Transformation to add a ”missing” numeric feature

Regression: missing feature

We have seem an example of a missing numeric feature in the past.

Recall our example illustrating linear regression

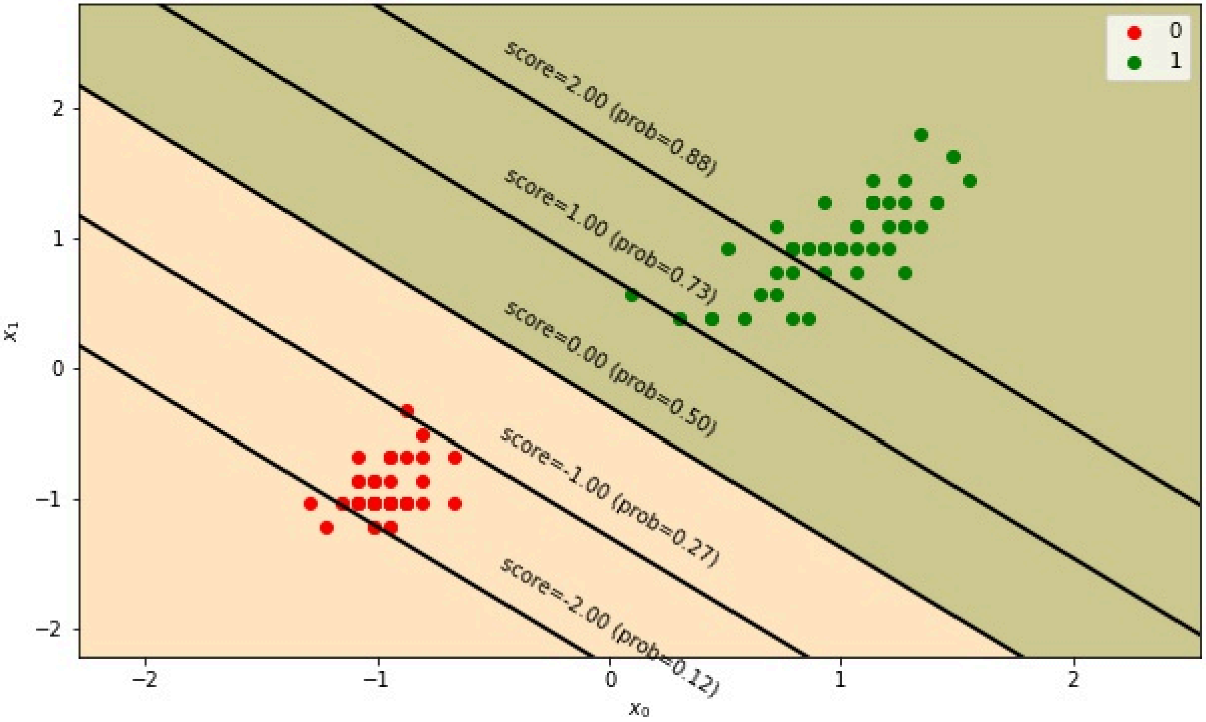
- the first model hypothesized the relationship as
$$\mathbf{y} = \Theta_0 + \Theta_1 \mathbf{x}$$
- Error Analysis revealed a systemic error
- Causing us to add another feature (the square of the first feature)
$$\mathbf{y} = \Theta_0 + \Theta_1 \mathbf{x} + \Theta_2 \mathbf{x}^2$$

