Assignment 6 Companion Notebook: Motivation for Neural Networks

Learning Objectives:

- Understand the limitations of logistic regression through an example
- Become familiar with feedforward, multi-layer neural networks
- Fit a neural network to a dataset and examine the results

Titanic: The Sequel

In order to motivate the need for neural networks, we're going to return to the Titanic dataset and examine a particular limitation of logistic regression.

We'll begin by loading the data.

In [1]:

```python
import gdown
import pandas as pd

gdown.download('https://drive.google.com/uc?authuser=0&id=1XIFiL3WxxR6M2nWgADi3xWvuRO6A-Ov8&export=download', 'titanic_train.csv', False)
df = pd.read_csv('titanic_train.csv')
df
```

```
Downloading...
From: https://drive.google.com/uc?authuser=0&id=1XIFiL3WxxR6M2nWgADi3xWvuRO6A-Ov8&export=download
To: /Users/pruvolo/Documents/assignments/Module 1/06/titanic_train.csv
100%|██████████| 61.2k/61.2k [00:00<00:00, 1.30MB/s]
```

Out[1]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C85	C
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S
5	6	0	3	Moran, Mr. James	male	NaN	0	0	330877	8.4583	NaN	Q
6	7	0	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	51.8625	E46	S
7	8	0	3	Palsson, Master. Gosta Leonard	male	2.0	3	1	349909	21.0750	NaN	S
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Berg)	female	27.0	0	2	347742	11.1333	NaN	S
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30.0708	NaN	C
10	11	1	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16.7000	G6	S
11	12	1	1	Bonnell, Miss. Elizabeth	female	58.0	0	0	113783	26.5500	C103	S
12	13	0	3	Saundercock, Mr. William Henry	male	20.0	0	0	A/5. 2151	8.0500	NaN	S
13	14	0	3	Andersson, Mr. Anders Johan	male	39.0	1	5	347082	31.2750	NaN	S
14	15	0	3	Vestrom, Miss. Hulda Amanda Adolfina	female	14.0	0	0	350406	7.8542	NaN	S

