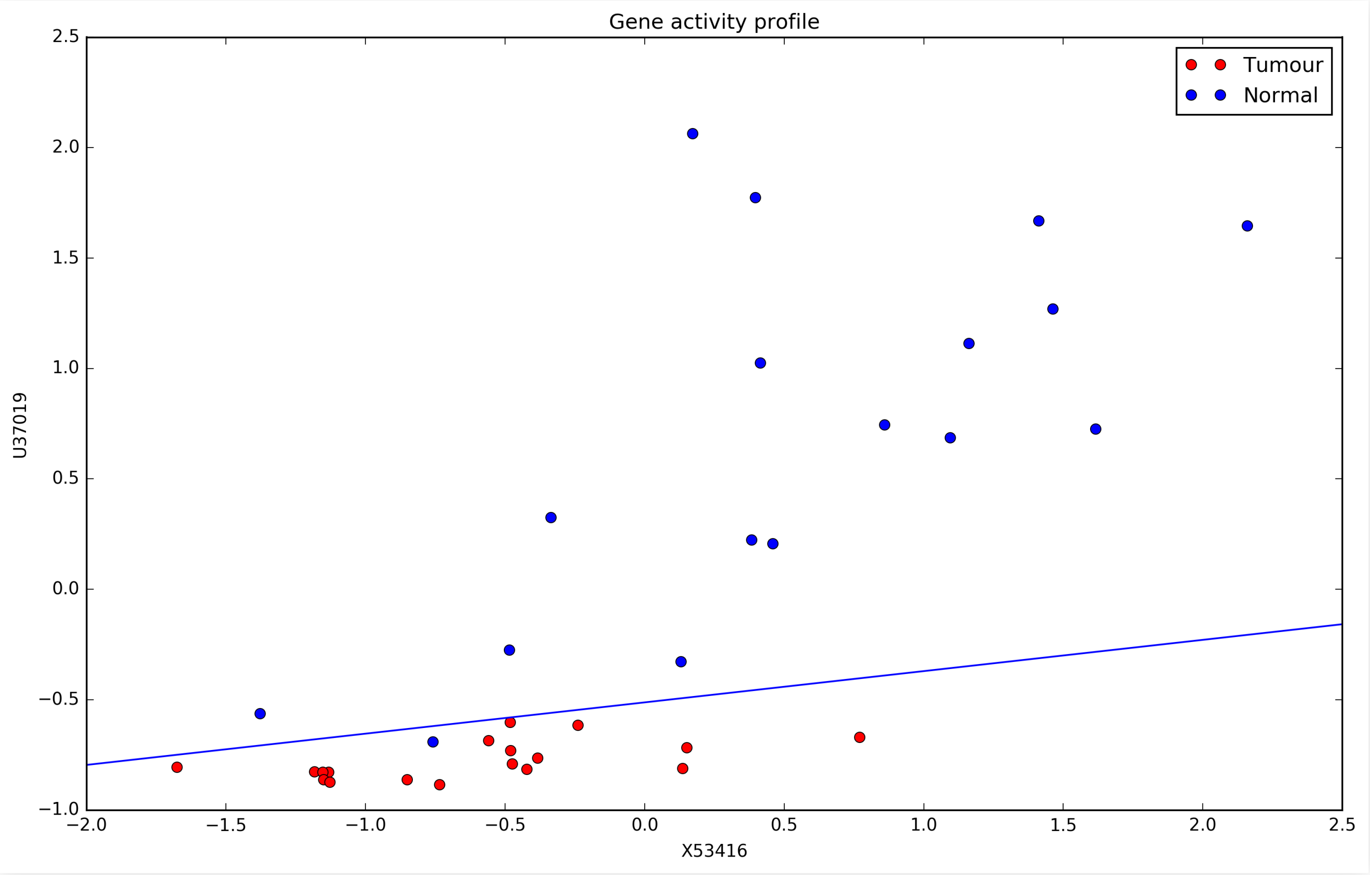
Actin-binding protein X53416, smooth muscle cell Ca binding protein U37019



Nonlinear Separability

This set is not linearly separable

- But we can expand the features (nonlinearly).



