q3

May 24, 2020

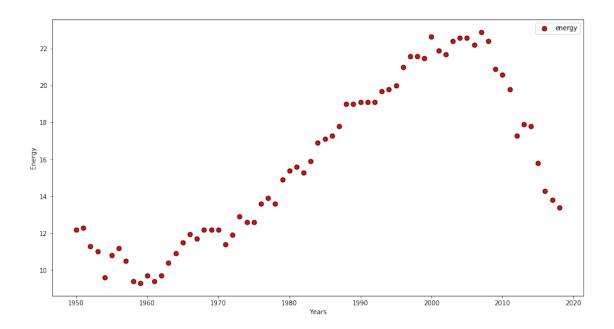
```
[1]: import numpy as np
  import pandas as pd
  import matplotlib.pyplot as plt
  from sklearn.metrics import mean_squared_error
  from sklearn.preprocessing import StandardScaler
  from skfda.representation.basis import BSpline
  import rpy2.robjects as robjects
  from multiprocessing import Process, Queue
  from IPython.core.display import display, HTML
  display(HTML("<style>.container { width:100% !important; }</style>"))
```

<IPython.core.display.HTML object>

0.0.1 Read in the Data

```
[2]: df = pd.read_csv('P04.csv', header=None)
```

0.0.2 View the Data



0.0.3 Separate x and y vectors

```
[4]: X = df[0].values
y = df[1].values
```

0.0.4 Cubic Splines Implementation

This implementation is a python recreation of the R example code. It utilizes OLS to find the weight vector

```
[5]: def cubic_splines(x, y, **kwargs):

''''

inputs
-----

x   -> Domain vector (independent variables)

y   -> Response vector (dependent variables)

kwargs -> should have any of the following options

knots --> [list]: list of knots

num_knots --> [int]: number of desired knots. These knots will

→be equidistant and calculated from input x

outputs
-----

B   -> Weight matrix found from OLS

yhat -> Fitted data
```

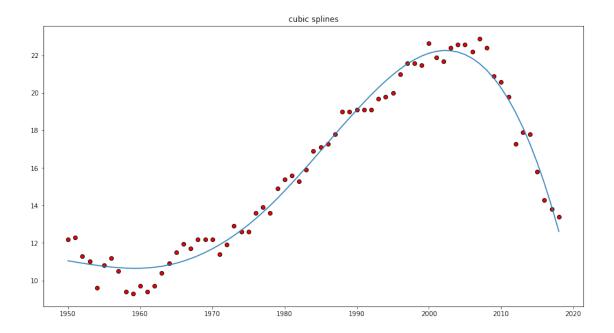
```
makeH -> Function needed to transform new unseen data
   111
   if 'knots' in kwargs.keys():
       assert isinstance(kwargs['knots'], list), 'knots should be a list'
       knots = np.array(kwargs['knots'])
   elif 'num_knots' in kwargs.keys():
       assert isinstance(kwargs['num_knots'], int), 'num_knots should be an_
→integer'
       knots = np.linspace(min(x), max(x), kwargs['num_knots'])
   111
   This is a closure function that is a returned object from this function so_{\sqcup}
\hookrightarrowa user can trasnform new unseen independent variables
   after initially fitting the training data with the supplied knots
   def wrapper(knots):
       def inner(x):
           basis = []
           h1 = 1
           h2 = x
           h3 = x**2
           h4 = x**3
           basis = [h1, h2, h3, h4]
           for i in range(len(knots)):
               h = (x - knots[i])**3
               if h <= 0:
                   h = 0
               basis.append(h)
           H = np.array(basis)
           return H
       return inner
   #create a transform function to be returned
   makeH = wrapper(knots)
   x = np.array(x)
   y = np.array(y)
   knots = np.array(knots)
   #1st basis function is all ones
```

```
h1 = np.ones(len(x))
   #2nd basis function is linear
   h2 = x
   #3rd basis function is quadratic
   h3 = x**2
   #4th basis function is cubic
   h4 = x**3
   basis = [h1, h2, h3, h4]
   \#get the truncated power basis for sigma_ki < x < sigma_ki+1
   for i in range(len(knots)):
       h = (x - knots[i])**3
       h[h \leftarrow 0] = 0
       basis.append(h)
   #transformation matrix
   H = np.array(basis)
   #weight vectors found from OLS
   B = np.dot(np.linalg.pinv(np.dot(H, H.T)), np.dot(H,y))
   #return weight vector, the fitted data, and the transformation function to \Box
→ transform new unseen data
   return B , np.dot(H.T,B), makeH
```