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
15	16	1	2	Amanda Adolfina Hewlett, Mrs. (Mary D Kingcome)	female	55.0	0	0	248706	16.0000	NaN	S
16	17	0	3	Rice, Master. Eugene	male	2.0	4	1	382652	29.1250	NaN	Q
17	18	1	2	Williams, Mr. Charles Eugene	male	NaN	0	0	244373	13.0000	NaN	S
18	19	0	3	Vander Planke, Mrs. Julius (Emelia Maria Vande...	female	31.0	1	0	345763	18.0000	NaN	S
19	20	1	3	Masselmani, Mrs. Fatima	female	NaN	0	0	2649	7.2250	NaN	C
20	21	0	2	Fynney, Mr. Joseph J	male	35.0	0	0	239865	26.0000	NaN	S
21	22	1	2	Beesley, Mr. Lawrence	male	34.0	0	0	248698	13.0000	D56	S
22	23	1	3	McGowan, Miss. Anna "Annie"	female	15.0	0	0	330923	8.0292	NaN	Q
23	24	1	1	Sloper, Mr. William Thompson	male	28.0	0	0	113788	35.5000	A6	S
24	25	0	3	Palsson, Miss. Torborg Danira	female	8.0	3	1	349909	21.0750	NaN	S
25	26	1	3	Asplund, Mrs. Carl Oscar (Selma Augusta Emilia...	female	38.0	1	5	347077	31.3875	NaN	S
26	27	0	3	Emir, Mr. Farred Chehab	male	NaN	0	0	2631	7.2250	NaN	C
27	28	0	1	Fortune, Mr. Charles Alexander	male	19.0	3	2	19950	263.0000	C23 C25 C27	S
28	29	1	3	O'Dwyer, Miss. Ellen "Nellie"	female	NaN	0	0	330959	7.8792	NaN	Q
29	30	0	3	Todoroff, Mr. Lalio	male	NaN	0	0	349216	7.8958	NaN	S
...	...	...	...	...	...	...	...	...	...	...	...	...
861	862	0	2	Giles, Mr. Frederick Edward	male	21.0	1	0	28134	11.5000	NaN	S
862	863	1	1	Swift, Mrs. Frederick Joel (Margaret Welles Ba...	female	48.0	0	0	17466	25.9292	D17	S
863	864	0	3	Sage, Miss. Dorothy Edith "Dolly"	female	NaN	8	2	CA. 2343	69.5500	NaN	S
864	865	0	2	Gill, Mr. John William	male	24.0	0	0	233866	13.0000	NaN	S
865	866	1	2	Bystrom, Mrs. (Karolina)	female	42.0	0	0	236852	13.0000	NaN	S
866	867	1	2	Duran y More, Miss. Asuncion	female	27.0	1	0	SC/PARIS 2149	13.8583	NaN	C
867	868	0	1	Roebling, Mr. Washington Augustus II	male	31.0	0	0	PC 17590	50.4958	A24	S
868	869	0	3	van Melkebeke, Mr. Philemon	male	NaN	0	0	345777	9.5000	NaN	S
869	870	1	3	Johnson, Master. Harold Theodor	male	4.0	1	1	347742	11.1333	NaN	S
870	871	0	3	Balkic, Mr. Cerin	male	26.0	0	0	349248	7.8958	NaN	S
871	872	1	1	Beckwith, Mrs. Richard Leonard (Sallie Monypeny)	female	47.0	1	1	11751	52.5542	D35	S
872	873	0	1	Carlsson, Mr. Frans Olof	male	33.0	0	0	695	5.0000	B51 B53 B55	S
873	874	0	3	Vander Cruyssen, Mr. Victor	male	47.0	0	0	345765	9.0000	NaN	S
874	875	1	2	Abelson, Mrs. Samuel (Hannah Wizosky)	female	28.0	1	0	P/PP 3381	24.0000	NaN	C
875	876	1	3	Najib, Miss. Adele Kiamie "Jane"	female	15.0	0	0	2667	7.2250	NaN	C
876	877	0	3	Gustafsson, Mr. Alfred Ossian	male	20.0	0	0	7534	9.8458	NaN	S
877	878	0	3	Petroff, Mr. Nedelio	male	19.0	0	0	349212	7.8958	NaN	S
878	879	0	3	Laleff, Mr. Kristo	male	NaN	0	0	349217	7.8958	NaN	S
879	880	1	1	Potter, Mrs. Thomas Jr (Lily Alexenia Wilson)	female	56.0	0	1	11767	83.1583	C50	C
880	881	1	2	Shelley, Mrs. William (Imanita Parrish Hall)	female	25.0	0	1	230433	26.0000	NaN	S
881	882	0	3	Markun, Mr. Johann	male	33.0	0	0	349257	7.8958	NaN	S

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
882	883	0	3	Dahlberg, Miss. Gerda Ulrika	female	22.0	0	0	7552	10.5167	NaN	S
883	884	0	2	Banfield, Mr. Frederick James	male	28.0	0	0	C.A./SOTON 34068	10.5000	NaN	S
884	885	0	3	Sutehall, Mr. Henry Jr	male	25.0	0	0	SOTON/OQ 392076	7.0500	NaN	S
885	886	0	3	Rice, Mrs. William (Margaret Norton)	female	39.0	0	5	382652	29.1250	NaN	Q
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.0000	NaN	S
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.0000	B42	S
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	23.4500	NaN	S
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.0000	C148	C
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.7500	NaN	Q

891 rows × 12 columns

From some of the exploratory analysis in the assignment 5 walkthrough, we know that both age and sex are good predictors of whether or not someone survived the Titanic sinking. That said, we saw that the effect surivival rate for women wasn't dramatically changed by age, but the survival rate for men was dramatically changed. Here are some plots showing this result.