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Nonlinear Separability

- First, we add a term $x_1 \times x_2$

```
def poly_3features(X):
    """append a column with the product of the two first features
    """
    X_exp = np.zeros((X.shape[0],X.shape[1]+1))
    X_exp[:,:-1] = X
    X_exp[:,-1] = X[:,0]*X[:,1]
    return X_exp
```

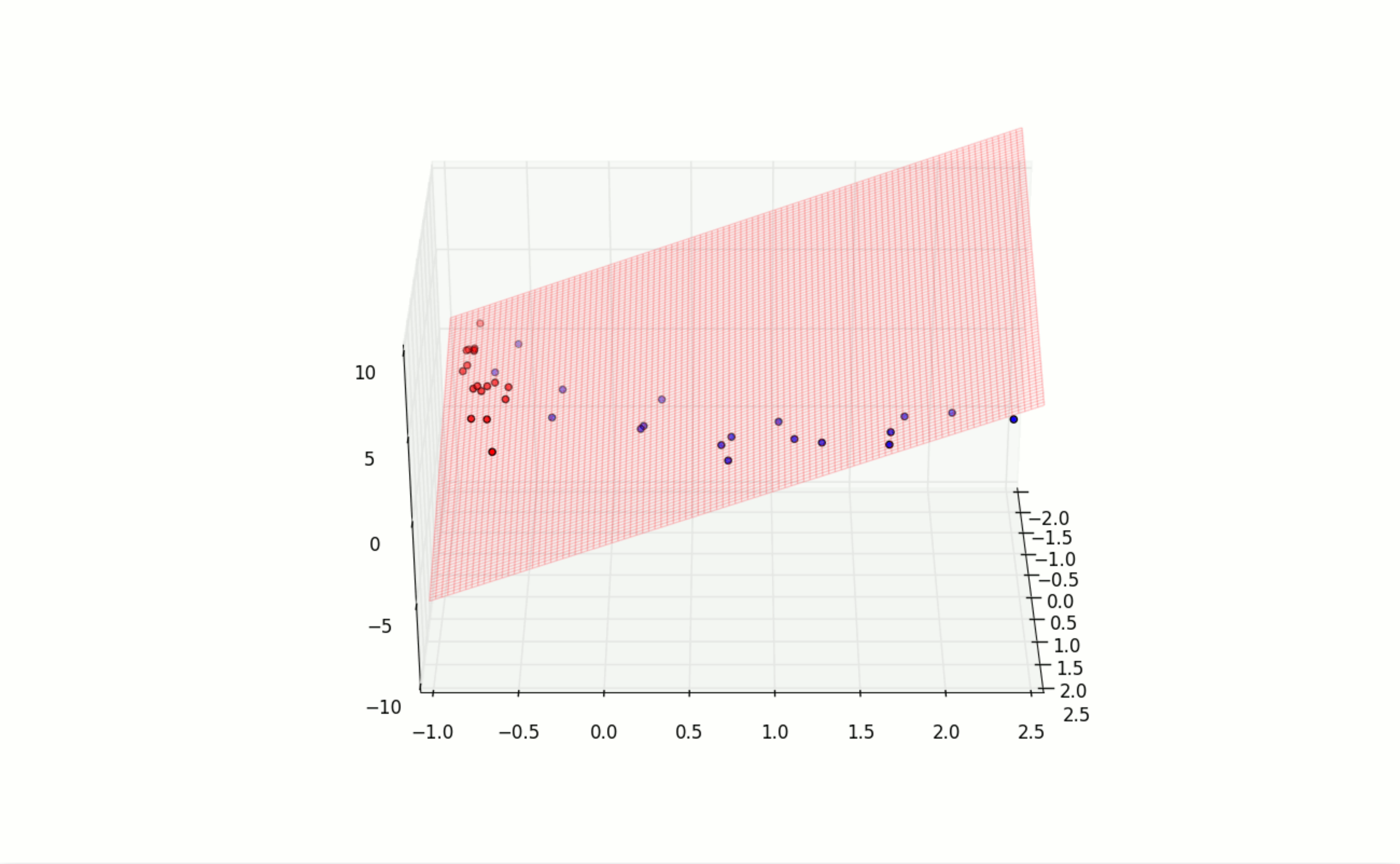
- And we do a logistic regression in 3D

```
from sklearn.linear_model import LogisticRegression

#load and standardize data
X_exp = poly_3features(Xs)
reg = LogisticRegression(C=1e12, tol=1e-10)
reg.fit(X_exp,Ys[:,0])
```