Classification: missing feature

The Logistic Regression Classifier

- is a type of Classifier
- that creates a *linear surface* to separate classes

Separation bounday as function of probability threshold

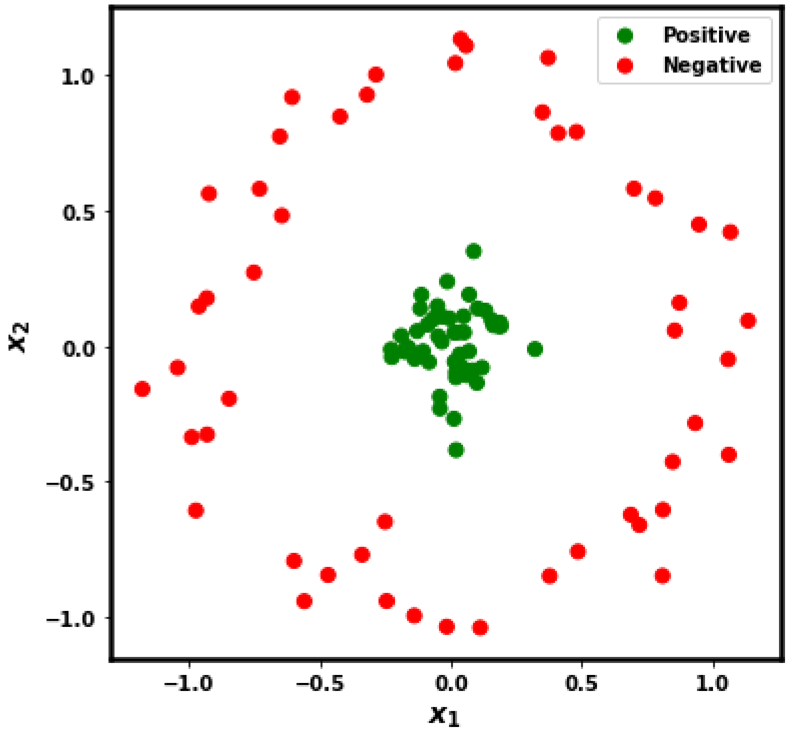


But what if the data is such that a linear surface cannot separate classes ?

- we can use a classifier that *does not* assume linear separability (KNN, Decision Trees)
- **or** we can add a feature to make the classes linearly separable
    - here: we illustrate with a numeric feature

Consider Binary Classification on the following "bulls-eye" dataset.

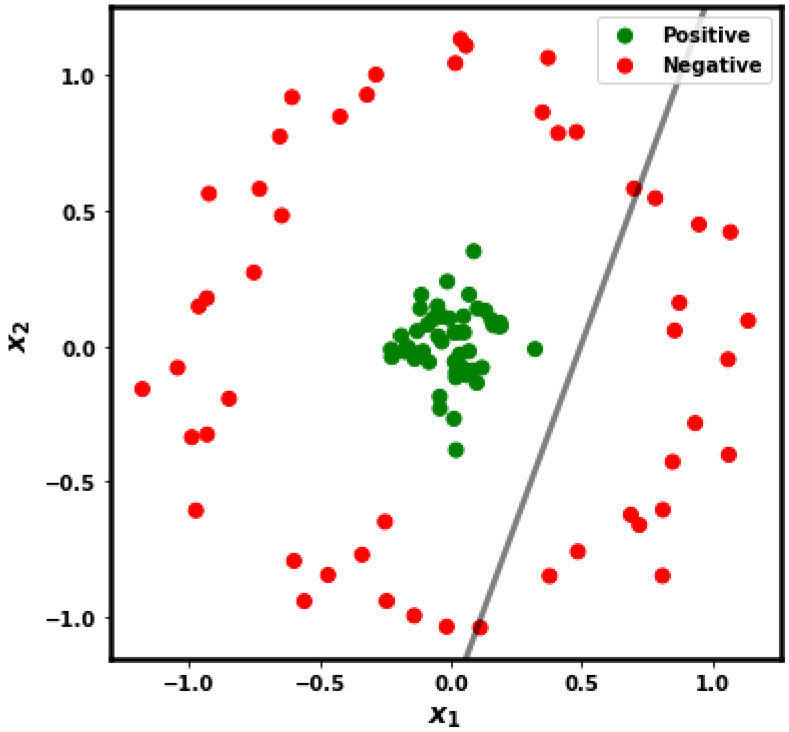
In [5]:
```
fig, ax = plt.subplots(1,1, figsize=(6,6) )
Xc, yc = svmh.make_circles(ax=ax, plot=True)
```



Visually, we can see that the classes are separable, but clearly not by a line.

Here's what one linear classifier (an SVC, which we will study later) produces

In [6]:
```
fig, ax = plt.subplots(1,1, figsize=(6,6) )
svm_clf = svmh.circles_linear(Xc, yc, ax=ax)
```



