

Numerical Analysis for Computer Scientists
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Project #2

Finding the line strength of stars for an
astronomer

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1 Introduction and Problem Background

This project is about solving real-world problems with their accompanied complexities and ambiguities. The best method must be determined and its limitations and possible errors must be known. In this project intensity of light from stars will be studied. Stars produces a continuous curve of light over a range of frequencies called the *spectrum* for that star. It can be measured in *relative intensity* ($\frac{\text{W}}{\text{m}^2 \times \text{Hz}}$) as a function of the frequency (Hz) which is defined as the spectrum. We want to measure in relative intensity because the energy is higher at higher frequencies and that known property is not the one we want to study. Therefore we normalize it with the frequency.

What is interesting is that the surrounding gases of a star will either absorb (cold gas) or emit (warm) light which is visible at discrete fixed frequencies in the spectrum as *spectral lines*. By identifying these spectral lines the components of the star can be found because each chemical composition have a unique fingerprint of discrete frequencies [1] [2].

In this project a measured continuous spectrum for a star is given which contains six spectral lines evenly divided in absorption lines and emissions lines. The task is to find the total intensity for each of these spectral lines called the *line strength* measured in $\frac{\text{M}}{\text{m}^2}$ [3]. This is achieved by finding the area under the curve at the peak-frequencies i.e. integrating the relative intensity over these frequencies.

The areas can not be found using analytical methods since we don't have the real spectrum and spectrum line functions – just observations from it. We must find a way of finding the area from just these observations.

The given data is a file with 4000 measurements of *Specific Intensity* in $\frac{\text{W}}{\text{m}^2 \times \text{Hz}}$ at frequencies in the range $[3.50 \times 10^{14}, 4.29 \times 10^{14}]$.

2 Numerical Considerations

For this problem there was no hints on what methods to be used. Therefore an iterative approach was used to find methods that works. The process will be describe in section 3. As described there, I used some *MATLAB*[®] features including polynomial fitting in the least squares sense with the command *polyfit* and estimation of areas using the trapezoidal method with the command *trapz*. As later described there was a problem with an ill-conditioned matrix which was solved my normalization.

3 Results & Analysis

All code used to get the results can be seen in Appendix B. The first thing to do is, as always, to get an understanding of what are the given. Since studying the raw data is hard a graphical plot over the curve is desired to grasp the main characteristics of what we have. The relative intensity spectrum can be seen in figure 1 and the spectrum itself in figure 2. In these two plots the six spectral lines are clearly visible. Just because it is interesting, the intensities are also show as a function of the wave lengths in figure 3 using the *MATLAB*[®] function *spectrumLabel*[4].

The first naïve thing to do is to see if we can fit a curve the data directly. Just by trying out some, one seen in figure 4, we can conclude that no polynomial can fit both the spectrum and the spectrum lines and give a good representation of the real

functions. From this the main idea for solving this project was developed. We want to find a function representing the spectrum and then approximate the area between this function and the peaks/dips.

To find this function we must first remove the distracting points from the spectrum lines and extrapolate the missing parts of the spectrum line. By plotting the data points as a function of their index in a graph the beginning, midpoints and endpoints for peaks/dips could be found. One had to zoom in very much in the graph to really see the hidden details of the slope. From these points some polynomial fittings was done as seen in figure 5. This of course depends on eye measurements which is not exact so I made sure to have some small marginals by removing possibly more points than needed. This is not a problem since this area is small and will not affect the end results. There are probably a better way of finding these points but I considered that this would require too much effort and that this method was good enough.

It was found that a polynomial of degree 4 followed the curve good enough. Higher degrees did not to much better. The tricky point is the small and steep segment between the first dip and the second peak. Because of the large variety in the frequencies the matrix A used by *polyfit* is ill-conditioned $cond(A^T \times A = 1.681060E + 27)$ giving results that can not be trusted the frequencies had to be normalized before fitting.

For all but two spectrum lines we can now calculate the area by using the trapezoidal method by giving the start and end frequencies and the corresponding difference between the fitted curve and the measure relative intensities to the *MATLAB*[®] command *trapz*. The results can be seen in table 1.

Spectral Line	Area (full)
1	3.555511E+06
2	5.030370E+06
3	1.586236E+06
4+5	2.127647E+07
6	3.250223E+06

Table 1: Full areas for the spectrum lines (double dip excluded).