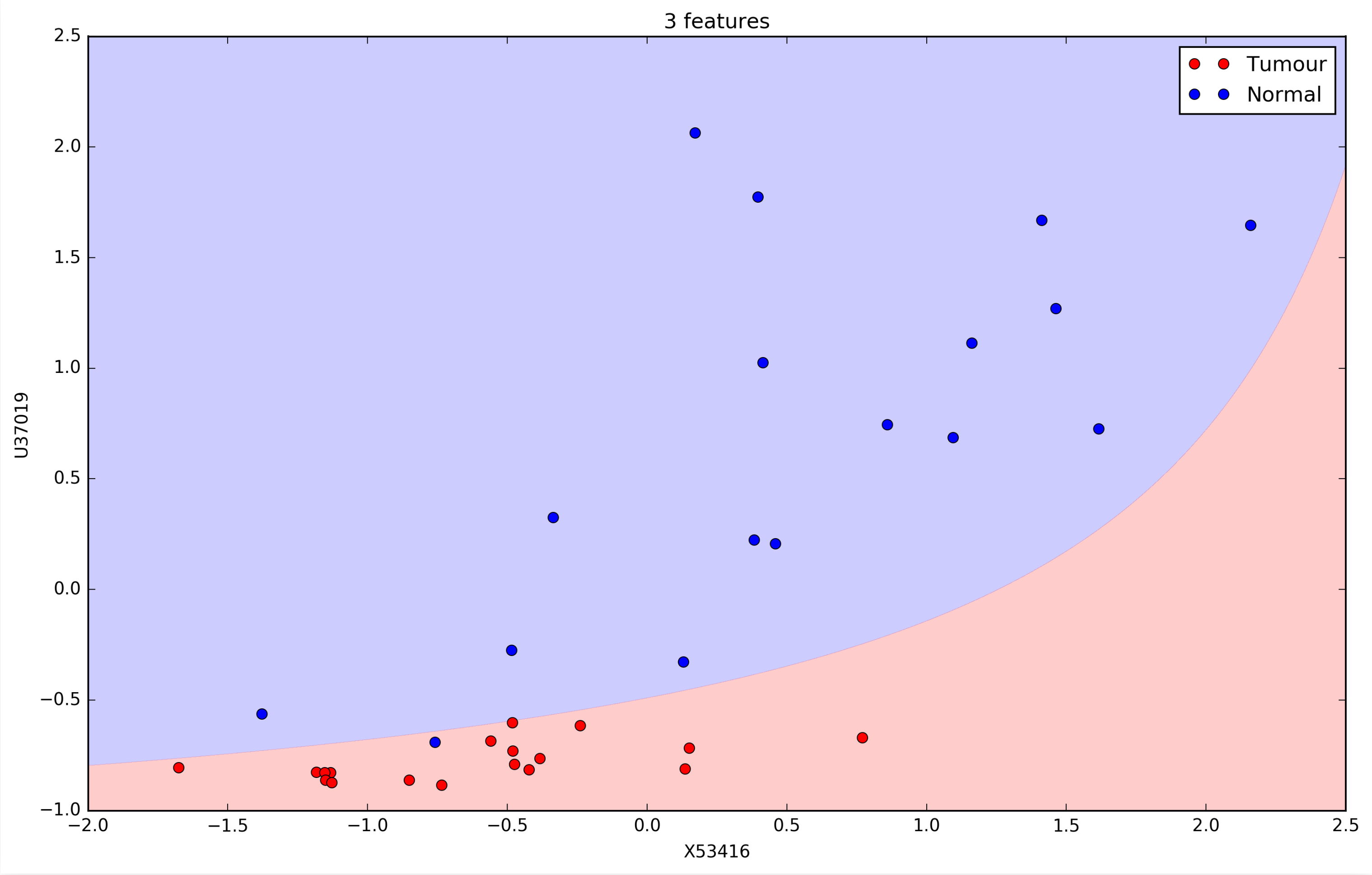
Nonlinear Separability

- This fits a plane in a 3D feature space



