Multiple Partition Regression Analysis Rhys Hawkins and Malcolm Sambridge September 24, 2012

This tutorial describes how to analyse discontinuous data using Monte-Carlo Markov-Chain based regression.

Pre-requisites

This tutorial is for the Python version of the rjmcmc library. The examples rely on the Matplotlib library for plotting. The versions used in the development of this tutorial are as follows:

- Python 2.7.1
- rjmcmc 0.1.0
- Matplotlib 1.1.0

The Data

Similar to the single partition tutorial we will use a non-trivial synthetic dataset with added noise. The difference this time is that we will add a series of discontinuities or step functions and a sign change.

The base function that is used is an exponentially increasing sine wave over the domain 0 \dots 10, ie:

$$y = \operatorname{stepsign}(x) \times e^{\frac{x}{3}} \sin \frac{2x}{3} + \operatorname{step}(x)$$
 (1)

Where the step and stepsign functions are defined as follows:

step(x) =
$$\begin{cases} 15 & x < 2.5 \\ -20 & 2.5 \ge x < 5 \\ 0 & otherwise \end{cases}$$
 (2)

stepsign(x) =
$$\begin{cases} -1 & x < 2.5\\ 1 & 2.5 \ge x < 5\\ -1 & otherwise \end{cases}$$
 (3)

The actual dataset unevenly (though with fairly good coverage) samples this function and adds some Gaussian noise and these values are save to an ASCII text file. A plot of the synthetic data points with the true function is shown in Figure 1.

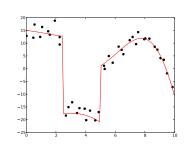


Figure 1: The Synthetic Data

Loading the Data

For those unfamiliar with Python, we discuss briefly the loading of data from a simple ASCII text file. The code for loading the data and doing a simple plot is shown in Listing 1.

Listing 1: Loading the Data

```
#
# Import the libraries we will need for analysis and plotting.
#
import imcmc
import matplotlib
import matplotlib.pyplot
#
# Open our data file which consists of one (x, y) coordinater per line
# separated by whitespace
#
f = open('data.txt', 'r')
lines = f.readlines()
x = []
y = []
for line in lines:
    columns = line.split()
    x.append(float(columns[o]))
    y.append(float(columns[o]))
    y.append(float(columns[o]))
f.close()
fig = matplotlib.pyplot.figure()
matplotlib.pyplot.plot(x, y, 'ko')
fig.savefig('ch1-loading.pdf', format='PDF')
matplotlib.pyplot.show()
```

The ASCII file contains an x, y pair per line separated by a space. On line 12, we use the built in function open to open the file. One lines 15 and 16 we initialize 2 list that will contain the x and y coordinates in the file. On line 18 we loop through the lines in the file and add each x, y pair to the 2 separate lists.

From line 26 onwards, we plot the data using the matplotlib library and save the plot to a PDF file. The plot resulting from this script can be seen in Figure 2.

Running the default analysis

For performing a regression analysis on a continuous dataset the function is called regression_part1d. The parameters for this function are mostly the same as the regression_single1d function with the only additional required parameter being pd.

The complete list of parameters for this function are as follows with default values shown where applicable:

- *dataset* The dataset object to run the analysis on. This is an rjmcmc.dataset1d object which wraps the x and y vectors you load from the file and includes individual point noise values. This is the only parameter which doesn't have a default value.
- *pd* The standard deviation for the perturbation of partition boundaries.

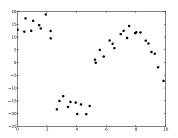


Figure 2: The Plot of the Data

burnin = 10000 The number of initial samples to throw away.

- *total* = 50000 The total number of samples to use for the analysis.
- *max_order* = 1 The maximum order of polynomial to use to fit the data.
- *xsamples* = 100 The number of points to sample along the x direction for the curve.
- *ysamples* = 100 The number of points to sample along the y directory for the statistics such as mode, median and confidence intervals. This is the number of bins for the histograms in the y direction.
- *confidence_interval* = 0.95 The confidence interval to use for minimum and maximum confidence intervals. This should be a value between 0 and 1.

For this analysis we are only going to use the default values and the listing is shown in Listing 2.