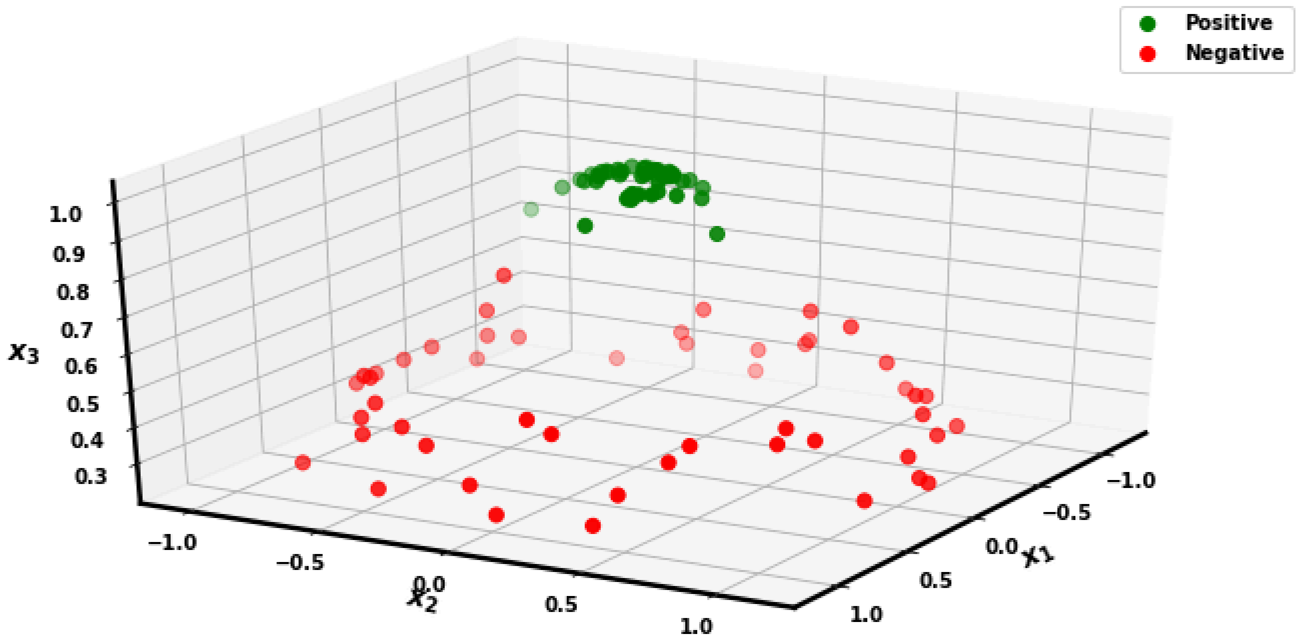
Let's add a new *numeric* feature defined by the (Gaussian) *Radial Basis Function (RBF)*

$$\mathbf{x}_3 = e^{-\sum_j \mathbf{x}_j^2}$$

Our features are now 3 dimensional; let's look at the plot:

In [7]:

```
X_w_rbf = svmh.circles_rbf_transform(Xc)
_= svmh.plot_3D(X=X_w_rbf, y=yc )
```



Magic !

The new feature is such that it is

- greatest at origin $(\mathbf{x}_1, \mathbf{x}_2) = (0, 0)$
- decreasing as you move away from the origin

The new feature enables a plane that is parallel to the $\mathbf{x}_1, \mathbf{x}_2$ plane to separate the two classes.

We can write the RBF transformation to reference an arbitrary origin $\mathbf{x}_c$

$$\text{RBF}(\mathbf{x}) = e^{-||\mathbf{x} - \mathbf{x}_c||}$$

- $||\mathbf{x} - \mathbf{x}_c||$ is a measure of the distance between example $\mathbf{x}$ and reference point $\mathbf{x}_c$
- In our case
    - $||\mathbf{x} - \mathbf{x}_c||$ is the L2 (Euclidean) distance
    - $\mathbf{x}_c$ is the origin $(0, 0)$

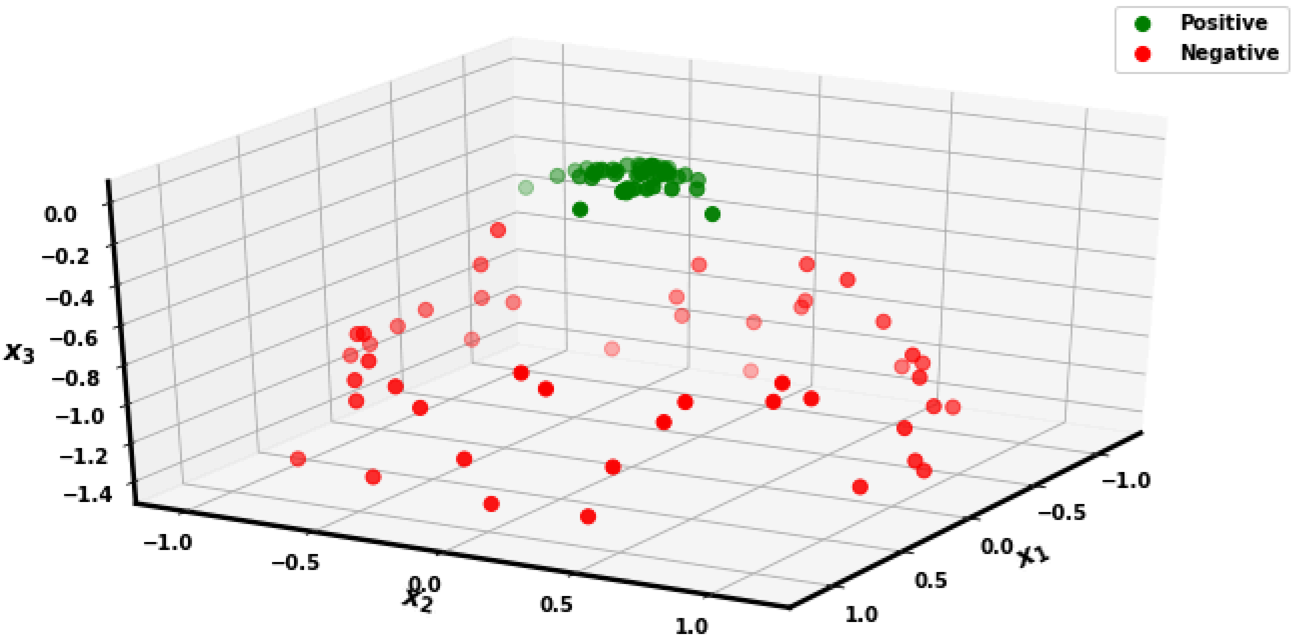
There is an even simpler transformation we could have used

