Coding Assignment 2

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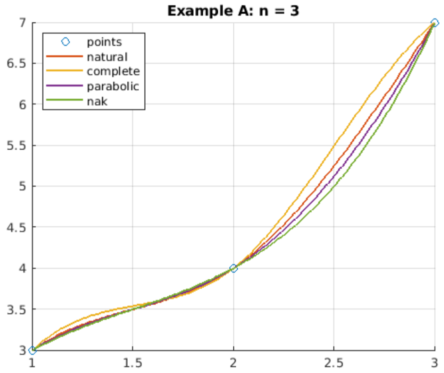
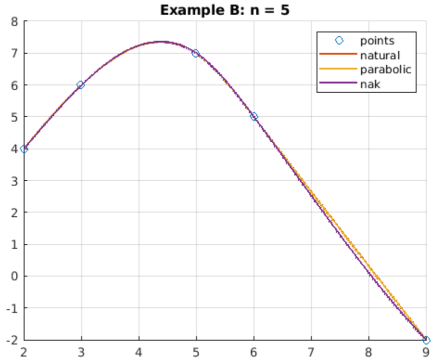
Problem 1 — Cubic Spline Implementation

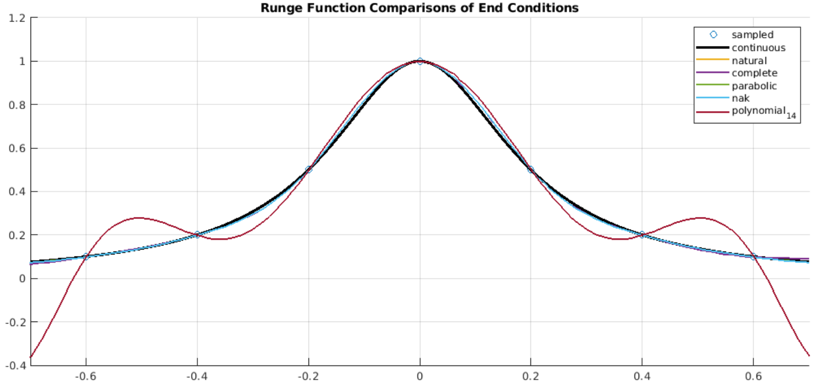
After implementing the spline equations, and solving the system of equations for the natural/free spline, complete spline, parabolically terminated, and not-a-knot end conditions, I generated these plots. The different end conditions are a parameter in my `spline_2()` function.





Problem 1 — Cubic Spline Implementation

I also checked this implementation using the Runge function $\frac{1}{1+25x^2}$:



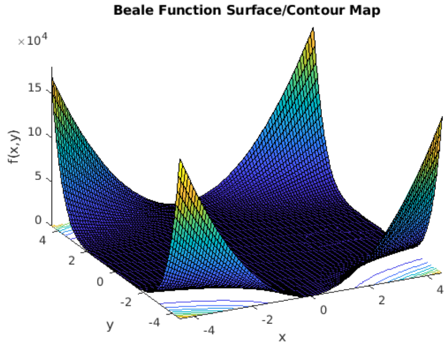
Note how the high-order polynomial fit is unstable/oscillatory at the ends, while the spline interpolations handle this problem nicely.

Problem 2 | Task 1 — Plotting

Here are my 2D & 3D contour maps for the:

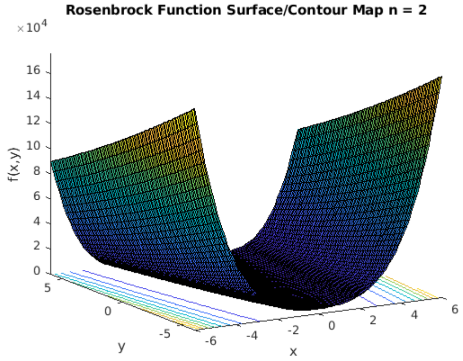
Beale Function:

$f(x,y) = (1.5 - x + xy) + (2.25 - x + xy^3)^2 + (2.625 - x + xy)^2$



Rosenbrock Function ($n = 2$):

$f(x) = \sum_{i=1}^{n-1} [100(x_{i+1} - x_i)^2]$

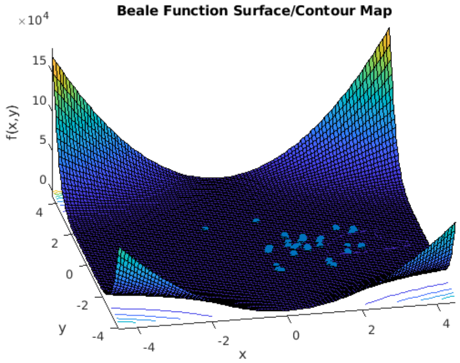


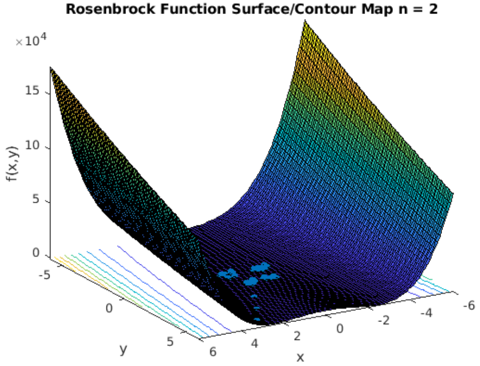
Problem 2 | Task 2a/b — Nelder-Mead Optimization