But what about the double dip? We're missing one boundary value for each of the dips and can thus not calculate the areas. Therefore we now assume that the distribution of spectrum frequencies are symmetric. By looking at the peaks/dips that we have we can see that they all seems to follow this. If we assume this the areas for the two dips can be found by finding the area for half of the line and multiply it by two. This was done for all points, in figure 2, so the results can be compared to the one in table 1

Spectral Line	Area (symmetry method)
1	3.546553E+06
2	5.039057E+06
3	1.576005E+06
4	1.416181E+07
5	9.521223E+06
6	2.841056E+06

Table 2: Areas found by calculating half the area and multiplying by two.

It is interesting to compare the full areas and the areas found by multiplying by two. So the infinity norm of the difference in areas (double dip excluded) was found

to be $4.091669E + 05$ and was for the last peak, spectral line 6. If we divide that with the corresponding more accurate area (the one found by using the whole known interval) we get that the quota in percent is 12.589. This must be considered high, also relative to the other differences but it has an explanation. By zooming in on the last peak (figure 6) we can see that there is no data point in the middle and the closest two points are not laid out symmetrically around the peak. Therefore it is hard to know where the mid point actually is. I chose to take the point closest to the real top and not spend time on approximating the real one. This is because there is no real need to find the area by using the symmetry for this point since both end and start points are known. The only reason for calculating the area in this way is for reference but we have 3 other peaks/dips that could be used to compare the full area with the symmetry methods that have clear points defining the middle.

But for the two dips with missing start/end points we somehow have to guess leading us to approximate by calculating the half we know. There are of course other methods that might give worse or better guesses. But all boils down to making smart guesses – we can not recover unknown information.

The difference between the full double dip area and sum of the symmetrically found individual areas are $2.406557E + 06$. The sum is 11.311% larger than the full double dip area. This difference is of course expected since the areas overlap for the two dips leading to a smaller area for the combined full dip.

For all results above we must know that all are affected by approximations and can not be taken for being exact. The first source of error is when I select begin and endpoints for the peaks/dips with eye-measurements. Comparison with other area results from friends that chose similar but not the exactly the same points gave no noticeable difference in the results. So hopefully the choice of points does not affect so much but is still a source of error. The curve fitting of the remaining points is also not perfect introducing errors in the final area difference. For the two dips that overlap can possibly have some more errors since half of the area is doubled to get the total area. If there is a large error in the half area (caused by any of the two previously mentioned sources) it will be doubled.

4 Lessons Learned

In this project I practiced on solving real problems as an engineer by combining previously learned knowledge in this and other courses to solve new types of problems. It was fun and instructive to find methods of solving the problem. I've also learned to use some new tools in *MATLAB*[®] like *trapz*, *setdiff* and how to import data from proprietary formats like *Microsoft Excel*[®]. Also I've practiced on normalizing to avoid ill-conditioning.

5 Acknowledgments

I worked tightly with Oscar Olsson, Tommy Ivarsson and Jonas Klauber when finding out the overall solution method. I also discussed the report with Fredrik Petterson and Simon Thörnqvist.

References

- [1] N. Strobel, "Production of light." Accessed 2012-04-21.
- [2] N. Strobel, "Discrete spectrum." Accessed 2012-04-21.
- [3] S. D. S. Survey, "Spectral types." Accessed 2012-04-21.

- [4] J. Mather, “Spectral and xyz color functions.” Downloaded 2012-04-21.