0.0.5 Test out cubic splines on the data with 6 knots

```
[6]: b, yhatcs, transformfunc = cubic_splines(X,y,num_knots=6)

[7]: plt.figure(figsize=(15,8))
   plt.scatter(X, y, color='r', edgecolor='k')
   plt.plot(X, yhatcs)
   plt.title('cubic splines')
   plt.show()
```



0.0.6 Cubic Splines MSE Function

The cubic_mse function can be ran as a single process but also supports a multiprocessing Queue object for multiprocessing of a hyperparameter gridsearch. It utilizes leave one out cross validation and aggregates the error for each left out independent variable predicted response. The errors from each LOO is then used to calculate the overall MSE. If a multiprocessing Queue object is supplied, the result is put on the queue and returned to the main process, otherwise the MSE is simply returned

```
#perform LOOCV
for i in range(len(y)):
    X = np.delete(x, i)
    Y = np.delete(y, i)
    #fit data on all indpendent variables except the value left out
    weights, fit, transform_func = cubic_splines(X, Y, num_knots=num_knots)
    #predict on the left out value
    xtest = x[i]
    xtest = transform func(xtest)
    pred = np.dot(weights, xtest)
    #calculate error
    preds[i] = pred
    y_true[i] = y[i]
#calculate mse
mse = mean_squared_error(y_true, preds)
#return mse
if q == None:
    return mse
else:
    q.put(mse)
```

0.0.7 b-splines implementation

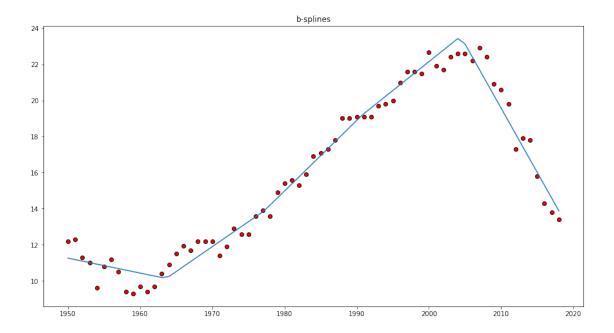
The b-splines implementation was created by using the skfda.representation.basis library and the BSpline object was utilized. The function takes in the independent and dependent variables along with the desired polynomial degree and returns the weight vector, the fitted data, and the object needed to transform new unseen data

```
outputs
   B -> Weight matrix found from OLS
   yhat -> Fitted data
   bss -> Object needed to transform new unseen data into an H tensor
  if 'knots' in kwargs.keys():
      assert isinstance(kwargs['knots'], (list, np.ndarray)), 'knots should
→be a list'
      knots = np.array(kwargs['knots'])
  elif 'num_knots' in kwargs.keys():
      assert isinstance(kwargs['num_knots'], int), 'num_knots should be anu
→integer'
      knots = np.linspace(min(x), max(x), kwargs['num_knots'])
   #instantiate a b-splines object
  bss = BSpline(knots=knots, order=order)
  #create the b-spline transformed tensors
  H = bss.evaluate(x)
  #find the weight vectors using OLS
  B = np.dot(np.linalg.pinv(np.dot(H, H.T)), np.dot(H,y))
  return B, np.dot(H.T,B), bss
```

0.0.8 Test out b-splines with 6 knots and 2nd order polynomial

```
[10]: weights, yhatbs, transform_object = bspline(X, y, 2, num_knots=6)

[11]: plt.figure(figsize=(15,8))
    plt.scatter(X,y, color='r', edgecolor='k')
    plt.plot(X, yhatbs)
    plt.title('b-splines')
    plt.show()
```



0.0.9 b-Spline MSE Function

The bspline_mse function can be ran as a single process but also supports a multiprocessing Queue object for multiprocessing of a hyperparameter gridsearch. It utilizes leave one out cross validation and aggregates the error for each left out independent variable predicted response. The errors from each LOO is then used to calculate the overall MSE. If a multiprocessing Queue object is supplied, the result is put on the queue and returned to the main process, otherwise the MSE is simply returned

```
#perform LOOCV
  for i in range(len(y)):
       X = np.delete(x, i)
      Y = np.delete(y, i)
       #fit the data on all indpendent variables except the left out value
      weights, fit, transform_object = bspline(X, Y, order=order,_
→num_knots=num_knots)
      xtest = x[i]
      xtest = transform_object.evaluate([xtest])
      pred = np.dot(weights, xtest)
      preds[i] = pred
      y_{true}[i] = y[i]
   #calculate mse
  mse = mean_squared_error(y_true, preds)
  if q == None:
      return mse
   else:
       q.put(mse)
```