Please see code `p2.m`. The Beale function was minimized successfully to $(3.0, 0.5)$ where $f(x, y) = 0$, as long as the starting point was $(4.5, 4.5)$ instead of $(-4.5, -4.5)$. The Rosenbrock function was minimize to $(1, 1, 1, 1)$ with the starting point being (2,2,2,2).

Problem 2 | Task 3

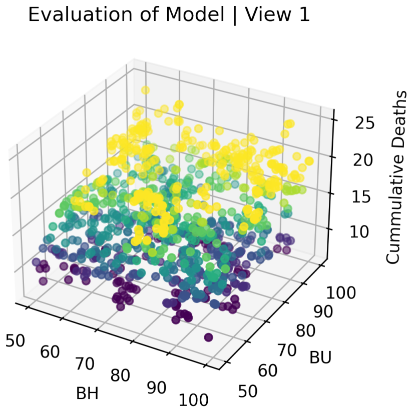
I had some issues with my implementation of Response Surface optimization of these two functions. Since we were asked to continuously fit a quadratic instead of a linear function *then* a quadratic, the minimization may have chosen points past the minimum, resulting in oscillations about the true minimum. Here are plots of where my minimum points (blue) ended up settling relative to these surfaces.

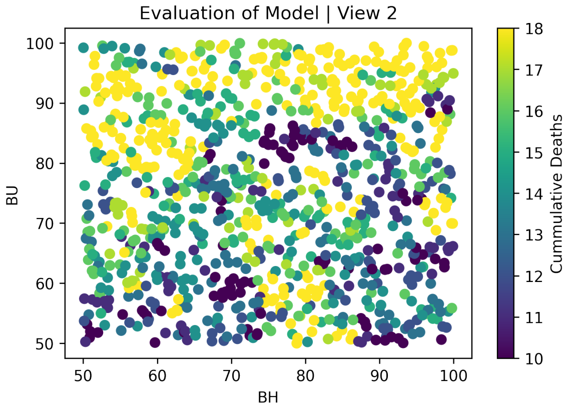




Problem 3

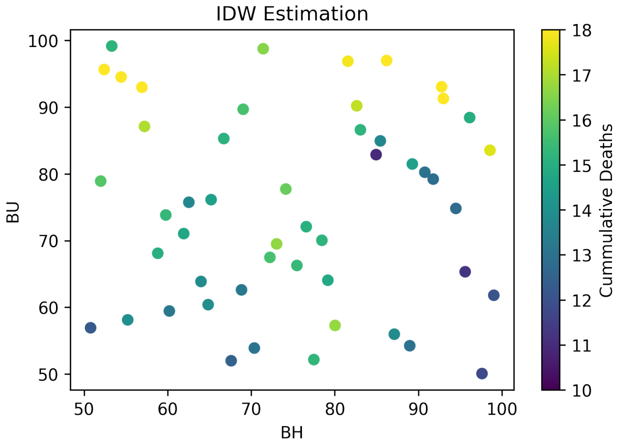
Here are the simulations I ran of the state-transition model. I ran 1000x1000 LHS design instead of 500, in order to better estimate a ground truth/better train my models. The data may be visualized as either a 2D or 3D plot, but I think the 3D one is prettier.





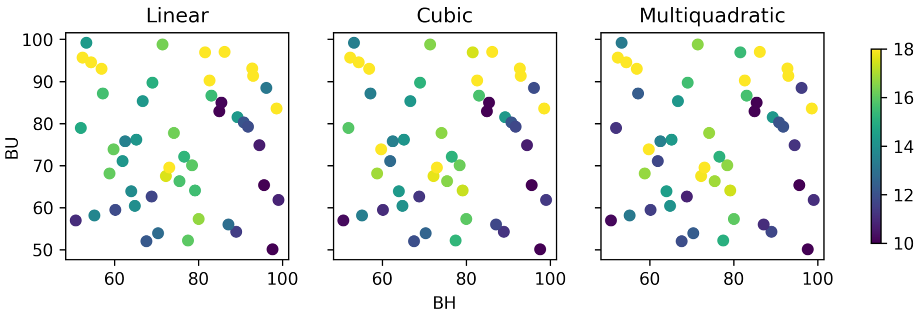
Problem 3 | Task 3a — IDW Approach

My Inverse Distance Weighted (IDW) attempt to metamodel the data is shown below. All the metamodeling methods are compared to the "ground truth" at the end of these slides.