Appendix

A Figures

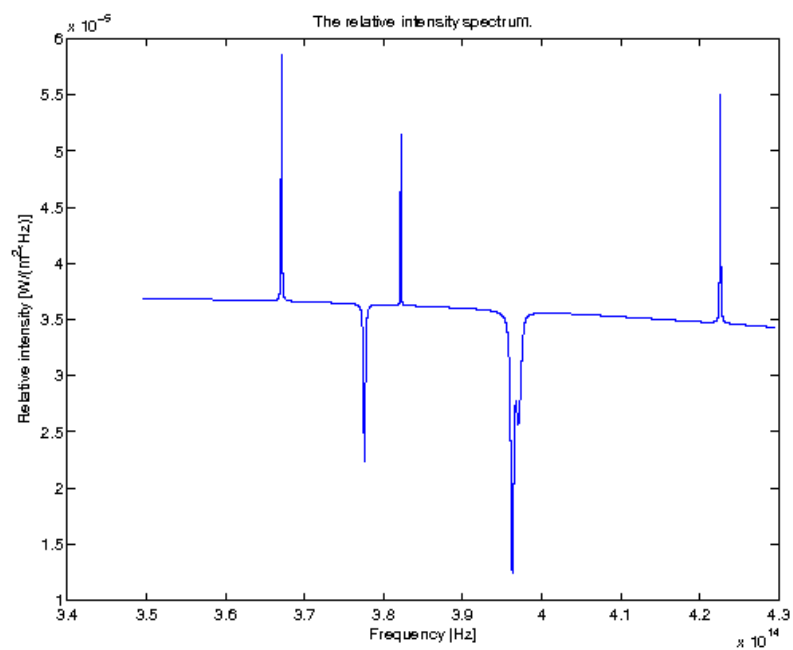


Figure 1:

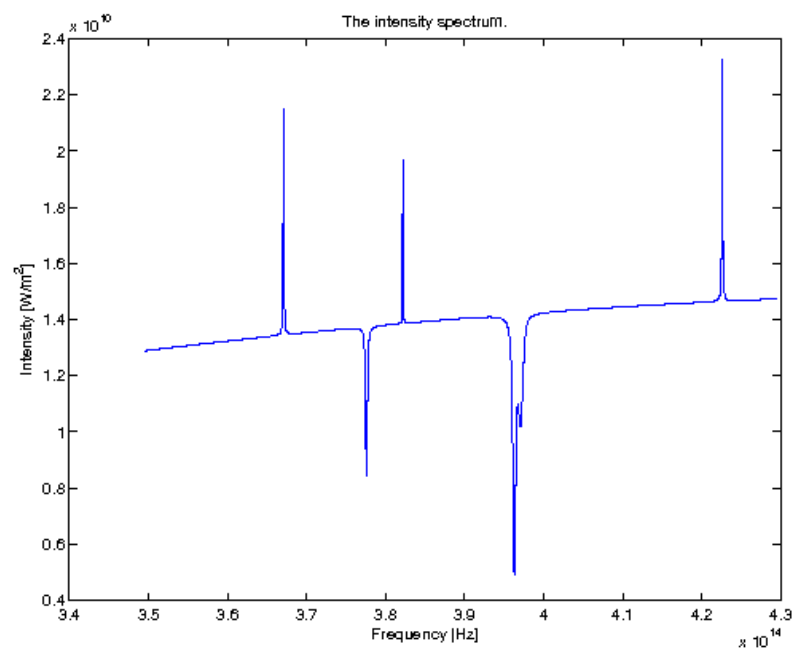


Figure 2:

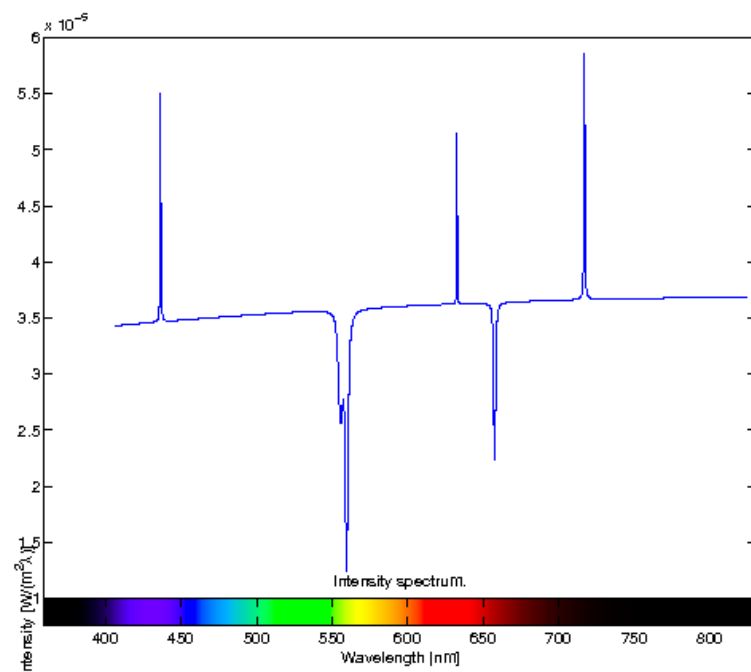


Figure 3:

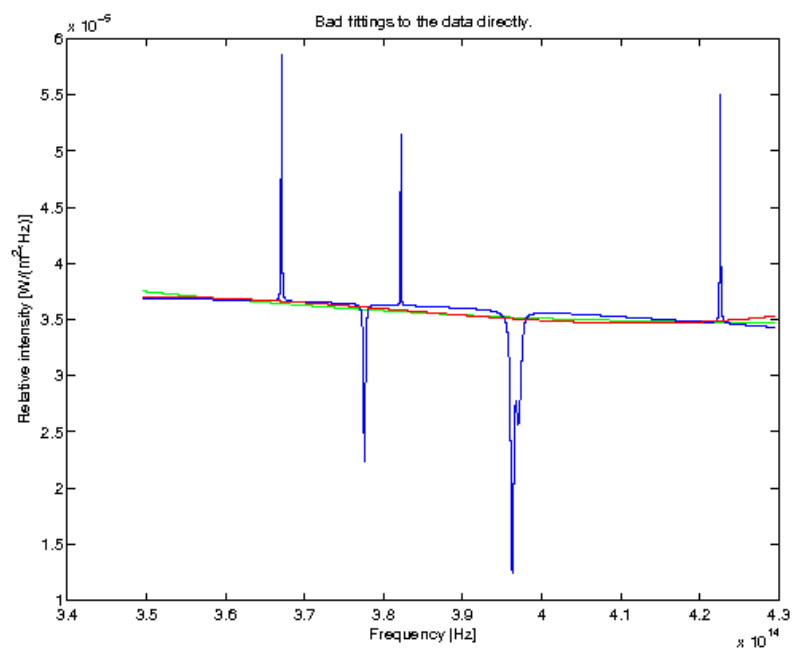


Figure 4:

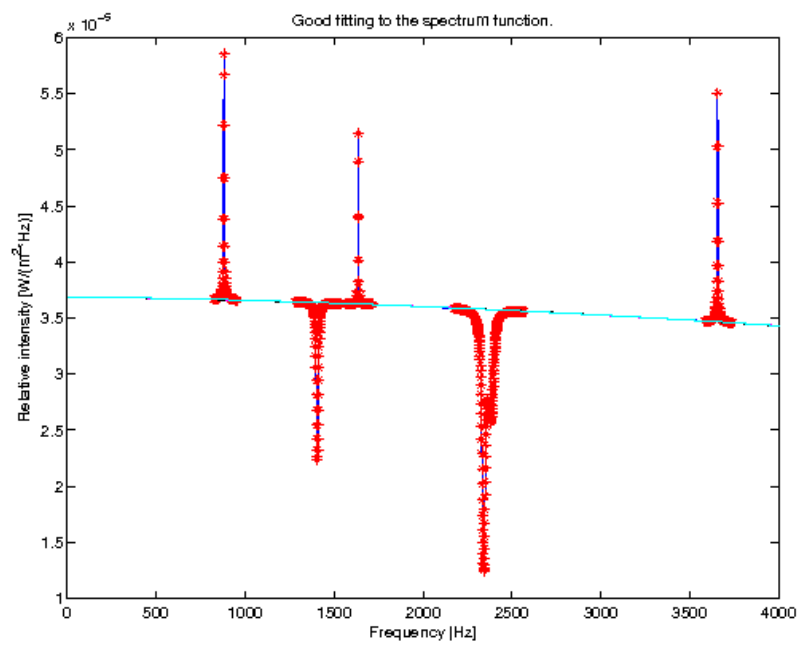


Figure 5:

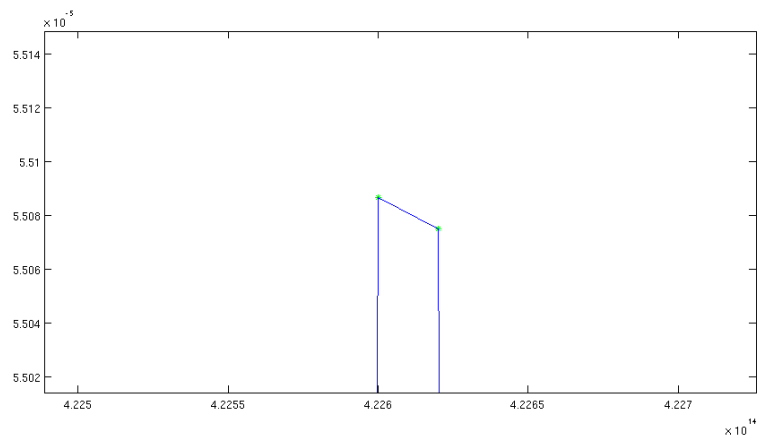


Figure 6: The two highest data points for the spectral line.

B Program listings

Here the *MATLAB*[®] functions and scripts used to achieve the results above are listed.

B.1 Scripts

The following scrips are the drivers for producing the results found in this report.

../src/pr2.m

```
1  clc % Clear command screen.
2  format long % Format of floating point numbers.
3  %format short e % Don't factor our common parts of numbers in
   matrices.
4  %clf % Clear current figure
5  close all % Close all figures.
6  fprintf(1, '—>Project #2.\n');
7  clear all
8  %warning on verbose % See MSGIDs for warnings.
9  %global d_freq, d_intens;
10 [ d_freq, d_intens ] = pr2.import_data('../spectrum_data.xls');
11
12 % Plot relative spectrum.
13 fig = figure('visible','off'); % Don't display the plot.
14 plot_relspectrum = plot(d_freq, d_intens, 'b');
15 xlabel('Frequency [Hz]')
16 ylabel('Relative intensity [W/(m^2*Hz)]')
17 title('The relative intensity spectrum.')
18 saveas(plot_relspectrum, '../img/spectrum_relative.eps', 'eps')
19 saveas(plot_relspectrum, '../img/spectrum_relative.png', 'png')
20 set(fig, 'visible','on') % Enable plots again.
21 close(fig);
22
23 % Plot spectrum
24 fig = figure('visible','off'); % Don't display the plot.
25 plot_spectrum = plot(d_freq, d_freq .* d_intens, 'b');
26 xlabel('Frequency [Hz]')
27 ylabel('Intensity [W/m^2]')
28 title('The intensity spectrum.')
29 saveas(plot_spectrum, '../img/spectrum.eps', 'eps')
30 saveas(plot_spectrum, '../img/spectrum.png', 'png')
31 set(fig, 'visible','on') % Enable plots again.
32 close(fig)
33
34 % Plot wavelengths spectrum.
35 fig = figure('visible','off'); % Don't display the plot.
36 ax = axes();
37 d_wavelen = 2.998e8 ./ d_freq; % wavelength = c / freq.
38 %d_wintens = d_wavelen .* d_intens;
39 plot_wave = plot(d_wavelen, d_intens, 'b');
40 spectral_color.spectrumLabel(ax);
41 xlabel('Wavelength [nm]')
42 ylabel('Intensity [W/(m^2\lambda)]')
43 title('Intensity spectrum.')
44 saveas(plot_wave, '../img/spectrum_wave.eps', 'eps')
45 saveas(plot_wave, '../img/spectrum_wave.png', 'png')
46 set(fig, 'visible','on') % Enable plots again.
47 close(fig)
48
49 % Try fitt polynomials to the data directly.
50 fig_badfit = figure('visible','off'); % Don't display the plot.
51 plot_badfit = plot(d_freq, d_intens, 'b');
```

```

52 hold on
53 xlabel('Frequency [Hz]')
54 ylabel('Relative intensity [W/(m^2*Hz)]')
55 title('Bad fittings to the data directly.')
56
57
58 warning off MATLAB:polyfit:RepeatedPointsOrRescale % I know about
    the problem.
59 badfit2 = polyfit(d_freq, d_intens, 2);
60 warning on MATLAB:polyfit:RepeatedPointsOrRescale
61 badfit2_v = polyval(badfit2, d_freq);
62 plot(d_freq, badfit2_v, 'g')
63 plot_badfit = plot(d_freq, d_intens, 'b');
64 hold on
65
66 warning off MATLAB:polyfit:RepeatedPointsOrRescale
67 badfit3 = polyfit(d_freq, d_intens, 3);
68 warning on MATLAB:polyfit:RepeatedPointsOrRescale
69 badfit3_v = polyval(badfit3, d_freq);
70 plot(d_freq, badfit3_v, 'r')
71
72 saveas(plot_badfit, '../img/bad_fits.eps', 'eps')
73 saveas(plot_badfit, '../img/bad_fits.png', 'png')
74 set(fig_badfit, 'visible', 'on') % Enable plots again.
75 close(fig_badfit)
76
77
78
79 %% Try to find a fit for the underlying spectrum function by
    deleting the peaks and dips.
80 % Plot relative spectrum.
81 d_indices = 1:length(d_freq); % Plot by index for easier
    adjustments later.
82 fig_goodfit = figure('visible','off');
83 %fig_goodfit = figure();
84 plot_goodfit = plot(d_indices, d_intens, 'b');
85 hold on
86 xlabel('Frequency [Hz]')
87 ylabel('Relative intensity [W/(m^2*Hz)]')
88 title('Good fitting to the spectrum function.')
89
90 peaks = []; % Row i is peak/dip i counted from the left with col1
    the left border and col2 the right border of the peak/dip.
91 % Found graphically with MATLABs data cursor in plots.
92 peaks(end+1,:) = [820 960];
93 peaks(end+1,:) = [1275 1540]; % Watch out for right boundary, deep
    zoom reveals heavy slope!
94 peaks(end+1,:) = [1560 1720];
95 peaks(end+1,:) = [2175 0];
96 peaks(end+1,:) = [0 2575];
97 peaks(end+1,:) = [3580 3745];
98
99 midpoints = [];
100 midpoints(end+1) = [881];
101 midpoints(end+1) = [1406];
102 midpoints(end+1) = [1636];
103 midpoints(end+1) = [2341];
104 midpoints(end+1) = [2380];
105 midpoints(end+1) = [3656];
106
107
108 spectrum_indices = [1:peaks(1,1)]; % Indices excluding the peaks

