

Numerical Recipes: Hand-In 3

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Abstract

In this report we present the problems, solutions and scripts for the exercises from the third handout for the course Numerical Recipes.

Plotting styles in this report are set using the following code

```
1 def set_styles():
2     """For consistent plotting scheme"""
3     plt.style.use('default')
4     mpl.rcParams['axes.grid'] = True
5     plt.style.use('seaborn-darkgrid')
6     mpl.rcParams['font.family'] = 'serif'
7     mpl.rcParams['lines.linewidth'] = 1.5
8
```

Listing 1: Matplotlib Plotting Styles

1 Satellite Galaxies Around a Massive Central

In this section we will investigate the spherical distribution of satellite galaxies around a massive central galaxies, and attempt to fit a function to simulated data. Their density distribution n can be described as

$$n(x) = A \langle N_{sat} \rangle \left(\frac{x}{b} \right)^{a-3} \exp \left[- \left(\frac{x}{b} \right)^c \right] \quad (1)$$

Here x is the radius relative to the virial radius, i.e. $x \equiv r/r_{vir}$ with $x < x_{max} = 5$. a , b and c are free parameters, $\langle N_{sat} \rangle$ is the mean number of satellites per halo and $A = A(a, b, c)$ normalizes this profile such that $\int \int_V n(x) dV = \langle N_{sat} \rangle$. In this work we will mainly look at the number of satellites in the infinitesimal range $[x, x + dx]$. This is given by

$$N(x)dx = n(x)4\pi x^2 dx \quad (2)$$

```

1 # Main Equations
2 def n(x, A, Nsat, a, b, c):
3     """Density profile of the spherical distribution of
4     satellite galaxies around a central as a function of
5     x = r/r_vir. The values given come from hand-in 2"""
6     return A*Nsat*((x/b)**(a-3))*np.exp(-(x/b)**c)
7
8 def N(x, A, Nsat, a, b, c):
9     """Number of satellites at a distance x. This is the
10    function n(x, ..) integrated over the full sphere at x"""
11    return 4.*np.pi*x*x*n(x, A, Nsat, a, b, c)

```

Listing 2: Satellite galaxy distribution code

1.1 Maximization

We start by searching for the maximum of the distribution given by equation 2, for this we will assume $a = 2.4$, $b = 0.25$, $c = 1.6$. $x_{max} = 5$, $\langle N_{sat} \rangle = 100$ and $A = 256/(5\pi^{3/2})$. Instead of searching for the maximum, we instead search for the minimum of $-N(x)dx$ which gives the equivalent resulting x . Visually inspecting the distribution (Figure 1), we see a clear peak at $x \sim 0.5$. To be safe we set the edges of our initial bracket at $x_{min} = 0$ and $x_{max} = 5$ and then apply a bracketing algorithm to find a three-point bracket around the minimum. Then we use this bracket as input to the golden section search algorithm to find the x -value at the peak. We find the following brackets and minimization results:

```

1 Minimization Results
2 Bracket: [5.00000000e+00 1.00000000e-04 8.09010814e+00]
3 x at Max: 0.22998248152335327
4 N(x) Max: 267.84553313361295

```

Listing 3: Results of the maximization algorithm.

We also show the distribution and the exact location of this peak in Figure 1. We can see that the algorithms have perfectly discovered the maximum of this distribution.