$$\mathbf{x}_3 = -||\mathbf{x} - \mathbf{x}_c||^2$$

That is: the (negative) of the L2 distance.

The advantage of the RBF is that it has little effect on points far from the reference point.

In [8]:
```
X_w_rad = svmh.circles_radius_transform(Xc)
_= svmh.plot_3D(X=X_w_rad, y=yc )
```



The common aspect of each transformation

- observation that there are a set of examples with green labels
- centered around a point (origin)

The transformation added a feature that was greatest in magnitude around those points.mm

Curved boundaries and Linear Classifiers

Recall the transformation of adding a higher order polynomial feature for the "curvy" dataset

$$\mathbf{y} = \Theta_0 + \Theta_1 \mathbf{x} + \Theta_2 \mathbf{x}^2$$

This equation is *still linear* in the two features $\mathbf{x}_1$ and $\mathbf{x}_1^2$.

In Classification, we can created *curved boundaries* that are *still linear* in their features.

- But clearly not linear in raw features

The two plots below use a Classifier requiring Linear Separability of the examples

- the right plot adds a polynomial feature
- creating a curved boundary
- even though the equation is still linear in the features

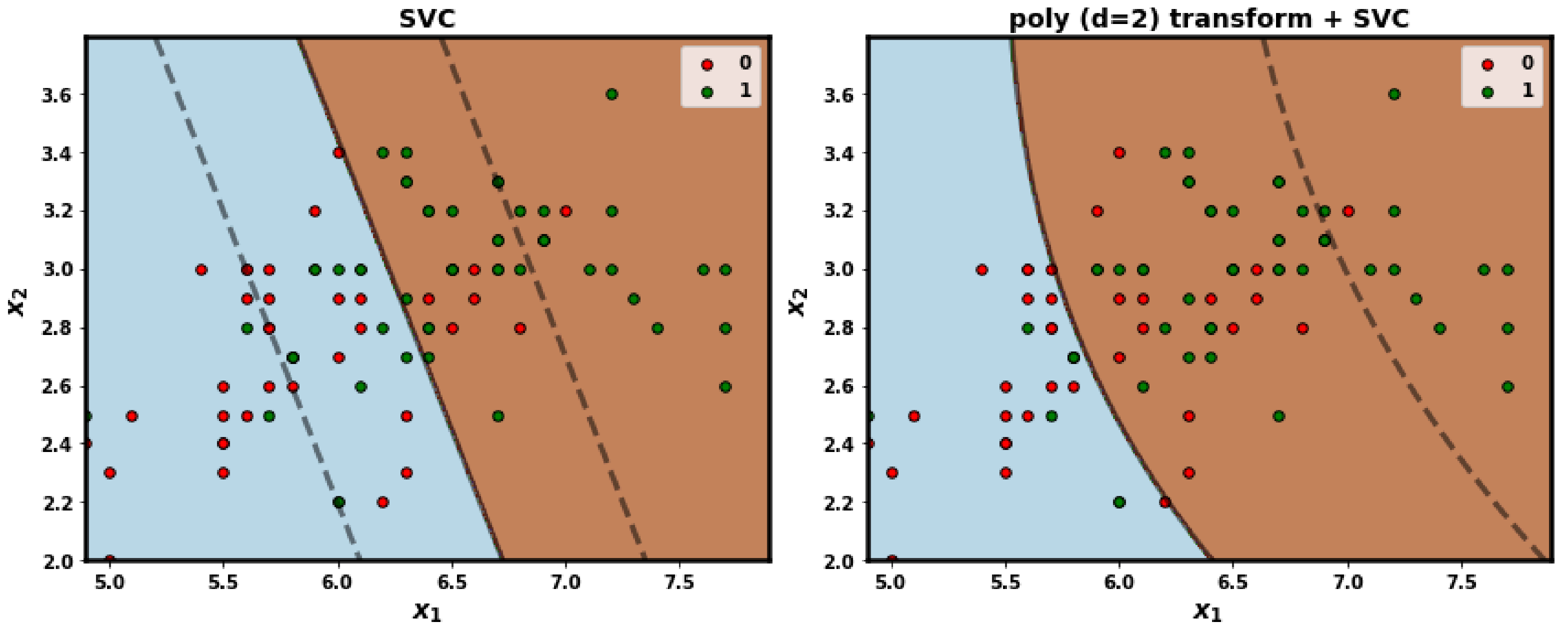
In [9]:

```
svmh = svm_helper.SVM_Helper()

_= svmh.create_kernel_data()

gamma=1
C=0.1

linear_kernel_svm = svm.SVC(kernel="linear", gamma=gamma)

# Pipelines
feature_map_poly2 = PolynomialFeatures(2)
poly2_approx = pipeline.Pipeline( [ ("feature map", feature_map_poly2),
                                    ("svm", svm.LinearSVC())
                                  ])

classifiers =  [ ("SVC", linear_kernel_svm),
                 ("poly (d=2) transform + SVC", poly2_approx)
               ]
_= svmh.create_kernel_data(classifiers=classifiers)
fig, axs = svmh.plot_kernel_vs_transform()
plt.close()
```

```
/home/kjp/anaconda3/lib/python3.7/site-packages/sklearn/svm/base.py:929: Conve
rgenceWarning: Liblinear failed to converge, increase the number of iteration
s.
  "the number of iterations.", ConvergenceWarning)
```