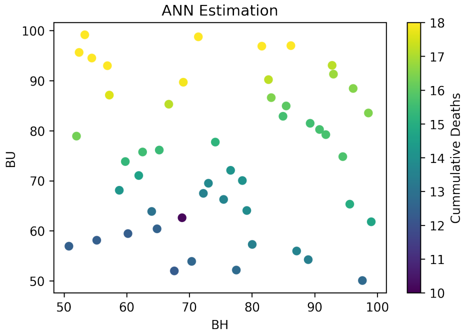
Problem 3 | Task 3b — RBF Approach

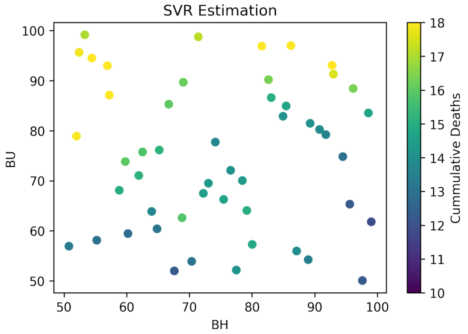
My Radial Basis Function (RBF) approach was as follows. I simulated this using a linear, cubic, and multiquadratic approach. I was not sure what was meant by combining cubic and linear approach...



Problem 3 | Task 3c/d — Neural Net and SVR Approaches

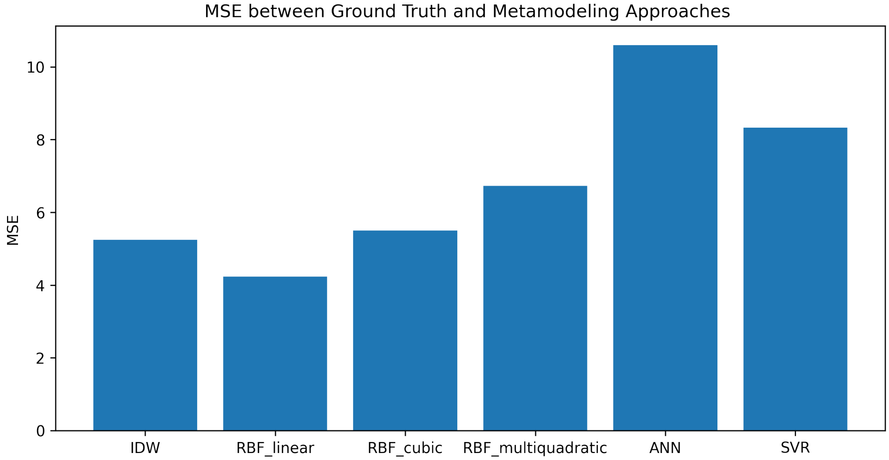
Here are my ANN and Support Vector Regression (SVR). For the ANN approach, I allowed a maximum of 1000 iterations.





Problem 3 | Comparisons to Ground Truth

To compare these metamodeling approaches to the ground truth, I used mean square error (MSE). It appears the RBF linear and IDW approaches resulted in the best representation of the model, with MSE $\approx$ 6. I am attaching my ipythonnotebook output to this slide deck in case there are any dependency-related issues to whomever may read this.