0.0.10 Smoothing Spline implementation

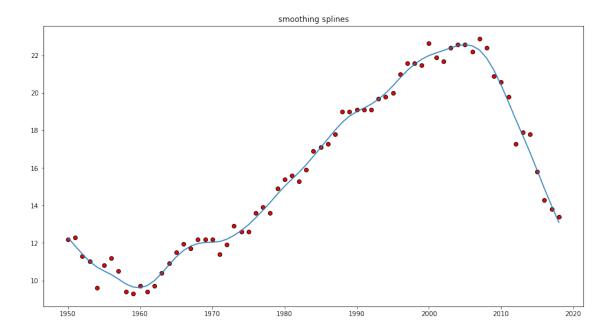
The smoothing spline implementation using the rpy2 library which allows for the direct usage of R function in python. The code is a Python implementation of the R example code provided. A closure function is created so new predictions can be made on unseen data with respect to the fit

```
#qet the smooth.spline function used by r
   smooth_spline = robjects.r['smooth.spline']
   #conver x and y to r objects
   x = robjects.FloatVector(list(x))
   y = robjects.FloatVector(list(y))
   #fit the data
   spline_obj = smooth_spline(x=x, y=y, spar=float(spar))
   111
   This closure function is returned so predictions can be made on new unseen \sqcup
\hookrightarrow data.
   def wrapper(spline_obj):
       def inner(x):
           x = robjects.FloatVector(list(x))
           yspline = robjects.r['predict'](spline_obj,x).rx2('y')
           return np.array(yspline)
       return inner
   #create the prediction function
   predict_obj = wrapper(spline_obj)
   #return yhat and prediction function
   return np.array(spline_obj.rx2('y')) , predict_obj
```

0.0.11 test out smoothing splines with a smoothing parameter of 0.5

```
[14]: yhatss, predict_obj = smoothing_splines(x=X, y=y, spar=0.5)

[15]: plt.figure(figsize=(15,8))
    plt.scatter(X,y,color='r', edgecolor='k')
    plt.plot(X,yhatss)
    plt.title('smoothing splines')
    plt.show()
```



0.0.12 Smoothing Spline MSE Function

The smoothing_mse function can be ran as a single process but also supports a multiprocessing Queue object for multiprocessing of a hyperparameter gridsearch. It utilizes leave one out cross validation and aggregates the error for each left out independent variable predicted response. The errors from each LOO is then used to calculate the overall MSE. If a multiprocessing Queue object is supplied, the result is put on the queue and returned to the main process, otherwise the MSE is simply returned

```
#perform LOOCV
for i in range(len(y)):
    X = np.delete(x, i)
    Y = np.delete(y, i)
    #fit data except left out indpendent variable
    fit, predict_object = smoothing_splines(X, Y, spar)
    #predict on left out value
    xtest = x[i]
    pred = predict_object([xtest])
    preds[i] = pred
    y_true[i] = y[i]
#calculate mse
mse = mean_squared_error(y_true, preds)
if q == None:
    return mse
else:
    q.put(mse)
```

0.0.13 Gaussian kernel implementation

The guassian kernel function is a Python refactor of the R example code provided - It creates a closure function use for real time evaluation of independent variables

```
def wrapper(x,y,lambda_):
    def inner(xtest):
        if not isinstance(xtest, (list, np.ndarray)):
            xtest = [xtest]
        N = len(xtest)
        f = np.zeros(N)

        for k in range(N):
            z = kerf((xtest[k] - x) / lambda_)
            f[k] = np.sum(z * y) / np.sum(z)

        return f
    return inner

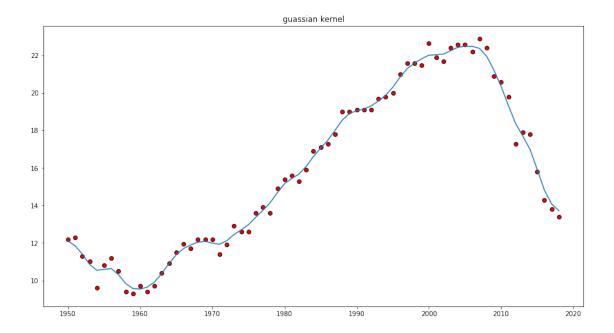
func = wrapper(x, y, lambda_)

return func
```