In [10]:
```
fig
```

Out[10]:



- Left plot shows a boundary that is linear in raw features
- Right plot show a boundary that is linear in transformed features
    - plotted in the dimensions of raw features

The transformation results in a boundary shape with greater flexibility.

Transformations should be motivated by logic, not magic !

Although the transformation on the "bulls-eye" dataset seems magical, we must be skeptical of magic

- There should be some *logical* justification for the added feature
- Without such logic: we are in danger of overfitting and will fail to generalize to test examples

For example:

- Perhaps $\mathbf{x}_1, \mathbf{x}_2$ are geographic coordinates (latitude/longitude)
- There is a distinction (different classes) based on distance from the city center $(\mathbf{x}_1, \mathbf{x}_2) = (0, 0)$
    - e.g. Urban/Suburban

Transformation to add a ”missing” categorical feature

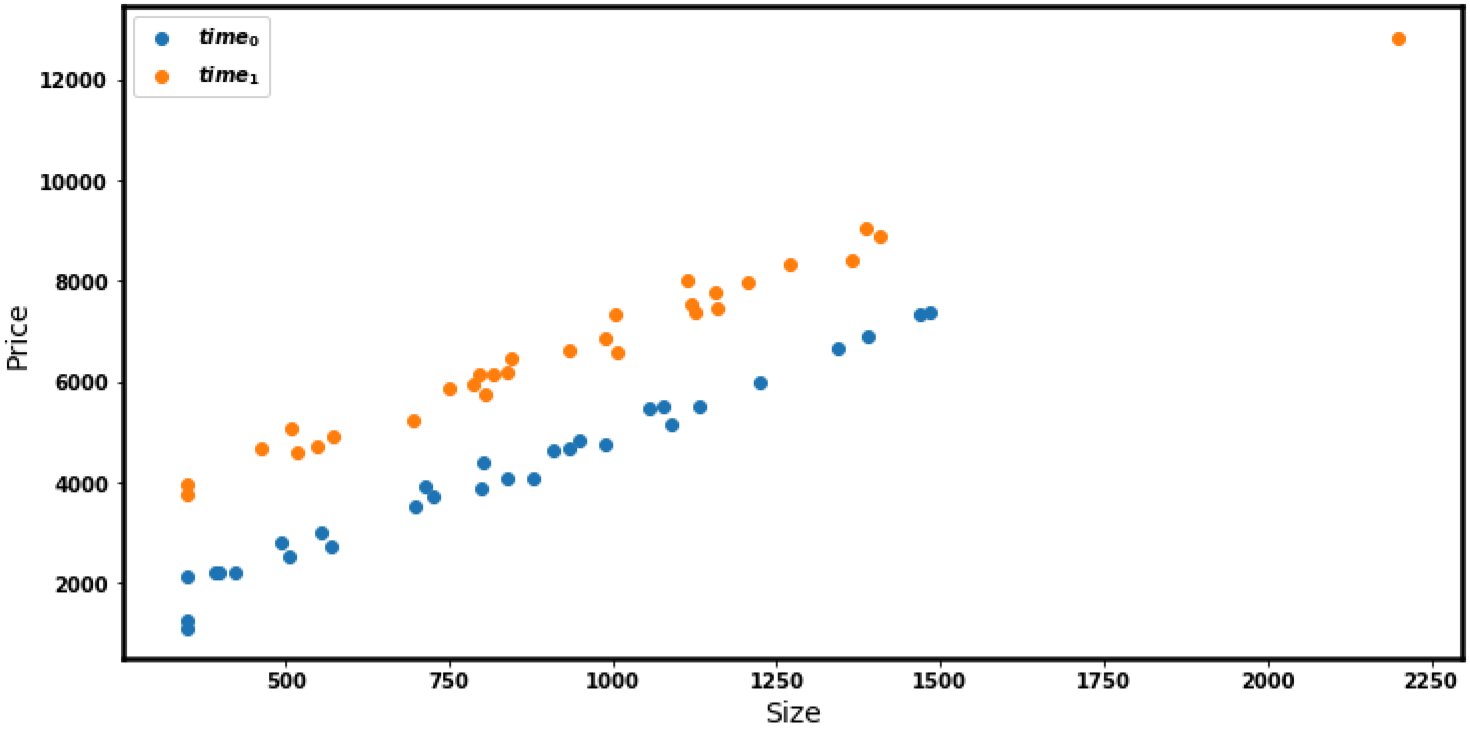
Recall the dataset where training examples formed two distinct groups