p3

April 19, 2021

1 Coding Assignment 2 | Problem 3:

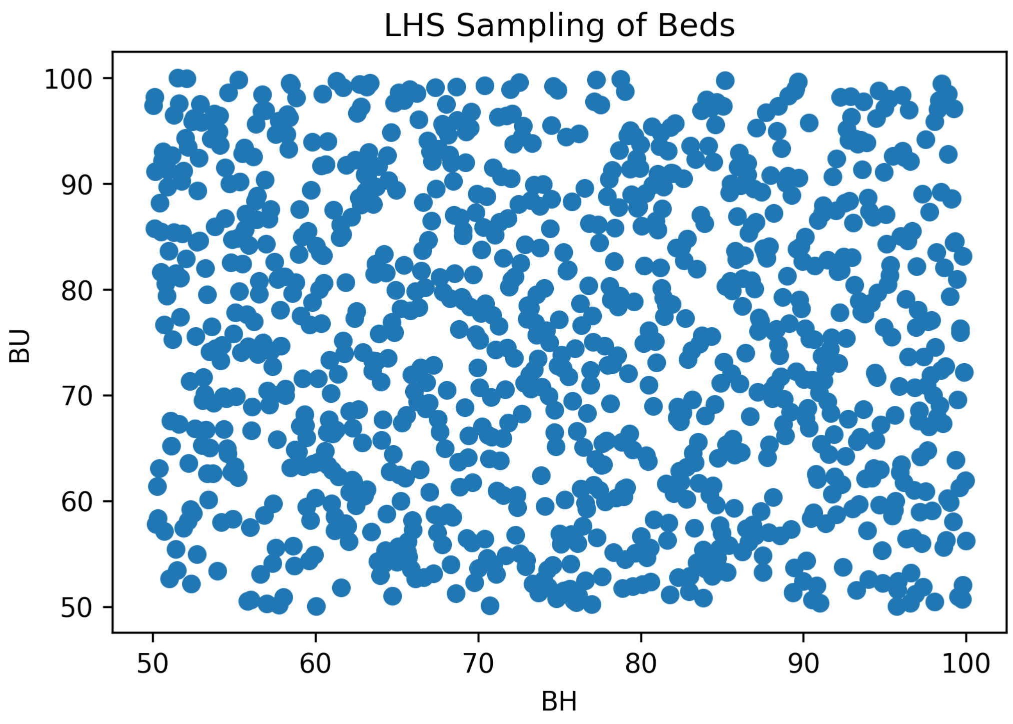
Andrew Sivaprakasam

BME 695 Numerical Methods

Dependent on a few packages, see import statments.

1.1 Task 3 | LHS Design

[3]:
```python
from main import main
import pandas as pd
import matplotlib.pyplot as plt
from pyDOE import lhs
import numpy as np
import pickle
from joblib import Parallel, delayed


%matplotlib inline

bed_min = 50;
bed_max = 100;
bed_range = bed_max-bed_min;

#Generate the lhs samples
test = lhs(2, samples = 1000)
test = bed_min + test*(bed_range);
test = np.asarray(test);

#verify samples
BH,BU = test.T;
plt.figure(dpi=300)
plot1 = plt.scatter(BH,BU);
plt.title('LHS Sampling of Beds');
plt.xlabel('BH');
plt.ylabel('BU');
plt.savefig('LHS_GT.png', bbox_inches='tight')
```



1.2 For Easy Parallelization:

This also runs the ground truth simulation used for training models.

[12]:
```
def main_p(bh,bu):
    r = main(bh,bu,5)

    print(r);
    return r
```

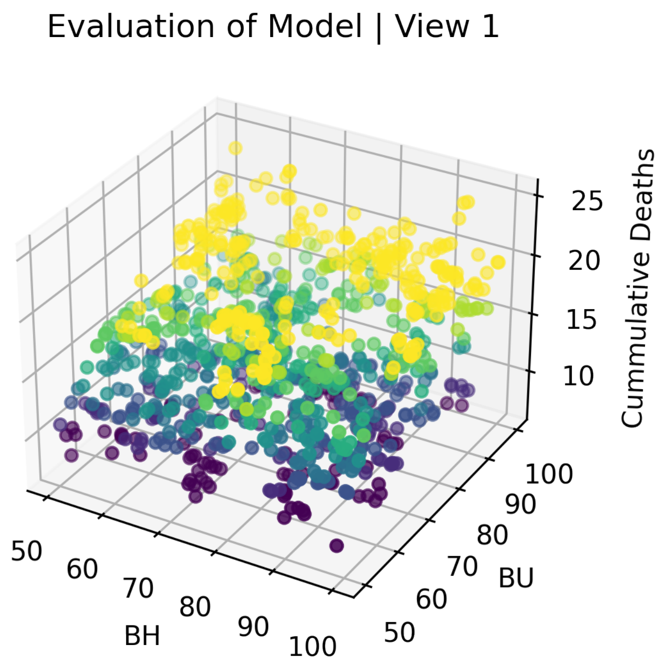
[2]:
```
#simulate
r = np.zeros(len(BH));
r = Parallel(n_jobs = -1, verbose = 0)(delayed(main_p)(BH[i],BU[i]) for i in␣
↪range(0,len(BH)))
```

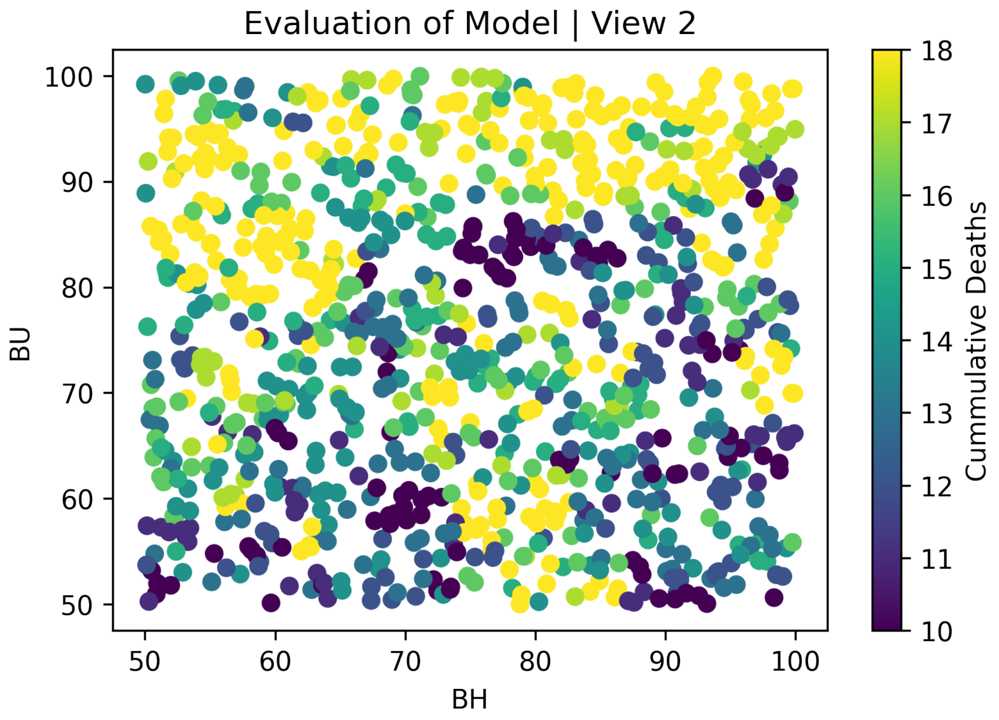
1.3 Pickle to save time:

Just saves everthing nicely in a file.

[4]:
```
#save data to file:
#pickle.dump([BH,BU,r], open("1000_sims", "wb"))
BH,BU,r = pickle.load(open("1000_sims","rb"))
```

[5]:
```
#plot data:
fig, ax = plt.subplots(subplot_kw={"projection": "3d"},dpi=300)
surf = ax.scatter(BH, BU, r,c = r,vmin=10, vmax=18)
plt.title('Evaluation of Model | View 1')
plt.ylabel('BU');
plt.xlabel('BH');
ax.set_zlabel('Cummulative Deaths');
plt.savefig('GT_Sim1.png', bbox_inches='tight')

plt.figure(dpi=300)
plot1 = plt.scatter(BH,BU,c = r,vmin=10, vmax=18)
plt.colorbar(label = 'Cummulative Deaths')
plt.ylabel('BU')
plt.xlabel('BH')
plt.title('Evaluation of Model | View 2')
plt.savefig('GT_Sim2.png', bbox_inches='tight')
```





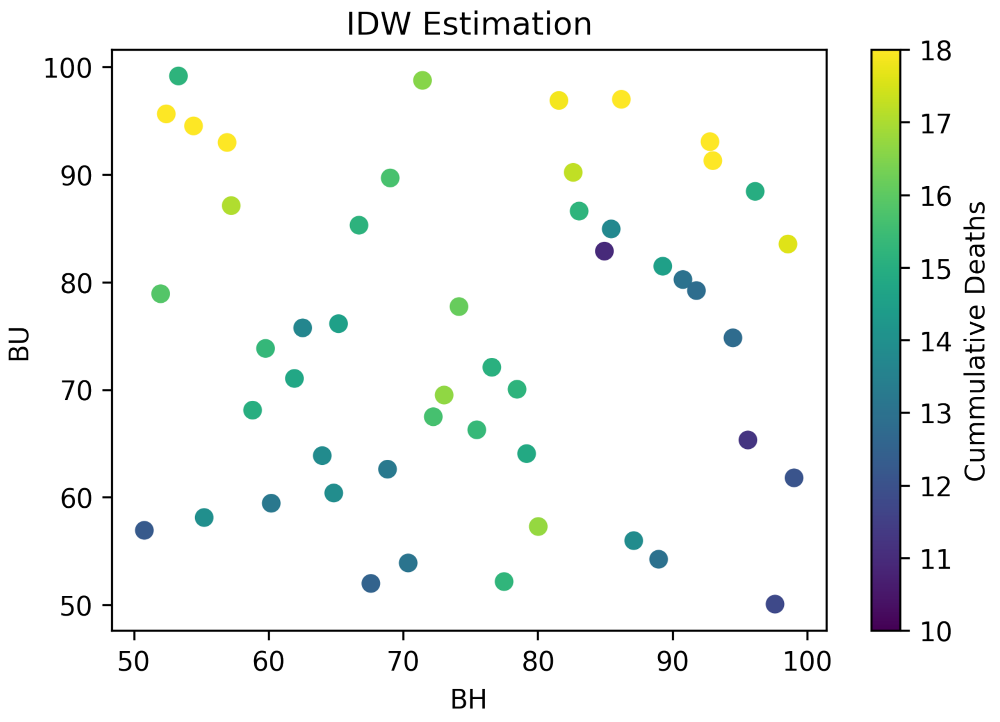
[6]:
```
#generate LHS samples at lower res for metamodeling

test = lhs(2, samples = 50)
test = bed_min + test*(bed_range);
test = np.asarray(test);

BH_i, BU_i = test.T;
```

1.4 Task 3a | IDW Implementation:

Based on the implementation found here https://rafatieppo.github.io/post/2018_07_27_idw2pyr/:

Modified to handle a pythagorean distance.