Nonlinear Separability

- Project back into the original plane



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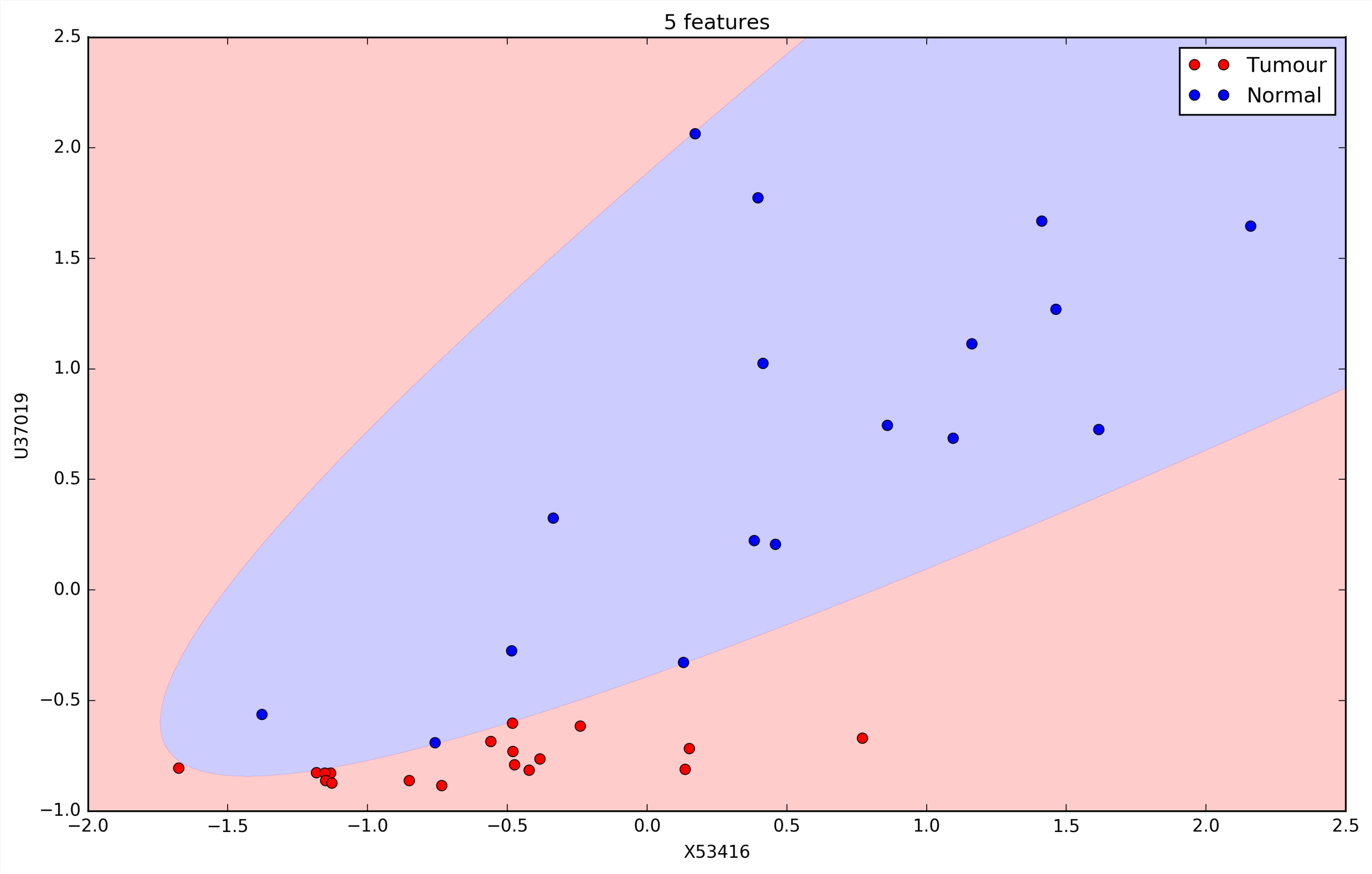
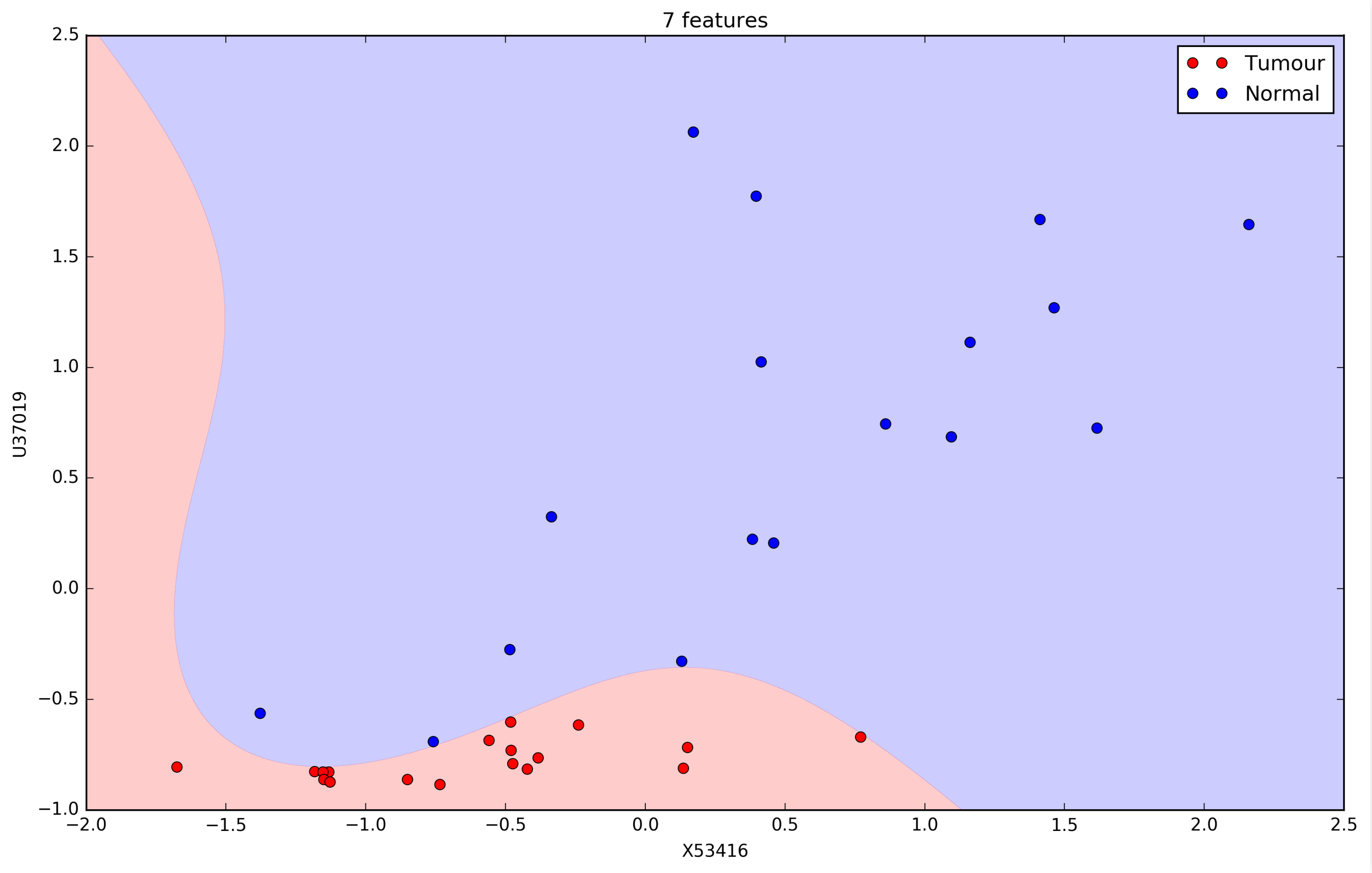
Nonlinear Separability