Listing 2: Running the Default Analysis

```
# Import the libraries we will need for analysis and plotting.
#
 3
4
5
6
         import rjmcmc
        import matplotlib
import matplotlib.pyplot
 _{8}^{7}
        # # Open our data file which consists of one (x, y) coordinate per line
# separated by whitespace
#
f = open('data.txt', 'r')
lines = f.readlines()
9
10
11
12
13
14
15
16
17
18
        x = []
y = []
        for line in lines:
    columns = line.split()
19
20
              x.append(float(columns[0]))
y.append(float(columns[1]))
21
22
        f.close()
24
25
26
27
28
        #
# Set our x range
#

    xmin = 0.0
    xmax = 10.0

\begin{array}{c} 29\\ 3^{0}\\ 3^{1}\\ 3^{2}\\ 3^{3}\\ 3^{4}\\ 3^{5}\\ 3^{6}\\ 3^{7}\\ 3^{8}\\ 3^{9}\\ 4^{1}\\ 4^{2}\\ 4^{3}\\ 4^{4}\\ 4^{5}\\ 4^{6}\\ 4^{7}\\ 4^{8} \end{array}
        #
# Estimate our error standard deviation
#
        sigma = 3.0
n = [sigma] * len(x)
        #
# Create the rjmcmc dataset
         data = rjmcmc.dataset1d(x, y, n)
        #
# Specify the standard deviation for the move partition
        pd = 1.0
        #
# Run an analysis with reduced max order to only allow linear
# segments
49
50
51
52
         burnin = 10000
        total = 50000
max_partitions = 10
max_order = 1
53
54
55
56
57
        results = rjmcmc.regression partid(data,
```

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8 9 0 1 2	pd, burnin, total, max_partitions, max_order)
3 4 5 6 7 8	# # Retrieve the mean curve for plotting # xc = results.x() meancurve = results.mean()
9 1 2 3 4	# # Retrieve the partition location and count information # partlocation = results.partition_location_histogram() partcount = results.partitions()
5 6 7 8 9	# # Plot the data with black crosses and the mean with a red line # fig = matplotlib.pyplot.figure(1)
1 2 3 4 5 6	<pre>a = matplotlib.pyplot.subplot(211) a.plot(x, y, 'ko', xc, meancurve, 'r-') a.set_xlim(xmin, xmax) b = matplotlib.pyplot.subplot(212)</pre>
7 8 9 1	<pre>b = matprofit subprof(12) b.bar(xc, partlocation , xc[1] - xc[0]) b.set_xlim (xmin, xmax) fig.savefig('ch2-analyse.pdf', format='PDF')</pre>
2 3 4 5 6	<pre>fig = matplotlib.pyplot.figure(2) a = matplotlib.pyplot.subplot(111) a.hist(partcount, bins=5, range=(0,5), align='left') figure for first the second s</pre>
7 8 9	fig.savefig('ch2-analyse-partcount.pdf', format='PDF') matplotlib.pyplot.show()

The preamble (lines $1 \dots 24$) consists of loading the file as in the previous section.

An important part of the analysis is estimating the error in the data. This is specified as a error value per data point and can be thought of a weighting as to how well the fit will attempt to fit an individual point. If the value is low, then the fit will be tight and conversely if the value is high then the fit will be loose. On lines 35 and 36 we set a value of 3.0 for all data points. Use this value for now, but try other values greater than 0.0 to see the effect.

On line 41 we construct the dataset1d object from the x, y and n lists we created. These lists must be the same length.

On line 46 we set the value for the pd parameter. With partition modelling, a variable number of discontinuities are trialed at random locations along the x-axis. As part of the fitting process, the locations of these discontinuities are perturbed by an amount determined by sampling from a normal distribution with a standard deviation given by the pd parameter. We will discuss how to choose this value latter, but for now a useful rule of thumb would be to set it to 5 to 10 percent of the range of the data. So in this case our range is 10, so a pd of 1 would seem a good first approximation.

On line 57 we run the analysis with this dataset1d object. The regression_single1d function returns a resultset1d object which contains various results and diagnostics about the analysis. For this simple analysis we simply take the x sampling coordinates and the mean of the fits. And plot the mean with the original data points to

see how representative the mean is. This plot is shown in Figure 3.

In the plot, rather than just plotting the mean of the fits, we have also plotted the histogram of the location of the partition boundaries which indicates the most likely location of the discontinuities. As can be seen in the figure, the histogram highlights the artificial discontinuities created at x = 2.5 and 5.

We have also plotted the histogram of the number of partitions as shown in Figure 4. From this we can infer the likelihood of the number of the partitions in the data.