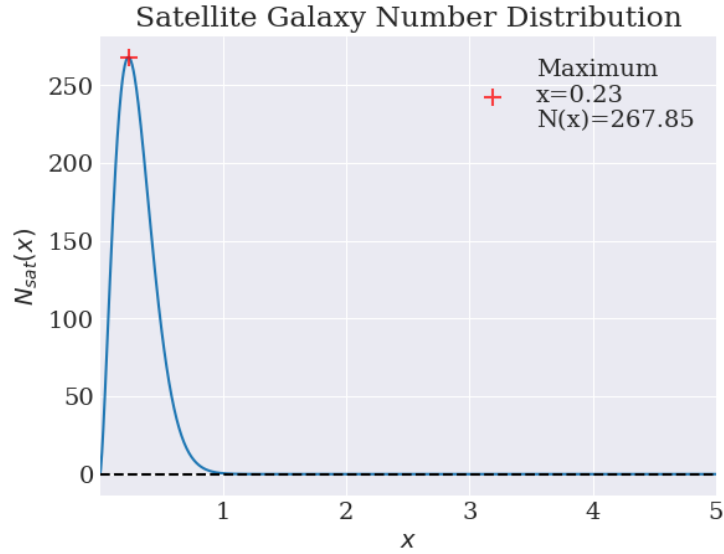


Figure 1: Distribution of the number of galaxies in the infinitesimal range $[x, x + dx]$ described by equation 2. The red cross indicates the position of the maximum of this distribution discovered using the golden search algorithm as described in Section 1.1

```

1 def maximization():
2     """Code for Q1a"""
3     # Constants
4     a = 2.4
5     b = 0.25
6     c = 1.6
7     xmin = 1e-4 # this cannot be zero because of the factor (x/b)^(
8     a-3) and a-3 < 0
9     xmax = 5
10    Nsat = 100
11    A = 256./(5.*np.pi**(3./2.))
12
13    # Maximizing a function f is equal to minimizing -f
14    minim_func = lambda x: -1*N(x, A, Nsat, a, b, c)
15
16    # Make a three-point bracket surrounding the minimum. As
17    # initial
18    # edges we take the edges of the interval [0, 5]
19    bracket, _ = make_bracket(minim_func, [xmin, xmax])
20    x_at_max, _ = golden_section_search(minim_func, bracket)
21    max_val = N(x_at_max, A, Nsat, a, b, c)
22
23    print(f'Maximum of N(x) found at x = {x_at_max}, N(x) = {
24    max_val}')
25
26    xx = np.linspace(xmin, xmax, 1000)
27    yy = N(xx, A, Nsat, a, b, c)
28    plt.plot(xx, yy)
29    plt.scatter(x_at_max, max_val, c='red', marker='+', alpha=0.75,
30    s=100, zorder=3, label=f'Maximum\ nx={x_at_max:.2 f }\nN(x)={
31    max_val:.2 f }')

```

```

27 plt.axhline(y=0, c='black', ls='—')
28 plt.xlim(xmin,xmax)
29 plt.xlabel(r'$x$')
30 plt.ylabel(r'$N_{\{sat\}}(x)$')
31 plt.title('Satellite Galaxy Number Distribution')
32 plt.legend()
33 plt.savefig('results/mini.png', bbox_inches='tight')
34
35 with open('results/mini.results.txt', 'w') as file:
36     file.write(f"""Minimization Results
37 Bracket: {bracket}
38 x at Max: {x_at_max}
39 N(x) Max: {max_val}""")

```

Listing 4: Code calling the maximization algorithm

```

1 # MINIMIZATION
2 def parabola_min_analytic(a, b, c, fa, fb, fc):
3     """Analytically computes the x-value of the minimum of a
4     parabola
5     that crosses a, b and c
6     """
7     top = (b-a)**2 * (fb-fc) - (b-c)**2 * (fb-fa)
8     bot = (b-a) * (fb-fc) - (b-c) * (fb-fa)
9     return b - 0.5*(top/bot)
10
11 def make_bracket(func, bracket, w=(1.+np.sqrt(5))/2, dist_thresh
12 =100, max_iter=10000):
13     """Given two points [a, b], attempts to return a bracket
14     triplet
15     [a, b, c] such that f(a) > f(b) and f(c) > f(b).
16     Note we only compute f(d) once for each point to save computing
17     time"""
18     a, b = bracket
19     fa, fb = func(a), func(b)
20     direction = 1 # Indicates if we're moving right or left
21     if fa < fb:
22         # Switch the two points
23         a, b = b, a
24         fa, fb = fb, fa
25         direction = -1 # move to the left
26
27     c = b + direction * (b - a) * w
28     fc = func(c)
29
30     for i in range(max_iter):
31         if fc > fb:
32             return np.array([a, b, c]), i+1
33         d = parabola_min_analytic(a, b, c, fa, fb, fc)
34         fd = func(d)
35         if np.isnan(fd):
36             print(f'New point d:{d} gives fd:{fd}. Breaking
37             function')
38             return np.array([a,b,c]), i+1
39         # We might have a bracket if b < d < c
40         if (d>b) and (d<c):
41             if fd > fb:
42                 return np.array([a, b, d]), i+1
43             elif fd < fc:
44                 return np.array([b, d, c]), i+1
45             # Else we don't want this d
46             #print('no parabola, in between b and c')