0.0.14 Test out gaussian kernel with a lambda value of 1.2

```
[18]: gk = gaussian_kernel(X,y,1.2)

[19]: plt.figure(figsize=(15,8))
    plt.scatter(X,y,color='r', edgecolor='k')
    plt.plot(X, gk(X))
    plt.title('guassian kernel')
    plt.show()
```



0.0.15 Gaussian Kernel MSE Function

The gaussian_mse function can be ran as a single process but also supports a multiprocessing Queue object for multiprocessing of a hyperparameter gridsearch. It utilizes leave one out cross validation and aggregates the error for each left out independent variable predicted response. The errors from each LOO is then used to calculate the overall MSE. If a multiprocessing Queue object is supplied, the result is put on the queue and returned to the main process, otherwise the MSE is simply returned

```
X = np.delete(x, i)
Y = np.delete(y, i)

xtest = x[i]
pred_obj = gaussian_kernel(x,y,lambda_)

pred = pred_obj(xtest)

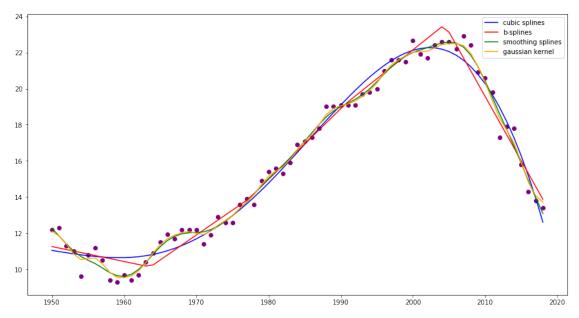
preds[i] = pred
y_true[i] = y[i]

mse = mean_squared_error(y_true, preds)

if q == None:
    return mse
else:
    q.put(mse)
```

0.0.16 Viewing all tests together

```
[21]: plt.figure(figsize=(15,8))
   plt.scatter(X,y, color='purple')
   plt.plot(X,yhatcs, color='blue', label='cubic splines')
   plt.plot(X,yhatbs, color='red', label='b-splines')
   plt.plot(X,yhatss, color='green', label='smoothing splines')
   plt.plot(X,gk(X), color='orange', label='gaussian kernel')
   plt.legend()
   plt.show()
```



0.1 LOOCV Implementation

This function utilizes multiprocessing and performs grid search across an array of hyperparameters for each algorithm. It returns a dictionary for each algorithm containing the best hyperparameter and the subsequent MSE value from the LOOCV

```
[22]: def LOOCV(x,y):
          111
          inputs
          x \rightarrow independent variable
          y -> dependent variable
          outputs
          results -> dictionary containing results for each algorithm
          #range of knots to grid search over (knots low = 6, knots high = 15)
          knots = range(6,16)
          #polynomial orders to grid search over (order low = 1, order high = 5)
          orders = range(1,6)
          #smoothing parameters to grid search over (spar low = 0, spar high = 1)
          spars = np.linspace(0,1,100)
          #lambda parameters to grid search over (lambda low = 1, lambda high = 4)
          lambdas_ = np.arange(0.1,4,0.1)
          #initialize empty array to hold all caluclated MSEs for each hyperparameter_
       \rightarrow grid searched over
          cs_mse = np.zeros(len(knots))
          bs_mse = np.zeros(len(knots) * len(orders))
          ss_mse = np.zeros(len(spars))
          gk_mse = np.zeros(len(lambdas_))
          #create a multiprocessing Queue object for each process to write results to
          cs_q = Queue()
          bs_q = Queue()
          ss_q = Queue()
          gk_q = Queue()
          #list to maintain PID for all created processes
          cs_process = []
          bs_process = []
          ss_process = []
```