In [2]:

```python
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
legend_entries = []
plt.subplot(1,2,1)
for groups in df[df['Sex'] == 'male'].groupby('Survived'):
    sns.distplot(groups[1]['Age'].dropna(), kde=False)
    legend_entries.append('Survived=%d'% groups[0])
plt.legend(legend_entries)
plt.title('Survival for sex="male"')

plt.subplot(1,2,2)
legend_entries = []
for groups in df[df['Sex'] == 'female'].groupby('Survived'):
    sns.distplot(groups[1]['Age'].dropna(), kde=False)
    legend_entries.append('Survived=%d'% groups[0])
plt.legend(legend_entries)
plt.title('Survival for sex="female"')
plt.show()

# while we're at it, silence annoying sklearn warnings
# import warnings filter
from warnings import simplefilter
# ignore all future warnings
simplefilter(action='ignore', category=FutureWarning)
```
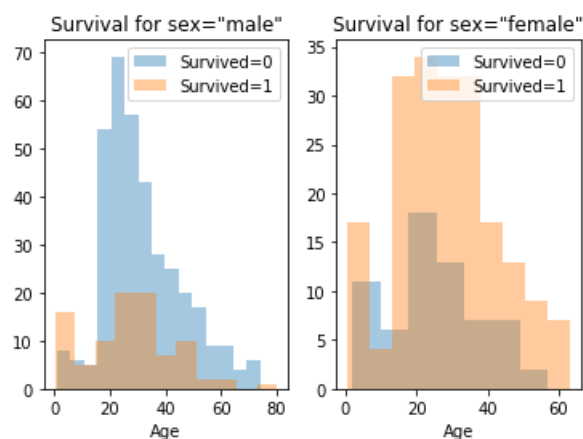

It would be great if we could use logistic regression in order to leverage this information. A good first pass would be to take both of these features (where we will encode `sex` using an `is_male` feature) and pass them into a logistic regression. The plot below

shows the results of this analysis where we represent the training data along with the lines of equal probability for the resultant model. We'll divide this into two cells, one where we prepare the data and the other where we fit the model and show the plot

In [3]:

```
# get rid of null values for age since this is just an illustrative example.
# this would not be a good thing to do if we were trying to evalutate the
# performance of a model.
df_filtered = df[['Age', 'Sex', 'Survived']].dropna()
experiment_1_data = pd.concat((pd.get_dummies(df_filtered['Sex'], drop_first=True),
df_filtered['Age']), axis=1)
experiment_1_outputs = df_filtered['Survived']
experiment_1_data
```

Out[3]:

	male	Age
0	1	22.0
1	0	38.0
2	0	26.0
3	0	35.0
4	1	35.0
6	1	54.0
7	1	2.0
8	0	27.0
9	0	14.0
10	0	4.0
11	0	58.0
12	1	20.0
13	1	39.0
14	0	14.0
15	0	55.0
16	1	2.0
18	0	31.0
20	1	35.0
21	1	34.0
22	0	15.0
23	1	28.0
24	0	8.0
25	0	38.0
27	1	19.0
30	1	40.0
33	1	66.0
34	1	28.0
35	1	42.0
37	1	21.0
38	0	18.0
...	...	...
856	0	45.0
857	1	51.0
858	0	24.0
860	1	41.0
861	1	21.0
862	0	48.0

	male	Age
862	0	48.0
864	1	24.0
865	0	42.0
866	0	27.0
867	1	31.0
869	1	4.0
870	1	26.0
871	0	47.0
872	1	33.0
873	1	47.0
874	0	28.0
875	0	15.0
876	1	20.0
877	1	19.0
879	0	56.0
880	0	25.0
881	1	33.0
882	0	22.0
883	1	28.0
884	1	25.0
885	0	39.0
886	1	27.0
887	0	19.0
889	1	26.0
890	1	32.0