```

```

42         d = c + direction * (c - b) * w
43     elif (d-b) > 100*(c-b): # d too far away, don't trust it
44         #print('no parabola, too far away')
45         d = c + direction * (c - b) * w
46     elif d < b:
47         pass#print('d smaller than b')
48
49     # we shifted but didn't find a bracket. Go again
50     a, b, c = b, c, d
51     fa, fb, fc = fb, fc, fd
52
53     print('WARNING: Max. iterations exceeded. No bracket was found.
54           Returning last values')
55     return np.array([a, b, c]), i+1
56
57 def golden_section_search(func, bracket, target_acc=1e-5, max_iter=
58     int(1e5)):
59     """Once we have a start 3-point bracket surrounding a minima,
60     this function iteratively
61     tightens the bracket to search of the enclosed minima using
62     golden section search."""
63     w = 2. - (1.+np.sqrt(5))/2 # 2 - golden ratio
64     a, b, c = bracket
65     fa, fb, fc = func(a), func(b), func(c)
66
67     for i in range(max_iter):
68         # Set new point in the largest interval
69         # We do this separately because the bracket propagation can
70         # just not be generalized sadly
71         if np.abs(c-b) > np.abs(b-a): # we tighten towards the
72             right
73             d = b + (c-b)*w
74             fd = func(d)
75             if fd < fb: # min is in between b and c
76                 a, b, c = b, d, c
77                 fa, fb, fc = fb, fd, fc
78             else: # min is in between a and d
79                 a, b, c = a, b, d
80                 fa, fb, fc = fa, fb, fd
81             else: # we tighten towards the left
82                 d = b + (a-b)*w
83                 fd = func(d)
84                 if fd < fb: # min is in between a and b
85                     a, b, c = a, d, b
86                     fa, fb, fc = fa, fd, fb
87                 else: # min is in between d and c
88                     a, b, c = d, b, c
89                     fa, fb, fc = fd, fb, fc
90
91     if np.abs(c-a) < target_acc:
92         return [b,d][np.argmin([fb, fd])], i+1 # return the x
93         point corresponding to the lowest f(x)
94
95     print("Maximum Number of Iterations Reached")
96     return b, i+1