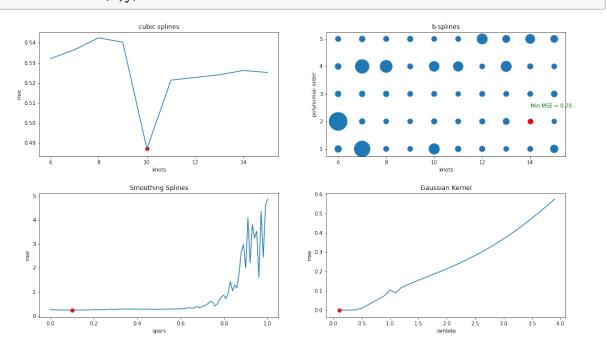
```
gk_process = []
#cubic mse multiprocessing
for i in knots:
    p = Process(target=cubic_mse, args=(x, y, i, cs_q))
    p.start()
    cs_process.append(p)
#join results from each cubic process
for pos, p in enumerate(cs_process):
    p.join()
    cs_mse[pos] = cs_q.get()
#b-spline mse multiprocessing
for i in knots:
    for j in orders:
        p = Process(target=bspline_mse, args=(x, y, j, i, bs_q))
        p.start()
        bs_process.append(p)
#join results from each b-spline process
for pos, p in enumerate(bs_process):
    p.join()
    bs_mse[pos] = bs_q.get()
#smoothing splines mse multiprocessing
for i in spars:
    p = Process(target=smoothing_mse, args=(x,y,i,ss_q))
    p.start()
    ss_process.append(p)
#join results from each smoothing spline process
for pos, p in enumerate(ss_process):
    p.join()
    ss_mse[pos] = ss_q.get()
#guassian mse multiprocessing
for i in lambdas_:
    p = Process(target=gaussian_mse, args=(x,y,i, gk_q))
    p.start()
    gk_process.append(p)
#join results from each gaussian process
for pos, p in enumerate(gk_process):
```

```
p.join()
       gk_mse[pos] = gk_q.get()
   #plot results
   fig, axes = plt.subplots(nrows=2, ncols=2, figsize=(18,10))
   ax1 = plt.subplot(221)
   ax1.plot(knots, cs_mse)
   ax1.scatter(knots[np.argmin(cs_mse)], cs_mse[np.argmin(cs_mse)],
⇔color='red', s=50)
   ax1.set_xlabel('knots')
   ax1.set_ylabel('mse')
   ax1.set_title('cubic splines')
   ax2 = plt.subplot(222)
   points = [(k,o) for k in knots for o in orders]
   xp = [x[0] \text{ for } x \text{ in points}]
   yp = [x[1] \text{ for } x \text{ in points}]
   ax2.scatter(xp,yp, s=bs_mse * 300)
   ax2.scatter(xp[np.argmin(bs_mse)], yp[np.argmin(bs_mse)], color='r', __
⇒s=bs_mse[np.argmin(bs_mse)]*300)
   plt.text(xp[np.argmin(bs_mse)], yp[np.argmin(bs_mse)] + 0.5, 'Min MSE = {}'.
→format(round(bs_mse[np.argmin(bs_mse)],2)), color='green')
   ax2.set xlabel('knots')
   ax2.set_ylabel('polynomial order')
   ax2.set_title('b-splines')
   ax3 = plt.subplot(223)
   ax3.plot(spars, ss_mse)
   ax3.scatter(spars[np.argmin(ss_mse)], ss_mse[np.argmin(ss_mse)], color='r', u
   ax3.set_xlabel('spars')
   ax3.set ylabel('mse')
   ax3.set_title('Smoothing Splines')
   ax4 = plt.subplot(224)
   ax4.plot(lambdas_, gk_mse)
   ax4.scatter(lambdas_[np.argmin(gk_mse)], gk_mse[np.argmin(gk_mse)],_u
\hookrightarrowcolor='r', s=50)
   ax4.set_xlabel('lambda')
   ax4.set_ylabel('mse')
   ax4.set_title('Gaussian Kernel')
   plt.subplots_adjust(left=None, bottom=None, right=None, top=None,
⇒wspace=None, hspace=0.3)
```

```
plt.show()
   results = {
               'cubic_splines':{'knot': knots[np.argmin(cs_mse)], 'mse':
 'bsplines': {'knot':xp[np.argmin(bs_mse)], 'order':yp[np.
 →argmin(bs_mse)], 'mse':bs_mse[np.argmin(bs_mse)]},
               'smooth_splines': {'spar':spars[np.argmin(ss_mse)], 'mse':
 →ss_mse[np.argmin(ss_mse)]},
               'gaussian_kernel': {'lambda':lambdas_[np.argmin(gk_mse)], 'mse':
}
   results_string = '''
Cubic Splines:
                  Optimal Knots {}
                  MSE {}
B-Splines:
                  Optimal Knots {}
                  Optimal Degree {}
                  MSE {}
Smoothing Splines: Optimal Smoothing Parameter {}
                  MSE {}
Gaussian Kernel:
                  Optimal Lambda {}
                  MSE {}
'''.format(results['cubic_splines']['knot'],
          results['cubic splines']['mse'],
          results['bsplines']['knot'],
          results['bsplines']['order'],
          results['bsplines']['mse'],
          results['smooth_splines']['spar'],
          results['smooth_splines']['mse'],
          results['gaussian_kernel']['lambda'],
          results['gaussian_kernel']['mse'])
   print(results_string)
   return results
```