- samples at different points in time

In [12]:

```
fig
```

Out[12]:



How do we pool data that is similar intra-group but different across groups ?

In the above example, it appears that

- The groups are defined by examples gathered at different times: time_0, time_1
- There is a linear relationship *in each group* in isolation
- There slope of the relationship is *the same* across time
- But the intercept differs across groups
    - Perhaps this reflects a tax or rebate that is independent of price.

If we are correct in hypothesizing that each group is from the same distribution *except for* different intercepts

- the following set of equations describes the data (separately for each of the two groups):

$$
\begin{aligned}
\mathbf{y}_{(\text{time}_0)} &= \Theta_{(\text{time}_0)} + \Theta_1 * \mathbf{x} \\
\mathbf{y}_{(\text{time}_1)} &= \Theta_{(\text{time}_1)} + \Theta_1 * \mathbf{x}
\end{aligned}
$$

Trying to fit a line (Linear Regression) as a function of the combined data will be disappointing.

- it will try to force a common intercept

$$\mathbf{y} = \Theta_0 + \Theta_1 * \mathbf{x}$$

when we know that the intercepts are different

We can derive a *single equation* describing both groups by adding

- a Categorical feature `Group`
- with two possible class values
- indicating which group the example belongs to

Using OHE to encode this categorical feature. we create two binary indicators Is_0, Is_1

$$\text{Is}_j^{(\mathbf{i})} = \begin{cases} 1 & \text{if } \mathbf{x}^{(\mathbf{i})} \text{ is in group } j \\ 0 & \text{if } \mathbf{x}^{(\mathbf{i})} \text{ is NOT in group } j \end{cases}$$

To illustrate: for example i in time 0 group, we have

$$\text{Is}_0^{(\mathbf{i})} = 1$$
$$\text{Is}_1^{(\mathbf{i})} = 0$$

This results in the following equation

$$\mathbf{y} \quad = \quad \Theta_{(\text{time}_0)} * \text{Is}_0 + \Theta_{(\text{time}_1)} * \text{Is}_1 + \Theta_1 * \mathbf{x}$$

Effectively, the equation allows each group to have its own intercept !

- because Is_0 and Is_1 are complementary

This transformation caused examples

- that appear different *at the surface level*
- to become *similar* by revealing the *deeper* relationship

Here's what the design matrix $\mathbf{X}''$ looks like when we add the two indicators:

$$\mathbf{X}'' = \begin{array}{c} \\ \begin{pmatrix} \mathbf{Is}_0 & \mathbf{Is}_1 & \mathbf{other\ features} \\ 1 & 0 & \cdots \\ 0 & 1 & \cdots \\ \vdots & & \end{pmatrix} \end{array} \begin{array}{l} \\ \text{time}_0 \\ \text{time}_1 \\ \\ \end{array}$$

- Examples from the first time period look similar to the first row
- Examples from the second time period look similar to the second row

Because $\mathbf{Is}_0$ and $\mathbf{Is}_1$ are complementary

- we have an instance of the *Dummy Variable Trap*
- we need the usual solution of dropping one binary indicator
    - resulting in

$$\mathbf{y} = \Theta_0 + \Theta'_{(\text{time}_1)} * \text{Is}_1 + \Theta_1 * \mathbf{x}$$

    - the intercept term Θ_0 captures the contribution to $\mathbf{y}$ of examples in group 0
    - the coefficient $\Theta'_{(\text{time}_1)}$ captures the *incremental* contribution to $\mathbf{y}$ of being in group 1 rather than group 0

Bucketing: making a numeric feature into a Categorical feature

The effect of some features may not have a linear effect on the probability predicted by a Classifier.