```

Listing 5: Code for the maximization algorithm

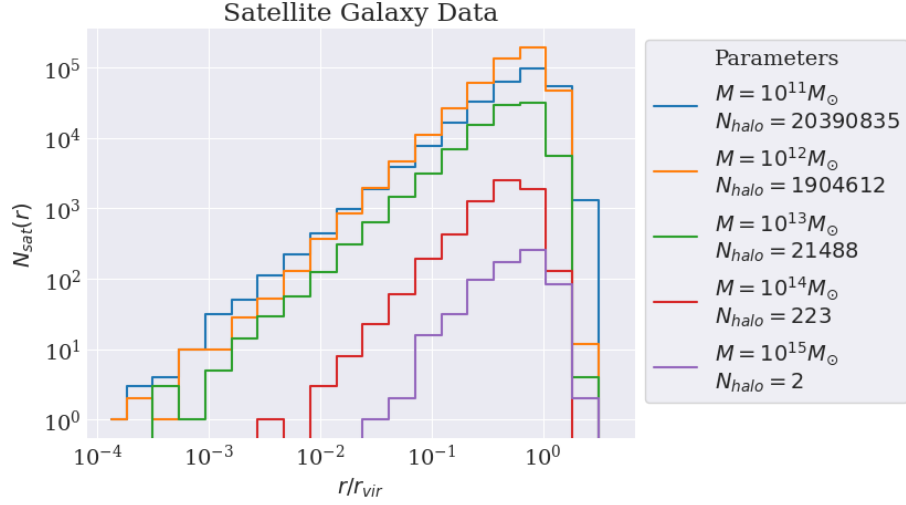


Figure 2: Binned satellite galaxy distance data divided into five mass bins of their massive galaxy halo as indicated on the right. The total number of halos over which the satellite galaxies are distributed is also indicated on the right.

1.2 Data Fitting

We import the five datafiles provided for this hand-in which contain satellite galaxies for halos in increasing mass bins ranging from $10^{11} M_{\odot}$ up to $10^{15} M_{\odot}$. Each file contains a number of halos, N_{halo} , and the distances of each satellite galaxy from its center massive galaxy. For each dataset we can immediately compute $\langle N_{sat} \rangle$ by dividing the total number of satellite galaxies by N_{halo} . We bin the data in 20 bins from $x = 10^{-4}$ to $x = 5$ in log-space. We set the lower limit above $x = 0$ for computational reasons because equation 2 is not defined there. We opt to show the distributions in log-space to better visualize the low x region. The decision for 20 bins is relatively arbitrary but appears to result in plots that are easily interpretable. We show the binned data together with N_{halo} for each dataset in Figure 2.

In the next two subsections we will first describe our two approaches to fit equation 2 to these distributions. In Section 1.3 we present the results of our fitting algorithms applied to the data, combined with a brief statistical analysis.

```

1 def readfile(filename):
2     """Code to read in the halo data, copied from the hand in
3     instructions:
4     https://home.strw.leidenuniv.nl/~daalen/Handin_files/
5     satellites2.py"""
6     f = open(filename, 'r')
7     data = f.readlines()[3:] # Skip first 3 lines
8     nhalo = int(data[0]) # number of halos
9     radius = []
10
11     for line in data[1:]:
12         if line[-1] != '#':
13             radius.append(float(line.split()[0]))
14
15     radius = np.array(radius, dtype=np.float64)

```

```

14 f.close()
15 return radius, nhalo # Return the virial radius for all the
    satellites in the file, and the number of halos
16 def make_plot_alldata():
17     """Make a plot showcasing all raw, binned data for the report
        """
18     basename = 'data/satgals_m1'
19     xmin = 1e-4 # cannot take zero because it messes with log and
        powers
20     xmax = 5
21     Nbins = 20
22     do_log = True
23     fig, ax = plt.subplots(1,1)
24
25     for i in range(1, 6):
26         radius, nhalo = readfile(f'{basename}{i}.txt')
27         n, bin_edges = hist(radius, xmin, xmax, Nbins, do_log)
28
29         Nsat = len(radius)/nhalo
30         bin_centers = np.zeros(len(bin_edges)-1)
31         for j in range(len(bin_centers)):
32             bin_centers[j] = bin_edges[j] + 0.5*(bin_edges[j+1] -
        bin_edges[j])
33
34         ax.step(bin_centers, n, where='mid', label=rf'$M=10^{\{i\}+10\}}M_{\{\odot\}}$'+'\n'+rf'$N_{\{halo\}} = \{nhalo\}$')#+'\n'+rf'$
        \left<N_{\{sat\}}\right>= \{Nsat:.3E\}$')
35
36     xlim, ylim = ax.get_xlim(), ax.get_ylim() # For future plotting
        of individual sets
37     ax.set_xlabel(r'$r/r_{\{vir\}}$')
38     ax.set_ylabel(r'$N_{\{sat\}}(r)$')
39     ax.set_title('Satellite Galaxy Data')
40
41     ax.set_xscale('log')
42     ax.set_yscale('log')
43     plt.legend(title='Parameters', bbox_to_anchor=(1, 1), frameon=
        True, fancybox=True)
44     plt.savefig('results/satellite_data.png', bbox_inches='tight')
45
46     return xlim, ylim