0.1.1 Perform LOOCV on Unscaled X data First

[23]: results = LOOCV(X,y)



Cubic Splines: Optimal Knots 10

MSE 0.4869035180512312

B-Splines: Optimal Knots 14

Optimal Degree 2

MSE 0.2757741596820151

Smoothing Splines: Optimal Smoothing Parameter 0.10101010101010102

MSE 0.24488285318203684

Gaussian Kernel: Optimal Lambda 0.1

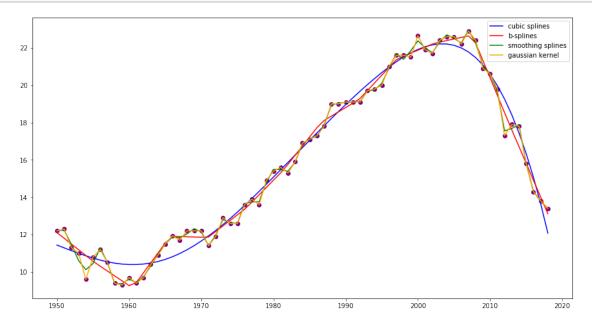
MSE 1.0060834733253483e-30

0.1.2 Utilizing best parameters for each algorithm

```
[24]: cs_knots = results['cubic_splines']['knot']
bs_knots = results['bsplines']['knot']
bs_degree = results['bsplines']['order']
ss_spar = results['smooth_splines']['spar']
gk_lambda = results['gaussian_kernel']['lambda']
```

```
[25]: b, yhatcs, transformfunc = cubic_splines(X,y,num_knots=cs_knots)
weights, yhatbs, transform_object = bspline(X, y, bs_degree, num_knots=bs_knots)
yhatss, predict_obj = smoothing_splines(x=X, y=y, spar=ss_spar)
gk = gaussian_kernel(X,y,gk_lambda)
```

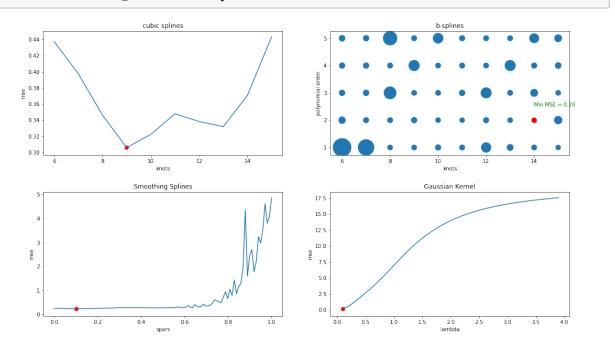
```
plt.figure(figsize=(15,8))
  plt.scatter(X,y, color='purple')
  plt.plot(X,yhatcs, color='blue', label='cubic splines')
  plt.plot(X,yhatbs, color='red', label='b-splines')
  plt.plot(X,yhatss, color='green', label='smoothing splines')
  plt.plot(X,gk(X), color='orange', label='gaussian kernel')
  plt.legend()
  plt.show()
```



0.1.3 Perform LOOCV on Scaled Data

```
[27]: scaler = StandardScaler()
scaler.fit(X.reshape(-1, 1))
X_transformed = scaler.transform(X.reshape(-1, 1))
X_transformed = np.array([i[0] for i in X_transformed.tolist()])
```

[28]: results = LOOCV(X_transformed,y)