714 rows × 2 columns

In [4]:

```python
from sklearn.linear_model import LogisticRegression
import numpy as np

model = LogisticRegression()
model.fit(experiment_1_data, experiment_1_outputs)

xx, yy = np.mgrid[-.1:1.1:.01, 0:85:.1]
grid = np.c_[xx.ravel(), yy.ravel()]
probs = model.predict_proba(grid)[:, 1].reshape(xx.shape)

f, ax = plt.subplots(figsize=(8, 6))
contour = ax.contourf(xx, yy, probs, 25, cmap="RdBu",
                      vmin=0, vmax=1)
ax_c = f.colorbar(contour)
ax_c.set_label("$P(survived)$")
ax_c.set_ticks([0, .25, .5, .75, 1])

ax.scatter(experiment_1_data['male'], experiment_1_data['Age'], c=experiment_1_outputs, s=50,
           cmap="RdBu", vmin=-.2, vmax=1.2,
           edgecolor="white", linewidth=1)

ax.set(xlim=(-.1, 1.1),
       ylim=(0, 85),
       xlabel="is male", ylabel="age (years)")
plt.show()
```
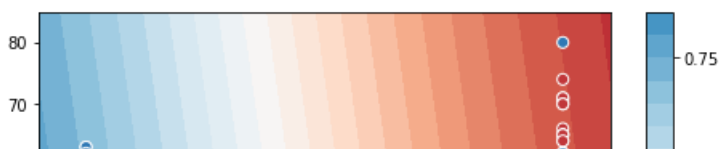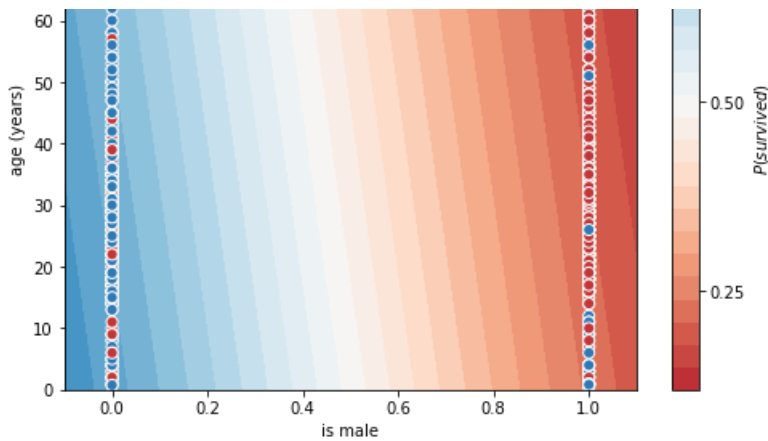
Notebook Exercise 1 (10 minutes)

(a) In English, explain what this graph is showing (defer interpretation for now, we just want to make sure you have an idea of what is represented in the plot, e.g., x-axis, y-axis, colored areas).

(b) Given the decision boundary, how does the model predict who will survive versus not survive? What does it predict for male babies?

Solution

(a) the graph shows a contour plot of the probability returned by the logistic regression model. Also shown on the graph are the training points (blue are passengers that survived and red are ones that did not).

(b) Even though the model is not quite as simple as one that just uses the is male feature, it never the less has a decisino boundary that will always predict that a male will not survive and a female will survive.

Adding the `is_young_male` feature

Based on this plot it seems that what we need is to have a model that is able to simulataneously predict that all women survived and that all very young boys survived. One way we can achieve this is by engineering a special `is_young_male` feature that is 1 if the person is under the age of 5 and male. The feature will take a value of 0 otherwise.

In [5]:

```
is_young_male = (experiment_1_data['male']) & (experiment_1_data['Age'] < 5).astype(int)
is_young_male.name = 'is_young_male'
experiment_2_data = pd.concat((experiment_1_data, is_young_male), axis=1)
experiment_2_data
# these don't change, but just to be consistent with variable naming
experiment_2_outputs = experiment_1_outputs
```

Next, we can take fit the model to this new dataset and create a plot that shows the results of fitting the model. To make the plot a bit easier to interpret, we'll just plot the model's binary output (0 or 1) rather than the probability. This will make it really clear what the model is doing with the points in the lower righthand corner.