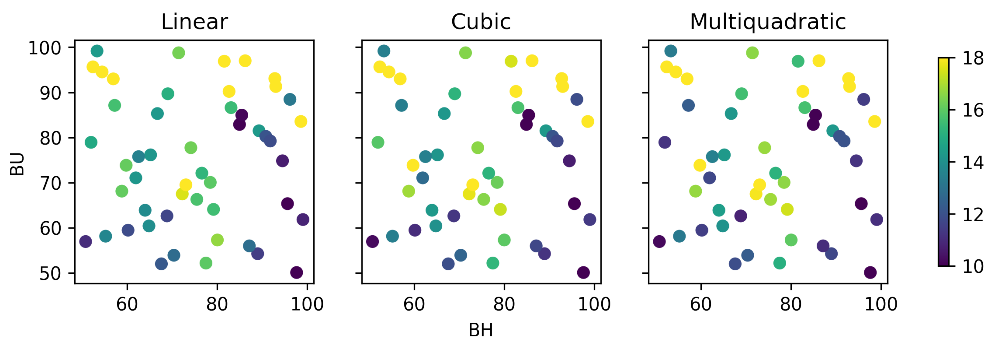
[7]:
```
#Implement IDW

def distance(x, y, xi, yi):
    d = np.sqrt((x-xi)**2 + (y-yi)**2);
    return(d)

def idwr(x, y, z, xi, yi):
    lstxyzi = []
    for p in range(len(xi)):
        lstdist = []
        for s in range(len(x)):
            d = distance(x[s], y[s], xi[p], yi[p])
            lstdist.append(d)
        sumsup = list((1 / np.power(lstdist, 2)))
        suminf = np.sum(sumsup)
        sumsup = np.sum(np.array(sumsup) * z)
        u = sumsup / suminf
        xyzi = u
        lstxyzi.append(xyzi)
    return(lstxyzi)

r_i_IDW = idwr(BH,BU,r,BH_i,BU_i);
plt.figure(dpi=300)
plot1 = plt.scatter(BH_i,BU_i,c = r_i_IDW,vmin=10, vmax=18)
plt.ylabel('BU')
plt.xlabel('BH')
plt.title('IDW Estimation')
plt.colorbar(label = 'Cummulative Deaths');
plt.savefig('IDW.png', bbox_inches='tight')
```



1.5 Task 3b | RBF Implementation:

Uses scipy:

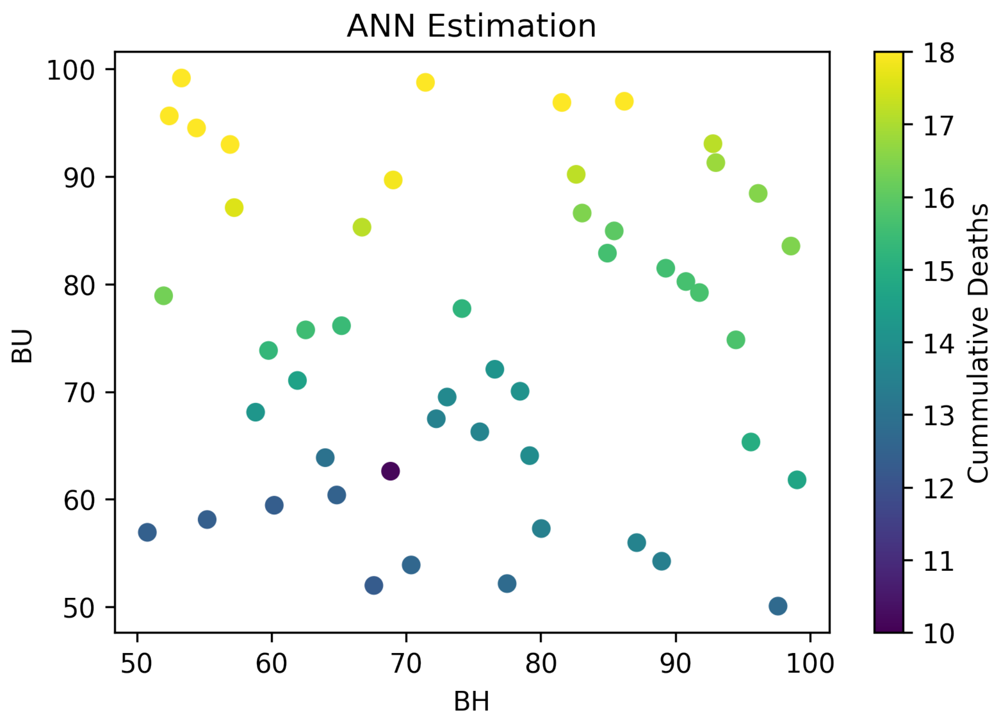
[8]:
```
#Implement RBF
from scipy.interpolate import Rbf

def cubilinear(self, r):
    return r**3 + r

rbf_i_lin = Rbf(BH, BU, r,function = 'linear');
rbf_i_cub = Rbf(BH, BU, r,function = 'cubic');
rbf_i_mq = Rbf(BH, BU, r)
r_i_RBF_lin = rbf_i_lin(BH_i, BU_i);
r_i_RBF_cub = rbf_i_cub(BH_i, BU_i);
r_i_RBF_mq = rbf_i_mq(BH_i, BU_i);



fig, axs = plt.subplots(1,3, sharex = True, sharey = True,figsize=(10, 3),␣
 ↪dpi=300)

axs[0].scatter(BH_i,BU_i,c = r_i_RBF_lin,vmin=10, vmax=18)
axs[0].set_title('Linear')
axs[0].set(adjustable='box', aspect='equal')

axs[1].scatter(BH_i,BU_i,c = r_i_RBF_cub,vmin=10, vmax=18)
axs[1].set_title('Cubic')
axs[1].set(adjustable='box', aspect='equal')
axs[1].set_xlabel('BH')



figend = axs[2].scatter(BH_i,BU_i,c = r_i_RBF_mq,vmin=10, vmax=18)
axs[2].set_title('Multiquadratic')
axs[2].set(adjustable = 'box', aspect='equal')

fig.colorbar(figend, ax=axs.ravel().tolist(), shrink = 0.7)

#plt.colorbar(im, label = 'Cummulative Deaths');
fig.add_subplot(111, frameon= False)
plt.tick_params(labelcolor='none', which='both', top=False, bottom=False,␣
 ↪left=False, right=False)
plt.ylabel('BU')
plt.savefig('RBF.png', bbox_inches='tight')
```