Cubic Splines: Optimal Knots 9

MSE 0.30610506353725286

B-Splines: Optimal Knots 14

Optimal Degree 2

MSE 0.27577415968201885

Smoothing Splines: Optimal Smoothing Parameter 0.10101010101010102

MSE 0.24488285318203865

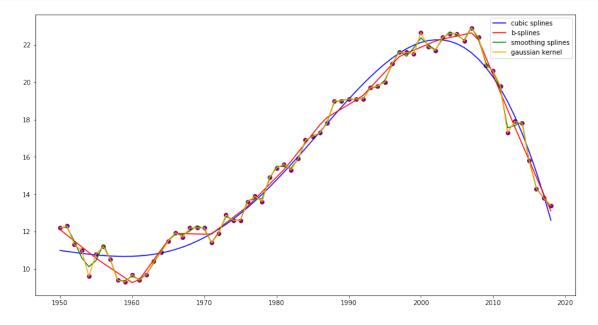
Gaussian Kernel: Optimal Lambda 0.1

MSE 0.21302888604096862

```
[29]: cs_knots = results['cubic_splines']['knot']
bs_knots = results['bsplines']['knot']
bs_degree = results['bsplines']['order']
ss_spar = results['smooth_splines']['spar']
gk_lambda = results['gaussian_kernel']['lambda']
```

[30]: b, yhatcs, transformfunc = cubic_splines(X,y,num_knots=cs_knots)
weights, yhatbs, transform_object = bspline(X, y, bs_degree, num_knots=bs_knots)
yhatss, predict_obj = smoothing_splines(x=X, y=y, spar=ss_spar)
gk = gaussian_kernel(X,y,gk_lambda)

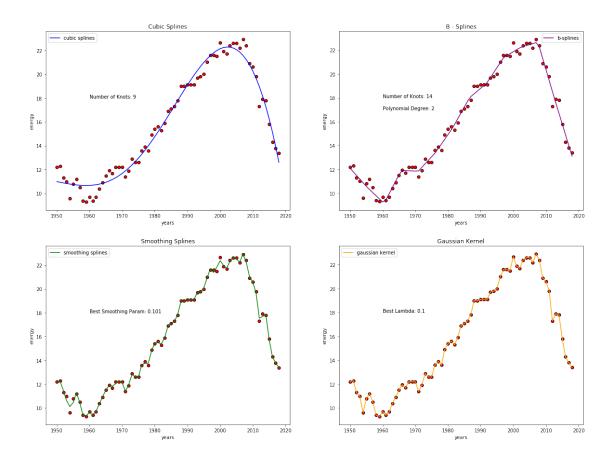
```
plt.figure(figsize=(15,8))
  plt.scatter(X,y, color='purple')
  plt.plot(X,yhatcs, color='blue', label='cubic splines')
  plt.plot(X,yhatbs, color='red', label='b-splines')
  plt.plot(X,yhatss, color='green', label='smoothing splines')
  plt.plot(X,gk(X), color='orange', label='gaussian kernel')
  plt.legend()
  plt.show()
```



```
[32]: fig, axes = plt.subplots(nrows=2, ncols=2, figsize=(20,15))

ax1 = plt.subplot(221)
ax1.scatter(X,y, color='red', edgecolor='k')
ax1.plot(X,yhatcs, color='blue', label='cubic splines')
ax1.set_xlabel('years')
ax1.set_ylabel('energy')
```

```
ax1.set_title('Cubic Splines')
plt.text(1960, 18, 'Number of Knots: {}'.format(cs_knots))
plt.legend()
ax2 = plt.subplot(222)
ax2.scatter(X,y, color='red', edgecolor='k')
ax2.plot(X,yhatbs, color='purple', label='b-splines')
ax2.set_xlabel('years')
ax2.set ylabel('energy')
ax2.set_title('B - Splines')
plt.text(1960, 18, 'Number of Knots: {}'.format(bs_knots))
plt.text(1960, 17, 'Polynomial Degree: {}'.format(bs_degree))
plt.legend()
ax3 = plt.subplot(223)
ax3.scatter(X,y,color='red', edgecolor='k')
ax3.plot(X,yhatss, color='green', label='smoothing splines')
ax3.set_xlabel('years')
ax3.set_ylabel('energy')
ax3.set_title('Smoothing Splines')
plt.text(1960, 18, 'Best Smoothing Param: {}'.format(round(ss_spar,3)))
plt.legend()
ax4 = plt.subplot(224)
ax4.scatter(X,y, color='red', edgecolor='k')
ax4.plot(X,gk(X), color='orange', label='gaussian kernel')
ax4.set_xlabel('years')
ax4.set_ylabel('energy')
ax4.set_title('Gaussian Kernel')
plt.text(1960, 18, 'Best Lambda: {}'.format(gk_lambda))
plt.legend()
plt.show()
```



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