In [6]:

```
model = LogisticRegression()
model.fit(experiment_2_data, experiment_1_outputs)

xx, yy = np.mgrid[-.1:1.1:.01, 0:85:.1]
grid = np.c_[xx.ravel(), yy.ravel()]
# Note: we are setting the is_young_male feature for a male value above 0.9 to
# aid in visualization.  Of course, the feature can only take on value 0 or 1
is_young_male_grid = np.logical_and(grid[:,0] >= 0.9, grid[:,1] < 5).astype(np.int)[:,np.newaxis]

grid = np.hstack((grid, is_young_male_grid))
outputs = model.predict(grid).reshape(xx.shape)

f, ax = plt.subplots(figsize=(8, 6))
contour = ax.contourf(xx, yy, outputs, 25, cmap="RdBu",
                      vmin=0, vmax=1)
```
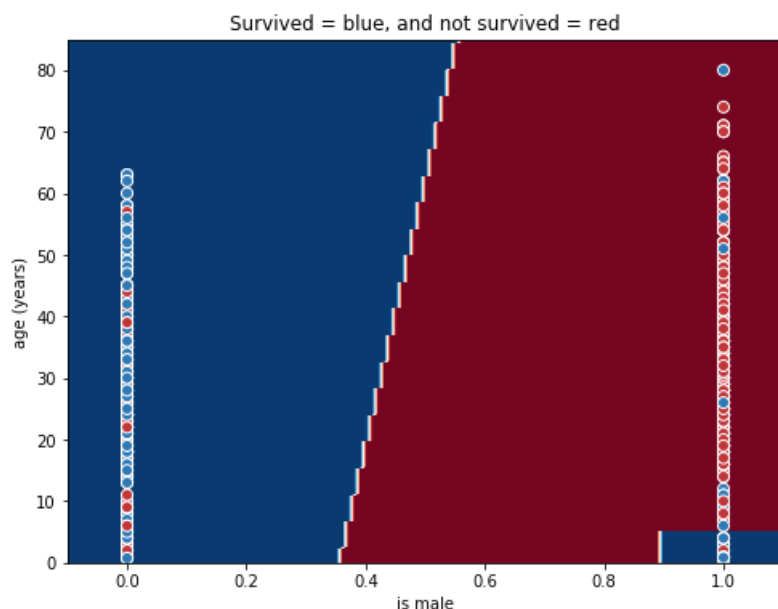
```
ax.set_title('Survived = blue, and not survived = red')

ax.scatter(experiment_1_data['male'], experiment_1_data['Age'], c=experiment_2_outputs, s=50,
           cmap="RdBu", vmin=-.2, vmax=1.2,
           edgecolor="white", linewidth=1)

ax.set(xlim=(-.1, 1.1),
       ylim=(0, 85),
       xlabel="is male", ylabel="age (years)")
plt.show()
```


Survived = blue, and not survived = red

Notebook Exercise 2 (10 minutes)

(a) Based on this graph, given a passenger's sex and age, what would the model predict?

(b) This seems to have achieved our goal of predicting that young males survived. What are the limitations of this approach of hand coding these sorts of features?

Solution

(a) The model predicts that all women and all males under the age of 5 will survive. Everyone else will not.

(b) Handcoding is very labor intensive and results in a lot of trial and error. There may be other useful trends in the sex / age data that we don't hand code since we don't have the right intuition.

Enter the Neural Network!

Next, we're going to learn about a particular type of neural network called a multilayer perceptron (you'll know exactly what one is by the end of this assignment!). For now, we won't give you a very sophisticated mental model of what this neural network is doing. Just think of it as automating the process of discovering useful representations for learning. We are trying to avoid needing to hand engineer features, such as we did with the `is young male` feature.