```

Listing 6: Code to import data, and make the plot of Figure 2

```

1 def fit_data():#xlim, ylim):
2     """Code for Q1b-d"""
3     basename = 'data/satgals_m1'
4     xmin = 1e-4 # cannot take zero because it messes with log and
        powers
5     xmax = 5
6     Nbins = 20
7     do_log = True
8     no_bins = False
9     guess = np.array([2.4, 0.25, 1.5])
10
11     fitres_txt = ""
12     full_fitres_txt = ""
13     stats_txt = ""
14     fig, axs = plt.subplots(3, 2, sharex=True, sharey=True,
        tight_layout=True, figsize=(8, 12))
15
16     # do all of the below for each dataset separately

```

```

17 for i in range(1,6):
18     ax = axs.flatten()[i-1]
19     radius, nhalo = readfile(f'{basename}{i}.txt')
20     n, bin_edges, bin_centers = hist(radius, xmin, xmax, Nbins,
    do_log, return_centers=True)
21
22     Nsat = len(radius)/nhalo
23     print(f'Imported Dataset M1{i}. {len(radius)} Objects.')
24
25     # 1b. Start with fitting a chi squared distribution to this
    using the Levenberg-Marquardt algorithm
26     # the biggest adaptation to it is that sigma is iteratively
    computed such that  $\sigma^2 = \mu$ 
27     print('Starting Chi Squared Fitting..')
28     params_chi2, chi2, niter_chi2 = fit_satellite_data_chisq(
    bin_centers, n, Nsat, guess, bin_edges)
29     print(f'\nChi Squared Fit:\n\Chi^2 = {chi2}\na, b, c = {
    params_chi2}\n')
30
31     # 1c. Now fit a Poisson distribution to this data using the
    Quasi-Newton method
32     print('Starting Poisson Fitting..')
33     if no_bins:
34         params_poisson, logL, niter_poisson =
    fit_satellite_data_poisson(radius, None, Nsat, guess, bin_edges
    , no_bins)
35     else: # feed it only nbins data points if wanted
36         params_poisson, logL, niter_poisson =
    fit_satellite_data_poisson(bin_centers, n, Nsat, guess,
    bin_edges, no_bins)
37     print(f'\nPoisson Fit:\nlog L = {logL}\n<Nsat> = {Nsat}\na,
    b, c = {params_poisson[0]}, {params_poisson[1]}, {
    params_poisson[2]}\n')
38
39     # Bin the Poisson and Chi squared models to match the data
40     xx = np.logspace(np.log10(xmin), np.log10(xmax), 100)
41     chi2_binned = nhalo * compute_mean_satellites(xx, *
    params_chi2, bin_edges, Nsat)
42     poisson_binned = nhalo * compute_mean_satellites(xx, *
    params_poisson, bin_edges, Nsat)
43
44     # Statistical Tests
45     DoF = Nbins - 4 # degrees of freedom
46
47     # G-test for the chi squared model because it is binned
48     # mask out all bins without observations:  $\lim_{O \rightarrow 0} [O \ln(O/E)] = 0$  for  $E \neq 0$ 
49     zero_mask = n != 0
50     G_chi2 = 2. * np.sum(n[zero_mask] * np.log((n/chi2_binned)[
    zero_mask])))
51     G_poisson = 2. * np.sum(n[zero_mask] * np.log((n/
    poisson_binned)[zero_mask])))
52     Q_chi2 = (gammaln(DoF/2., G_chi2/2.)/gamma(DoF/2.))
53     Q_poisson = (gammaln(DoF/2., G_poisson/2.)/gamma(DoF/2.))
54     print(f'G_chi2 = {G_chi2}, G_poisson = {G_poisson}')
55     print(f'Q_chi2 = {Q_chi2}, Q_poisson = {Q_poisson}')
56
57     # Plotting
58     ax.step(bin_centers, n, label='Data', where='mid')
59     ax.scatter(bin_centers, n, c='black', marker='X', s=25,
    zorder=5, label='Fit Points')
60     ax.step(bin_centers, chi2_binned, where='mid', label=r'$\