```

```

109     and dips.
110 for i = 2:length(peaks)
111     if i ~= 5 % No segment between these two dips.
112         spectrum_indices = [spectrum_indices peaks(i-1,2):peaks(i,1)];
113     end
114 end
115 spectrum_indices = [spectrum_indices peaks(length(peaks),2):
116     d_indices(end)];
117 peak_indices = setdiff(d_indices, spectrum_indices);
118 spectrum_v = d_intens(spectrum_indices)';
119 peak_v = d_intens(peak_indices);
120 %plot(spectrum_indices, spectrum_v, 'g*'); % Plot the spectrum
121 points.
122 plot(peak_indices, peak_v, 'r*'); % Plot points in the peak ranges,
123 now, adjust the boudaries manually.
124
125 %% Try fitting some lines to the spectrum.
126 spectrum_line2 = polyfit(spectrum_indices, spectrum_v, 2);
127 spectrum_line2_v = polyval(spectrum_line2, spectrum_indices);
128 plot(spectrum_indices, spectrum_line2_v, 'k') % black
129
130 warning off MATLAB:polyfit:RepeatedPointsOrRescale % I know about
131 the problem now.
132 spectrum_line3 = polyfit(spectrum_indices, spectrum_v, 3);
133 warning on MATLAB:polyfit:RepeatedPointsOrRescale
134 spectrum_line3_v = polyval(spectrum_line3, spectrum_indices);
135 plot(spectrum_indices, spectrum_line3_v, 'm') % magenta
136
137 warning off MATLAB:polyfit:RepeatedPointsOrRescale
138 spectrum_line4 = polyfit(spectrum_indices, spectrum_v, 4);
139 warning on MATLAB:polyfit:RepeatedPointsOrRescale
140 %spectrum_line4 = polyfit((spectrum_indices - mean(spectrum_indices
141 )) / std(spectrum_indices), spectrum_v, 4);
142 spectrum_line4_v = polyval(spectrum_line4, spectrum_indices);
143 plot(spectrum_indices, spectrum_line4_v, 'c') % cyan
144
145 % Check conditioning, see Sauer p.203.
146 A = [ones(length(spectrum_indices),1) spectrum_indices'
147     spectrum_indices.^2' spectrum_indices.^3' spectrum_indices
148     .^4'];
149 condition = cond(A'*A); % Ill conditioned!
150 fprintf(1, 'The conditon of A for the normal equation for a
151 polynomial fit of degree %i is %E\n', 4, condition);
152
153 % Centering and normalization to solve bad condition.
154 % Normalize frequencies.
155 d_freq_norm = (d_freq - mean(d_freq)) / std(d_freq);
156
157 saveas(plot_goodfit, '../img/spectrum_goodfit.eps', 'eps')
158 saveas(plot_goodfit, '../img/spectrum_goodfit.png', 'png')
159 set(fig_goodfit, 'visible', 'on') % Enable plots again.
160 close(fig_goodfit);
161 close all
162
163 spectrum_line = polyfit(d_freq_norm(spectrum_indices), d_intens(
164     spectrum_indices), 4);
165 line_v = polyval(spectrum_line, d_freq_norm);
166 peak_intens = d_intens - line_v; % We want the arean between the
167 curves.
168
169