In [7]:

```
from sklearn.neural_network import MLPClassifier

model = MLPClassifier(hidden_layer_sizes=(2), activation='logistic', solver='lbfgs', random_state=5
0)
model.fit(experiment_1_data, experiment_1_outputs)
```

Out[7]:

```
MLPClassifier(activation='logistic', alpha=0.0001, batch_size='auto',
              beta_1=0.9, beta_2=0.999, early_stopping=False, epsilon=1e-08,
              hidden_layer_sizes=2, learning_rate='constant',
              learning_rate_init=0.001, max_iter=200, momentum=0.9,
              n_iter_no_change=10, nesterovs_momentum=True, power_t=0.5,
```

```
                  random_state=50, shuffle=True, solver='lbfgs', tol=0.0001,
                  validation_fraction=0.1, verbose=False, warm_start=False)
```

In [8]:

```
xx, yy = np.mgrid[-.1:1.1:.01, 0:85:.1]
grid = np.c_[xx.ravel(), yy.ravel()]
outputs = model.predict(grid).reshape(xx.shape)

f, ax = plt.subplots(figsize=(8, 6))
contour = ax.contourf(xx, yy, outputs, 25, cmap="RdBu",
                      vmin=0, vmax=1)
ax.set_title('Survived = blue, and not survived = red')

ax.scatter(experiment_1_data['male'], experiment_1_data['Age'], c=experiment_2_outputs, s=50,
           cmap="RdBu", vmin=-.2, vmax=1.2,
           edgecolor="white", linewidth=1)

ax.set(xlim=(-.1, 1.1),
       ylim=(0, 85),
       xlabel="is male", ylabel="age (years)")
plt.show()
```


Survived = blue, and not survived = red
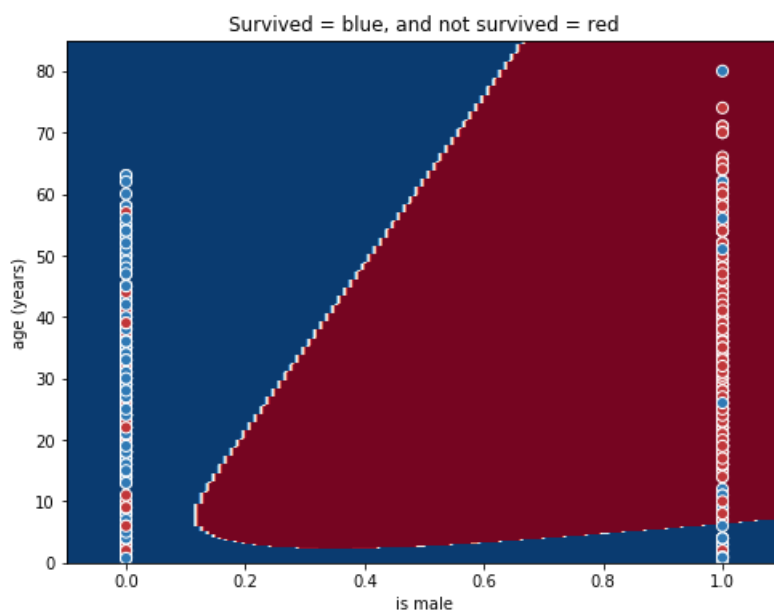
Notebook Exercise 3 (5 minutes)

Based on this graph how does the network decide whether a passenger will survive or not survive.

Solution

All women and all males under the age of 6ish are predicted to survive. All others are predicted not to survive.

Examining the Intermediate Representations in the Network

While we have yet to really unpack *how* the neural network was able to achieve this feat, we can start to interrogate the learned model to undrestand a bit of what it is doing.

For the purposes of this next set of plots and exercise, you should have the following mental model of what the network is doing (all of this will be made 100% precise when you go through the rest of the assignmnet document, but for now things will be explained on a conceptual level).

- Neural networks learn internal representations of the input data that help them make predictions (you may recall that this was Big Idea #4 in assignment 1).
- In this case we instructed the neural network to learn exactly 2 internal representations of the input data.
- The network will use these two internal representations, not the original input data, in order to arrive at its final decision.

In the plot below, we show the values for each of the 2 learned internal representations in the network. You can think of these representations as providing a remapping of the data into a new space that is then used to make the prediction as to whether the

representations as providing a remapping of the data into a new space that is then used to make the prediction as to whether the person was likely to surive or not survive.