It should be noted here that there are two discontinuities in function and one less prominent change in gradient in the real data. Looking at the plot of the number of partitions, we see strong support for 4 partitions, as the algorithm has identified the four segments in the original curve.

Increasing the maximum order of the polynomial

Partition modelling and allowing higher order polynomials are in conflict to some degree. A higher order polynomial can fit a discontinuity to some degree and therefore obviate the need to create an extra partition.

To show this, we can increase the maximum order allowed for the polynomials in each partition to 5. This means that the fitting procedure may use up to a 5th order polynomial instead of line segments. The script to do this is shown in Listing 3.

Listing 3: Increasing the maximum order of the polynomials

```
#
# Import the libraries we will need for analysis and plotting
import rjmcmc
import matple
import matplotlib
import matplotlib.pyplot
"
# Open our data file which consists of one (x, y) coordinate per line
# separated by whitespace
f = open('data.txt', 'r')
lines = f.readlines()
x = []
y = []
for line in lines:
      columns = line.split()
     x.append(float(columns[o]))
     y.append(float(columns[1]))
f.close()
#
# Set our x range
#

\begin{array}{l} xmin = 0.0 \\ xmax = 10.0 \end{array}

#
# Estimate our error standard deviation
sigma
n = [sigma] * len(x)
  Create the rjmcmc dataset
```

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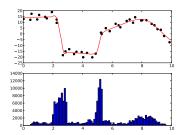


Figure 3: The Default Analysis Plot

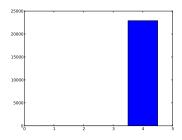


Figure 4: The Partition Count Histogram

41	data = rjmcmc.dataset1d(x, y, n)
42	4
43	# # Specify the standard deviation for the move partition
44	# Specify the standard destation for the move partition
45 46	m = 1.0
	pu – 1.0
47 48	<u>н</u>
49	"# Run the default analysis
49 50	#
51	results = rjmcmc.regression_partid(data, pd)
52	
53	#
54	# Retrieve the mean curve for plotting
55	#
56	xc = results . x()
57	meancurve = results.mean()
58	
59	#
60	# Retrieve the partition location and count information
61	#
62	partlocation = results.partition_location_histogram()
63	partcount = results.partitions()
64	
65	
66	# Plot the data with black crosses and the mean with a red line
67	
68	fig = matplotlib.pyplot.figure(1)
69 70	a = matplotlib.pyplot.subplot(211)
70	a - matpioniti.pypiot.subpiot(211)
71 72	a.plot(x, y, 'ko', xc, meancurve, 'r-')
73	a. set_xlim(xmin, xmax)
73	
75	b = matplotlib.pyplot.subplot(212)
76	b.bar(xc, particulation, $xc[1] - xc[o]$)
77	b.set_xlim(xmin, xmax)
78	
79	fig.savefig('ch3-order.pdf', format='PDF')
80	
81	fig = matplotlib.pyplot.figure(2)
82	
83	a = matplotlib.pyplot.subplot(111)
84	a.hist(partcount, bins=5, range=(0,5), align='left')
85	
86	fig.savefig('ch3-orderpartcount.pdf', format='PDF')
87	
88	matplotlib.pyplot.show()

The results of running this script can be seen in Figures 5 and 6. As can be seen, the fit is more smooth than the previous analysis and supports a fewer number of partitions. In particular we can see that there is some support for no discontinuities, but it is more likely that there are 1 or 2 which matches our artificially created boundaries (the discontinuity at x = 5 is not that large so it can be accommodated by a higher order polynomial). Try changing the maximum allowed order to, say, 2, i.e. allow up to a quadratic, and examine what happens to the Partition Count Histogram.

Confidence

So far we have only plotted the mean of the fits, however this gives only a glimpse as to how the data is being fitted. One way to look at the fitting is to takes samples of the fitting curves. The script to do this is showing in Listing 4.