Recall the `Age` feature from the Titanic Survival Classification problem.

Our analysis suggested that the Survival probability

- is **not** linear in Age

Trying to force `Age` into a linear model would not be appropriate.

Instead, we can create a Categorical synthetic feature `AgeBucket`

- with class values indicating whether age is in buckets of width 15 years
$$[0, 15), [15, 30), [30, 45), [45, 60), [60, 75)$$

Using OHE: we have a binary indicator for each bucket.

This is an example of

- replacing a numeric raw feature
- with a Categorical synthetic feature

to better match the characteristics of the model

Cross features

In our EDA for the Titanic Classification problem we discovered

- being a Female *seemed* to increase the chances of being in the `Survived` class
- but [deeper analysis (Classification_and_Non_Numerical_Data.ipynb#Conditional-survival-probability-(condition-on-multiple-attributes))](Classification_and_Non_Numerical_Data.ipynb#Conditional-survival-probability-(condition-on-multiple-attributes)) should this to be true *conditional* on not being in Third Class

It seems that we need to identify a group defined by the *intersection* of two conditions

- $\text{Is}_{\text{Female}}$ and $\text{Is}_{\substack{\text{PClass} \\ \neq 3}}$

That is, we want to create a feature FNTC (Female Not Third Class)

- that is True
- only for examples whose features are `Sex = Female` and `PClass` $\ne 3$

We first create two separate binary features

$$\text{Is}_{\text{Female}}$$

and

$$\text{Is}_{\text{PClass} \ne 3}$$

We can create a binary indicator that is the **intersection** of two binary indicators by multiplication

$$\mathrm{Is}_{\mathrm{FNTC}} = \mathrm{Is}_{\mathrm{Female}} * \mathrm{Is}_{\mathrm{PClass} \neq 3}$$

This is called a *cross feature* or a *cross term*.

This cross-feature serves the same purpose as the numeric feature we added to the bulls-eye dataset

- a feature that isolates a subset of examples

In fact, we can use a cross-feature for the bulls-eye dataset

- two binary features
  - one indicating $\mathbf{x}_1^{(\mathbf{i})}$ is close to 0
  - one indicating $\mathbf{x}_2^{(\mathbf{i})}$ is close to 0
- a cross-feature that indicates that $\mathbf{x}^{(\mathbf{i})}$ is close to $(0, 0)$
  - as the product of the two binary features

Here we create a cross feature that is `True` if two simpler features hold simultaneously

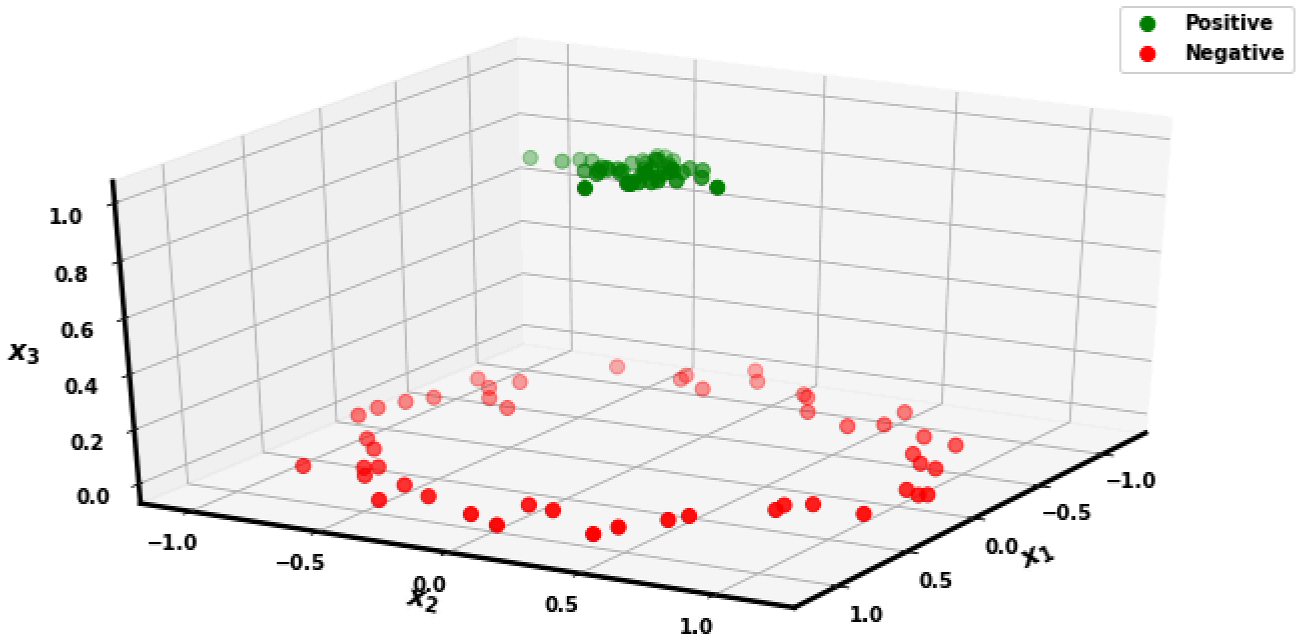
- $\text{Is}_{\text{near zero } \mathbf{x}_1}$ near zero indicator: $= -\epsilon \le \mathbf{x}_1 \le \epsilon$
- $\text{Is}_{\text{near zero } \mathbf{x}_2}$ near zero indicator: $= -\epsilon \le \mathbf{x}_2 \le \epsilon$