1.6 Task 3c | ANN Implementation:

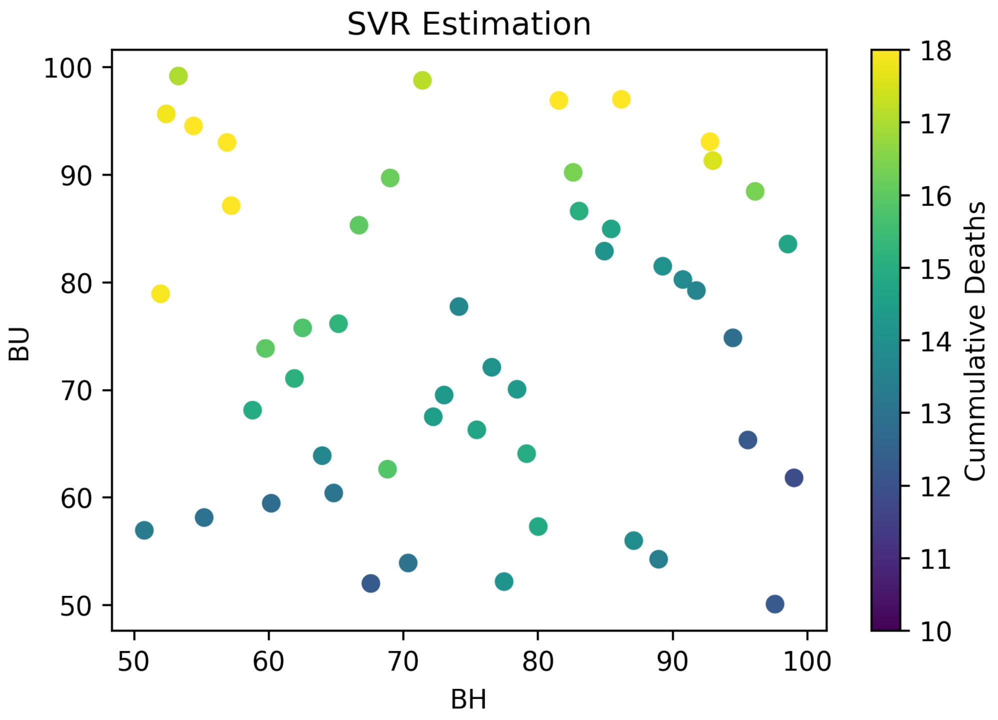
Uses SciKitLearn tools.

[9]:
```
#Implement ANN

from sklearn.neural_network import MLPRegressor

#set up dataframe:
r = np.squeeze(r);
#r = np.reshape(r[:],(500,-1))
data_x = np.zeros((len(BH),2));
data_x_i = np.zeros((len(BH_i),2));

data_y = r;

for i in range(0,len(BH)-1):
    data_x[i] = [BH[i],BU[i]];

for i in range(0, len(BH_i)-1) :
    data_x_i[i] = [BH_i[i],BU_i[i]];

regr = MLPRegressor(random_state=1,max_iter = 2000).fit(data_x,data_y);
regrs = regr.score(data_x,data_y);
r_i_ANN = regr.predict(data_x_i);

plt.figure(dpi=300)
plot2 = plt.scatter(BH_i,BU_i,c = r_i_ANN,vmin=10, vmax=18)
plt.colorbar(label = 'Cummulative Deaths');
plt.ylabel('BU')
plt.xlabel('BH')
plt.title('ANN Estimation');
plt.savefig('ANN.png', bbox_inches='tight')
```