```

```

160 % Assume symmetrical spectral lines.
161 half_areas = zeros(6,1);
162 for i = 1:length(peaks)
163     if i == 5 % We only have right start point
164         half_areas(i) = trapz(d_freq(midpoints(i):peaks(i,2)),
                                peak_intens(midpoints(i):peaks(i,2)));
165     else
166         half_areas(i) = trapz(d_freq(peaks(i,1):midpoints(i)),
                                peak_intens(peaks(i,1):midpoints(i)));
167     end
168 end
169
170 areas_symm = abs(2 .* half_areas);
171 areas_symm_str = sprintf('\t%E\n', areas_symm);
172 fprintf(1, 'Areas in W/m^2 found using symmetry is: \n[\n%s]\n',
          areas_symm_str);
173
174 % Calculate full areas for the 4 peaks we have left and right
    border for. The double dip (index 4) is counted as one dip.
175 full_areas = zeros(6,1);
176 for i = 1:length(peaks)
177     if ~(i == 4 || i == 5) % Skip the double dip.
178         full_areas(i) = trapz(d_freq(peaks(i,1):peaks(i,2)),
                                peak_intens(peaks(i,1):peaks(i,2)));
179     elseif i == 4
180         full_areas(i) = trapz(d_freq(peaks(i,1):peaks(i+1,2)),
                                peak_intens(peaks(i,1):peaks(i+1,2)));
181     end
182 end
183
184 % Areas found by using trapezoidal method for the whole peak/dip
    interval.
185 areas = abs(full_areas);
186 areas_str = sprintf('\t%E\n', areas);
187 fprintf(1, 'Areas found using thw whole peak/dip interval is: \n[\n
    %s]\n', areas_str);
188
189 % Find the largest difference in area between full and half.
190 areas_symm_parts = areas_symm([1:3 6]); % Skip double dip.
191 areas_parts = areas([1:3 6]); % Skip double dip.
192 area_diff = areas_symm_parts - areas_parts;
193 %area_norm = norm(area_diff, Inf);
194 [area_norm norm_pos] = max(abs(area_diff));
195 norm_quota = (area_norm / areas_parts(norm_pos)) * 100;
196 fprintf(1, 'The infinity norm of the difference in the two set of
    areas (double dip excluded) is %E. That is %.3f%% of the full
    area.\n', area_norm, norm_quota);
197
198 dip_diff = abs(areas(4) - (areas_symm(4) + areas_symm(5)));
199 dip_diff_quota = (dip_diff / areas(4)) * 100;
200 fprintf(1, 'The difference between the full double dip area and sum
    of the symmetrically found individual areas are %E. The sum is
    %.3f%% larger than the full double dip area.\n', dip_diff,
    dip_diff_quota);

```

B.2 Functions

The following functions implements the algorithms and the rest serves as helper functions to these algorithms and the scripts. To distinguish these from other *MATLAB*[®]-functions in the global namespace these reside in a own package called *pr2*.

../src/+pr2/import_data.m

```
1 function [ d_freq, d_intens ] = import_data( filename )
2 % Reads the data from the excel file filename and returns the
   frequencies
3 % d_freq and the intensities d_intens.
4     warning off MATLAB:xlsread:ActiveX % I don't have Excel or
       Windows.
5     num = xlsread( filename );
6     d_freq = num(:,1);
7     d_intens = num(:,2);
8 end
```