- Expand more: $x_1, x_2, x_1x_2, x_1^2, x_2^2$



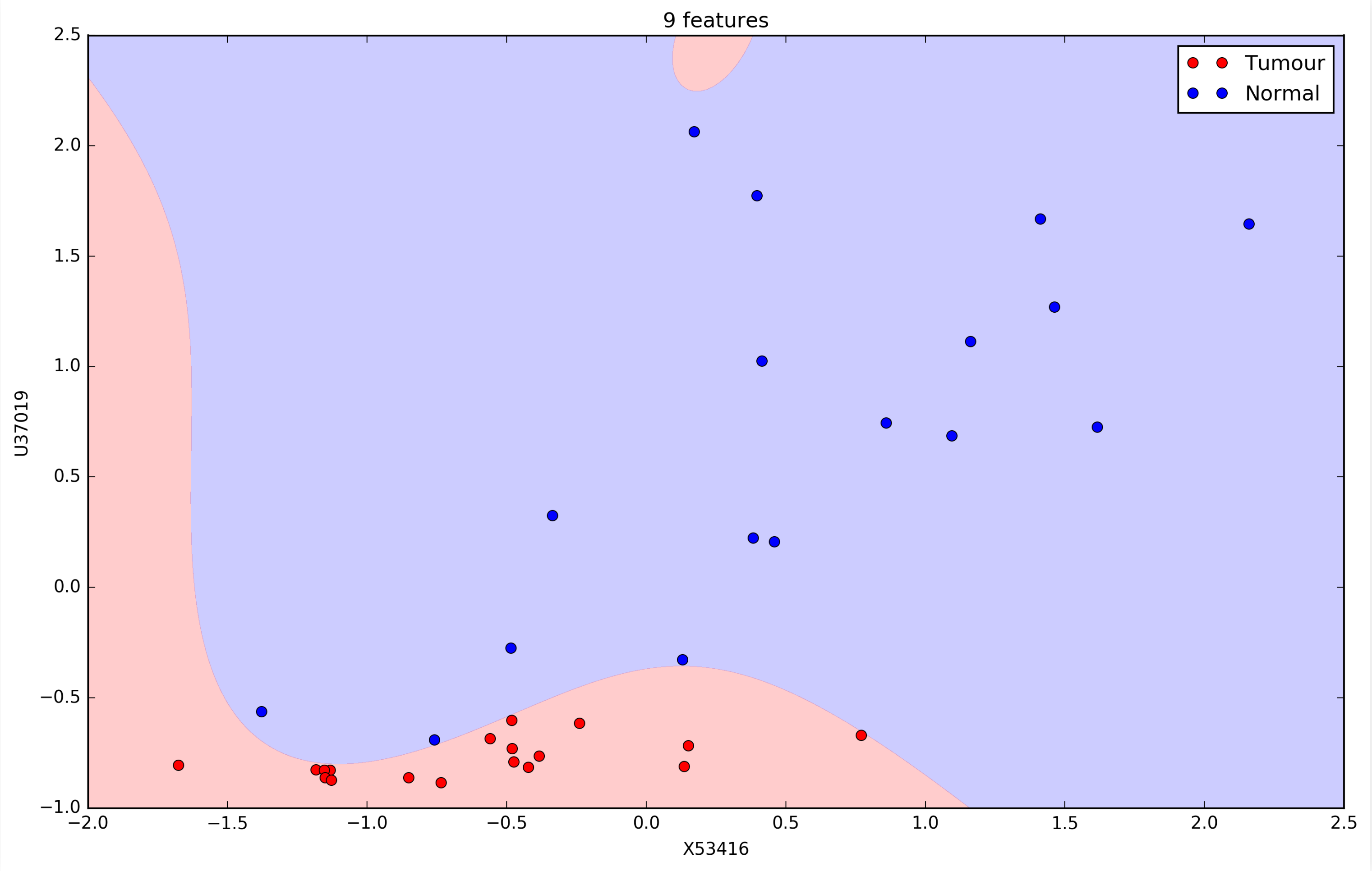
Nonlinear Separability

- Expand more: $x_1, x_2, x_1 x_2, x_1^2, x_2^2, x_1^3, x_2^3$



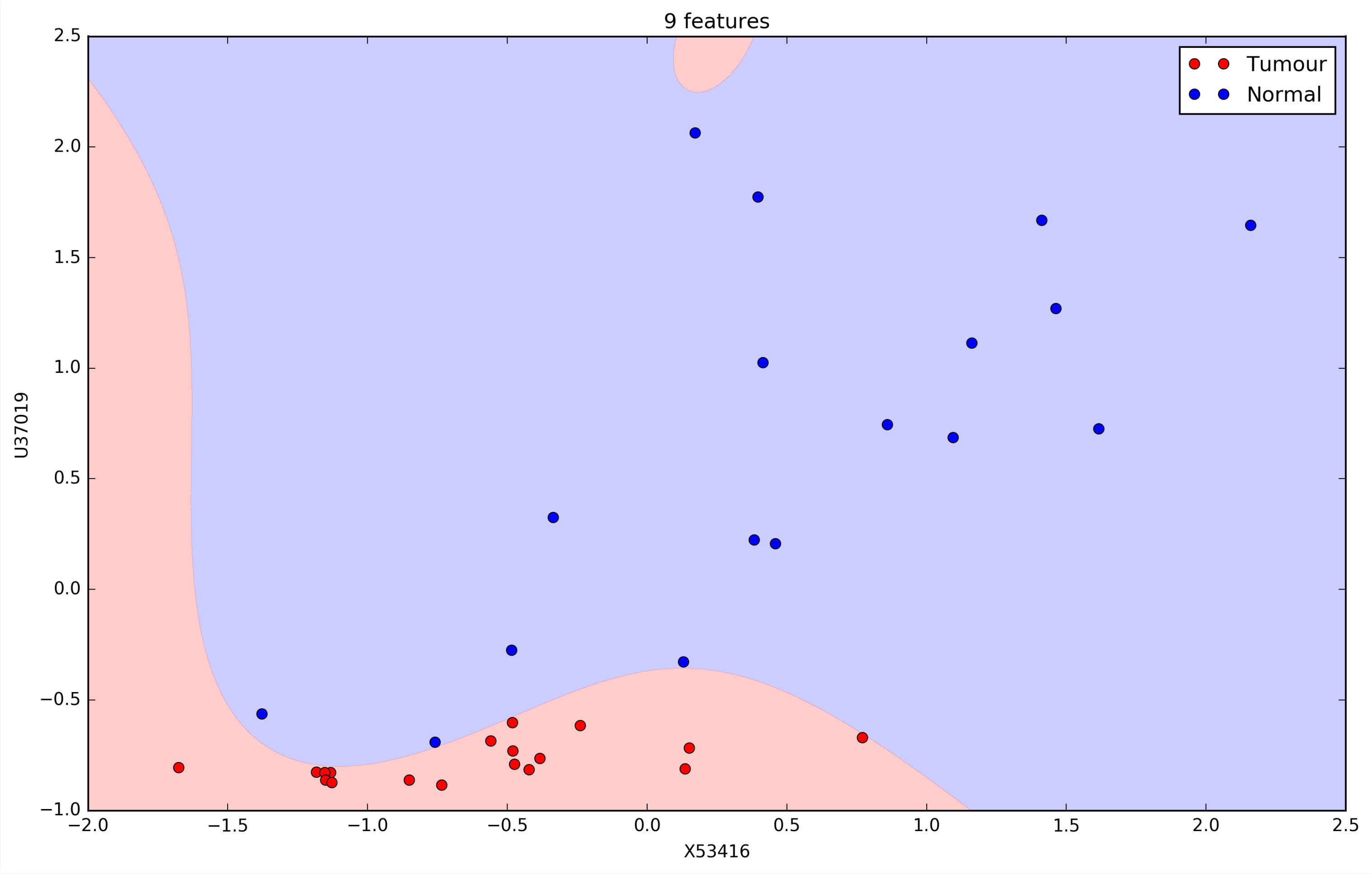
Nonlinear Separability

- Expand more: $x_1, x_2, x_1x_2, x_1^2, x_2^2, x_1^3, x_2^3, x_1^2x_2, x_1x_2^2$



Nonlinear Separability

- Is this too much? Overfitting?



Summary

Logistic Regression

Summary

- Linear separability
- Linear discriminant (hyperplane)
- ~~Fitting the discriminant with LMS~~
- Logistic Regression
- Linear separability in higher dimensions
- Next lecture: overfitting in classification

Further reading

- Bishop, Sections 4.1.1, 4.1.3 and 4.3.2