1.7 Task 3d | SVR Implementation:

```
[10]: #Implement SVR

from sklearn.svm import SVR

regr = SVR().fit(data_x,data_y);
r_i_SVR = regr.predict(data_x_i);


plt.figure(dpi=300)
plot2 = plt.scatter(BH_i,BU_i,c = r_i_SVR,vmin=10, vmax=18)
plt.colorbar(label = 'Cummulative Deaths');
plt.ylabel('BU')
plt.xlabel('BH')
plt.title('SVR Estimation');
plt.savefig('SVR.png', bbox_inches='tight')
```

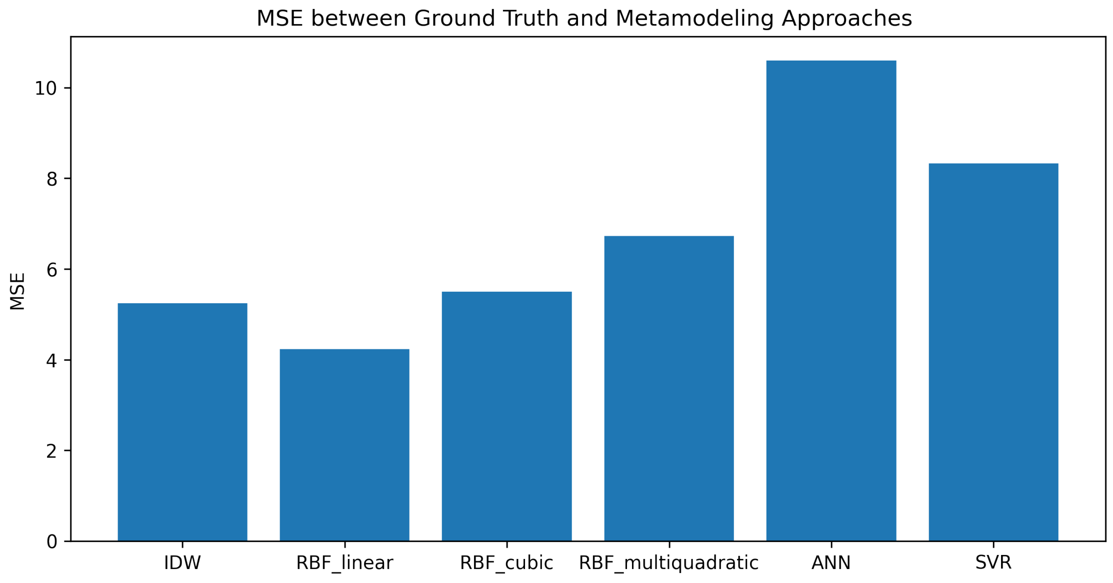


1.8 Comparison to Ground Truths:

[13]:
```
#Comparing all 4 Estimations:

#run 50x50 LHS samples with actual model to get a ground truth:
r_i_GT = np.zeros(len(BH_i));
r_i_GT = Parallel(n_jobs = -1, verbose = 0)(delayed(main_p)(BH_i[i],BU_i[i])␣
 ↪for i in range(0,len(BH_i)))
```

[14]:
```
#Compute MSE
#was already using scikit learn, so why not be lazy

from sklearn.metrics import mean_squared_error as mse

MSE_IDW = mse(r_i_GT,r_i_IDW)
MSE_RBF_lin = mse(r_i_GT,r_i_RBF_lin)
MSE_RBF_cub = mse(r_i_GT,r_i_RBF_cub)
MSE_RBF_mq = mse(r_i_GT,r_i_RBF_mq)
MSE_ANN = mse(r_i_GT,r_i_ANN)
MSE_SVR = mse(r_i_GT,r_i_SVR)

print('MSE_IDW = ', MSE_IDW)
print('MSE_RBF_lin = ', MSE_RBF_lin)
print('MSE_RBF_cub = ', MSE_RBF_cub)
print('MSE_RBF_mq = ', MSE_RBF_mq)
print('MSE_ANN = ', MSE_ANN)
print('MSE_SVR = ', MSE_SVR)


objects = ('IDW', 'RBF_linear','RBF_cubic','RBF_multiquadratic','ANN','SVR')
y_pos = np.arange(len(objects))

plt.figure(figsize=(10, 5), dpi=300)
plt.bar(y_pos, [MSE_IDW,MSE_RBF_lin,MSE_RBF_cub,MSE_RBF_mq,MSE_ANN,MSE_SVR])
plt.xticks(y_pos, objects)
plt.ylabel('MSE')
plt.title('MSE between Ground Truth and Metamodeling Approaches ')
plt.savefig('comparison.png', bbox_inches='tight')
```

```
MSE_IDW =  5.238969012918502
MSE_RBF_lin =  4.232139779082131
MSE_RBF_cub =  5.494961352184731
MSE_RBF_mq =  6.722711835960569
MSE_ANN =  10.593338128827456
MSE_SVR =  8.328352323570387
```


MSE between Ground Truth and Metamodeling Approaches
MSE
IDW
RBF_linear
RBF_cubic
RBF_multiquadratic
ANN
SVR