```



```

61     chi^2$ Fit', ls='—')
        ax.step(bin_centers, poisson_binned, where='mid', label='
Poisson Fit', ls='—')
62
63     ax.set_title(rf'M = $10^{\{i+10\}}$ M_{\odot}$')
64     ax.set_xscale('log')
65     ax.set_yscale('log')
66     ax.set_ylim(10**-5.5, 10**5.5)
67     ax.legend()
68
69     fitres_txt += f'$10^{\{i+10\}}$ & {Nsat:.2E} & {params_chi2
[0]:.2f} & {params_chi2[1]:.2f} & {params_chi2[2]:.2f} & {chi2
:.2E} & \\\ \n'
70     fitres_txt += f' & {params_poisson[0]:.2f} & {
params_poisson[1]:.2f} & {params_poisson[2]:.2f} & {logL:.2E
}\\\ \n'
71     full_fitres_txt += f'$10^{\{i+10\}}$ & {Nsat} & {
params_chi2[0]} & {params_chi2[1]} & {params_chi2[2]} & {chi2}
& \\\ \n'
72     full_fitres_txt += f' & {params_poisson[0]} & {
params_poisson[1]} & {params_poisson[2]} & {logL}\\\ \n'
73     stats_txt += f'$10^{\{i+10\}}$ & $\chi^2$ & {G_chi2} & {
Q_chi2} \\\ \n'
74     stats_txt += f'$10^{\{i+10\}}$ & Poisson & {G_poisson} & {
Q_poisson} \\\ \n'
75
76 # Figure Labels
77 for ax in axs[:,0]:
78     ax.set_ylabel(r'$N_{\text{sat}}(r)$')
79 for ax in axs[-1]:
80     ax.set_xlabel(r'$r/r_{\text{vir}}$')
81 plt.suptitle('Fit Results')
82 plt.savefig('results/fitresults.png', bbox_inches='tight')
83
84 fitres_txt = fitres_txt[:-3] # remove the last '\ \n'
85 stats_txt = stats_txt[:-3]
86 # Textfile writing
87 with open('results/fitresults.txt', 'w') as file:
88     file.write(fitres_txt)
89     file.close()
90 with open('results/stats.txt', 'w') as file:
91     file.write(stats_txt)
92     file.close()

```

Listing 7: Code that calls the fitting procedures and performs the statistical tests

1.2.1 Chi-Squared

These data are discrete counts, so therefore they should be fit by a Poisson distribution. However we start with an 'easy' χ^2 fit with Poisson variance (i.e. $\sigma^2 = \mu$) to compare to the proper unbiased fit. This means that we want to minimize the function

$$\chi^2 = \frac{(y_i - \mu(x_i|\mathbf{p}))}{\mu(x_i|\mathbf{p})}. \quad (3)$$

Where x_i and y_i are the bin center and bin counts respectively. μ is a function of the parameter describing the expected value in any particular bin, which is given by