In [9]:

```python
hidden_units = 1/(1+np.exp(-np.matmul(np.array(experiment_1_data), model.coefs_[0]) + model.interce
pts_[0]))

f = plt.figure(figsize=(12, 5))
hidden_units = 1/(1+np.exp(-np.matmul(grid, model.coefs_[0]) + model.intercepts_[0]))

for i in range(2):
    ax = f.add_subplot(1,2,i+1)
    contour = ax.contourf(xx, yy, hidden_units[:,i].reshape(xx.shape), 25, cmap="RdBu",
                          vmin=0, vmax=1)

    ax.scatter(experiment_1_data['male'], experiment_1_data['Age'], c=experiment_2_outputs, s=50,
            cmap="RdBu", vmin=-.2, vmax=1.2,
            edgecolor="white", linewidth=1)
    ax_c = f.colorbar(contour)
    ax_c.set_label("learned feature %d" %(i+1))
    ax_c.set_ticks([0, .25, .5, .75, 1])

    ax.set(xlim=(-.1, 1.1),
        ylim=(0, 85),
        xlabel="is male", ylabel="age (years)")
plt.show()
```
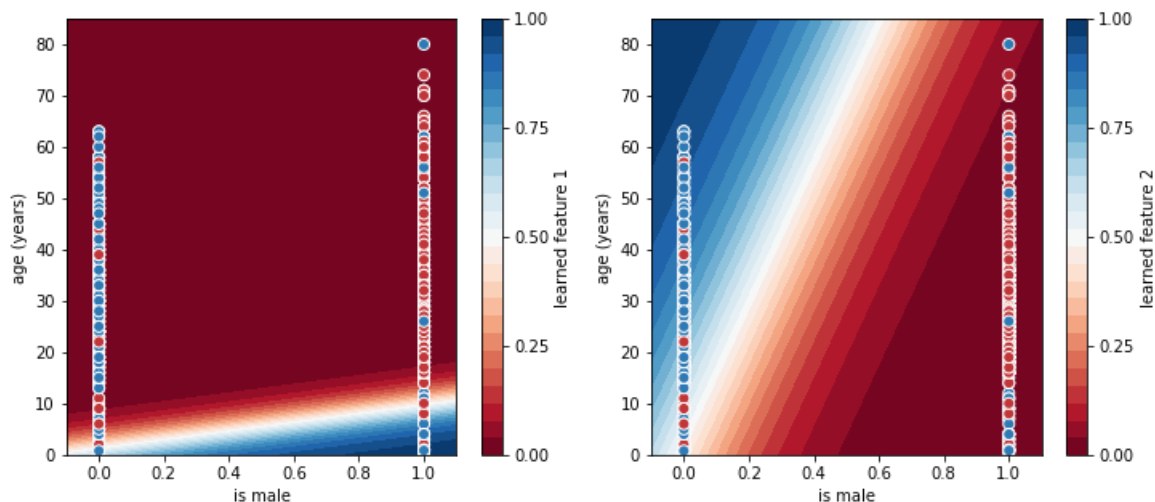

Notebook Exercise 4 (10 minutes)

(a) What does first learned feature (left plot) appear to encode?

(b) What does the second learned feature (right plot) appear to encode?

Solution

(a) The first feature appears to encode the notion of being a very young male (although female babies are also included).

(b) The second feature seems to encode whether or not the passenger is a female. The slant of the lines makes this more of an `is non infant female` feature.

Key takeaways

While this was a relatively simple example of how a neural network could be applied, the capabilities that you just saw in this notebook have immense significance. The ability of a neural network to take input data that may not be suited for prediction (e.g., sex and age) and transform it into a representation that is more useful for prediction is perhaps the most significant aspect of neural networks. Here is a summmary of what happened in this notebook.

- We reexamined the Titanic dataset and showed that adding the `age` feature doesn't really help in making predictions versus just using `sex`.
- We showed that we can manually add a feature called `is_young_male` that can help us in prediction.

- We showed that neural networks can automate this process of feature learning by developing their own internal representations.
- We showed that the neural network, in this case, learned an internal representation that is very similar to the `is_young_male` and `sex` representation.

In the rest of the assignment we'll be unpacking what exactly a neural network is. You'll learn how it functions and how you would fit the parameters of one.