The cross feature that identifies examples near $(0, 0)$ is

- $\text{Is}_{\text{near}(0,0)} = \text{Is}_{\text{near zero } \mathbf{x}_1} * \text{Is}_{\text{near zero } \mathbf{x}_2}$

In [13]:

```
X_w_sq = svmh.circles_square_transform(Xc)
_= svmh.plot_3D(X=X_w_sq, y=yc )
```



Cross-features can be abused

Cross terms are very tempting but can be abused when over-used.

- they can be used to identify small subsets of examples for special treatment
- taken to the extreme
    - they can create *one indicator for each training example*
    - essentially: memorizing the training dataset

Memorization of the training set

- usually results in failure to generalize out of sample
- is a hallmark of over-fitting

Here's a picture of the "per example" indicator

First, construct an indicator which is true

- if an example's feature j value is equal to the feature j value of example i:
$$\text{Is}_{\mathbf{x}_j^{(\mathbf{i})}} = (\mathbf{x}_j = \mathbf{x}_j^{(\mathbf{i})})$$

Now construct a cross feature that combines the indicators for all j and a single example i:

$$\text{Is}_{\text{example } i} \quad = \quad (\mathbf{x}_1 = \mathbf{x}_1^{(\mathbf{i})}) * (\mathbf{x}_2 = \mathbf{x}_2^{(\mathbf{i})})$$

This cross feature will be true on example i.

We can construct such a cross feature that recognizes any single example.

And here's the design matrix $\mathbf{X}''$ with a separate intercept per example.

$\mathbf{X}''$ has m intercept columns, one for each example, forming a diagonal of 1's

$$\mathbf{X}'' = \begin{array}{c} \begin{array}{cccccc} \textbf{const} & \mathrm{Is}_{\text{example 1}} & \mathrm{Is}_{\text{example 2}} & \mathrm{Is}_{\text{example 3}} & \dots & \textbf{other features} \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & \\ 1 & 0 & 1 & 0 & \dots & \\ 1 & 0 & 0 & 1 & \dots & \\ \vdots & & & & & \end{pmatrix} \end{array}$$

We can do the same for $\Theta_1, \Theta_2, \ldots, \Theta_n$ resulting in a design matrix $\mathbf{X}''$ with $m * n$ indicators

- One per example per parameter

Here's a design matrix $\mathbf{X}''$ with one set of parameters per example: \

$$\mathbf{X}'' = \begin{pmatrix} \textbf{const} & \text{Is}_{\text{example 1}} & (\text{Is}_{\text{example 1}} * \mathbf{x}_1) & (\text{Is}_{\text{example 1}} * \mathbf{x}_2) & \dots & \text{Is}_{\text{example 2}} & (\text{Is}_{\text{ex}} \\ 1 & 1 & \mathbf{x}_1^{(1)} & \mathbf{x}_2^{(1)} & \dots & 0 & \\ 1 & 0 & 0 & 0 & \dots & 1 & \\ \vdots & & & & & & \end{pmatrix}$$

Using this as the design matrix in Linear Regression

- Will get a perfect fit to training examples
- Would likely **not generalize** well to out of sample test examples.

When truly justified a small number of complex cross terms are quite powerful.

In [14]:

```
print("Done")
```

```
Done
```