Listing 4: Sampling the Fitting

```
1 #
#
1 mport the libraries we will need for analysis and plotting.
3 #
4 import natplotlib
6 import matplotlib.pyplot
7 form mpl_toolkits.mplot3d import axes3d, Axes3D
8
9 #
1 # Open our data file which consists of one (x, y) coordinater per line
```

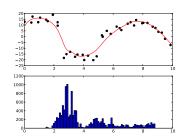


Figure 5: The Order Analysis Plot

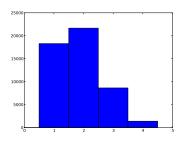


Figure 6: The Partition Count Histogram

```
# separated by whitespace
f = open('data.txt', 'r')
lines = f.readlines()
x = []
y = []
x.append(float(columns[o]))
y.append(float(columns[1]))
f.close()
#
# Estimate our error standard deviation
sigma = 3.0
n = [sigma] * len(x)
#
# Create the rjmcmc dataset
data = rjmcmc.dataset1d(x, y, n)
#
# Set our x range
#

\begin{array}{l} xmin = 0.0 \\ xmax = 10.0 \end{array}

#
# This is our callback function which samples the curves generated
# during the analysis
#
sample_x = None
sample_x = None
sample_curves = []
sample_rate = 250
def sample_rcb(x, y):
global sample_x, sample_curves, sample_i, sample_rate
     if sample_i == o:
    sample_x = x
     if sample_i % sample_rate == o:
    sample_curves.append(y)
      sample_i = sample_i + 1
#
# Run a series of analyses with varying maximum allowed order
#
#
# Specify the standard deviation for the move partition
#
pd = 1.0
#
# Run an analysis with reduced max order to only allow linear
segments
burnin = 10000
total = 50000
max_partitions = 10
max_order = 3
results = rjmcmc.regression_part1d_sampled(data,
                                                                  sampler_cb ,
                                                                  pd,
burnin,
                                                                  total ,
max_partitions ,
                                                                  max_order)
#
# Plot the data with black crosses, the sample curves as faint lines, and
# the mean as a red line
fig = matplotlib.pyplot.figure(1)
ax = fig.add_subplot(111)
yc = 0.5
yalpha = 1.0/((1.0 - yc) * float(len(sample_curves)))
for sy in sample_curves:
      ax.plot(sample_x, sy,
color = str(yc),
alpha = yalpha,
linestyle = '-',
linewidth = 10)
ax.plot(results.x(), results.mean(), 'r-')
ax.plot(x, y, 'ko')
ax.set_xlim(xmin, xmax)
fig.savefig('ch4-confidence.pdf', format='PDF')
fig = matplotlib.pyplot.figure(2)
ax = fig.add_subplot(111)
```

11

19 20 21

27 28

 $\begin{array}{c} 29\\ 30\\ 31\\ 32\\ 33\\ 34\\ 35\\ 36\\ 37\\ 39\\ 40\\ 41\\ 42\\ 44\\ 45\\ 46\\ 47\\ 48\\ 95\\ 51\\ 52\\ \end{array}$

59 60

 8_3 8_4 8_5 8_6 8_7 8_8 8_9 9_1 9_2 9_3 9_4 9_5 9_7 9_8

109 110 111

112

```
113
114 ax.plot(results.x(), results.mean(), 'r-')
115 ax.plot(x, y, 'ko')
116 ax.plot(results.x(), results.credible_min(), 'b:')
117 ax.plot(results.x(), results.credible_max(), 'b:')
118
119 ax.set_xlim(xmin, xmax)
120
121 fig.savefig('ch4-confidenceintervals.pdf', format='PDF')
122
123 matplotlib.pyplot.show()
```

The resulting plot is shown in Figure 7. This plot shows the mean as well as 200 curves sampled from the fitting process overplotted with transparency so that the darker regions are where the true curve is more likely to be. What should be noted is that there are large spikes about the discontinuities and this is to be expected as the fitting process will trial fitting curves across these discontinuities which will produce high order curves which will overshoot.

Another feature to notices is that at approximately x = 4.5, the curves tends to take 2 alternate paths. This type of feature is likely due to whether a partition boundary is located at approximately x = 5 or not.

An alternative look at the breadth of curves is to plot the confidence intervals that are generated during the fitting process. This result is shown in Figure 8.

The confidence interval curves are shown in blue dashed lines. What these curves represent is 95 percent of the curves generated during the fitting process were contained within these lines. Similarly to the sampled curves, there is some overshoot near severe discontinuities. Lowering the maximum order can sometimes alleviate these.

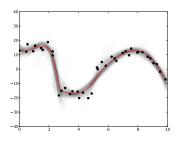


Figure 7: Sampled Curves from the Fitting

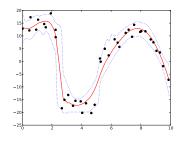


Figure 8: Confidence Intervals from the Curve Fitting