$$\mu(x_i|\mathbf{p}) = \tilde{N}_i = \int_{x_i}^{x_{i+1}} N(x) dx. \quad (4)$$

We minimize Equation 3 for each dataset separately using the Levenberg-Marquardt algorithm. As a good starting guess we use the same parameters as in Section 1.1, i.e. $a = 2.4$, $b = 0.25$, $c = 1.6$. Another important thing to note is that the normalization constant A is a function of these three parameters which keep changing. We therefore compute a new value for A each time the parameters are shift by first integrating over $N(x)$ from $x_{min} = 10^{-4}$ to $x_{max} = 5$ using Romberg integration and $A = 1$. We then compute A by dividing $\langle N_{sat} \rangle$ by the result of this integral.

```

1  ## CHI SQUARED FITTING ##
2  def compute_mean_satellites(x, a, b, c, bin_edges, Nsat):
3      """Chi squared function specifically for the distribution of
4      satellite
5      galaxies around a massive central, n(x, ..) which we attempt to
6      fit
7      using the assumption of Poisson variance \sigma^2 = \mu.
8      Therefore
9      sigma is not used, but we need to pass it for function
10     interoperability"""
11     # mean = variance = int(N(x))dx over the bin i
12     N_fit = lambda x: N(x, 1, Nsat, a, b, c)
13     integral = romberg_integration(N_fit, bin_edges[0], bin_edges
14     [-1], 8)
15     A = Nsat/integral
16     N_fit = lambda x: N(x, A, Nsat, a, b, c)
17
18     if len(x) == 1: # Evaluate only at a single data point
19         # the np.min clause is to ensure we never get an index
20         errors
21         bin_idx = np.min([np.argmin(bin_edges-x), len(bin_edges)])
22         return romberg_integration(N_fit, bin_edges[bin_idx],
23         bin_edges[bin_idx+1], 8)
24
25     mean_ar = np.zeros(len(bin_edges)-1)
26     for i in range(len(mean_ar)):
27         mean_ar[i] = romberg_integration(N_fit, bin_edges[i],
28         bin_edges[i+1], 8)
29
30     return mean_ar
31
32 def fit_satellite_data_chisq(bin_centers, n, Nsat, guess, bin_edges
33 ):
34     """Function applying the Levenberg-Marquadt algorithm to
35     implement the
36     'easy' fit to the data, with some slight modifications"""
37     # Need to add in the lambda function so we can pass in the
38     bin_edges we found
39
40     mean_func = lambda x, a, b, c: compute_mean_satellites(x, a, b,
41     c, bin_edges, Nsat)
42
43     # Fit 'fit_func' to the data using a minimization of chi^2
44     defined by chisq_func. It doesn't matter what values
45     # we use for sigma, because we will never use it. We set it to
46     0 here to ensure it's never used
47     return levenberg_marquardt(bin_centers, n, None, mean_func,
48     guess, linear=False,

```

```
34 | chisq_like_poisson=True)
```

Listing 8: Code for the chi-squared fitting computing \hat{N}_i and calling the Levenberg-Marquardt algorithm

```
1 | def determine_implicit_pivot_coeff(mat):
2 |     """Determines the coefficients for implicit pivoting in Crout's
3 |     Algorithm. It does this by finding
4 |     the absolute maximum value of each row in the matrix, and
5 |     storing its inverse.
6 |
7 |     NOTE: Requires a Matrix object (this script) as input. This
8 |     ensures correspondence with row_order
9 |     """
10 |     row_max_inverse = np.zeros(mat.num_rows)
11 |     for i in range(mat.num_rows):
12 |         row = mat.matrix[i]
13 |         row_max = row[np.argmax(np.abs(row))]
14 |         row_max_inverse[i] = 1. / row_max
15 |
16 |     return row_max_inverse
17 |
18 | def lu_decomposition(coefficients, implicit_pivoting=True, epsilon
19 |                      =1e-13):
20 |     """Decomposes a matrix into:
21 |         -L: A matrix with non-zero elements only in the lower-
22 |         triangle, and ones on the diagonal
23 |         -U: A matrix with non-zero elements only in the upper-
24 |         triangle, including the diagonal
25 |     These matrices are presented and stored into one.
26 |     The decomposition is done using Crout's Algorithm
27 |     """
28 |     if type(coefficients) == np.ndarray:
29 |         A = Matrix(values=coefficients)
30 |     else:
31 |         A = coefficients
32 |
33 |     # Combat round-off errors to dodge division by zero
34 |     A.matrix[np.abs(A.matrix)<epsilon] = epsilon
35 |
36 |     if implicit_pivoting:
37 |         row_max_inverse = determine_implicit_pivot_coeff(A)
38 |
39 |     imax_ar = np.zeros(A.num_columns)
40 |     # First pivot the matrix
41 |     for i in range(A.num_columns):
42 |         # A.matrix[i:, i] selects all elements on or below the
43 |         diagonal
44 |         if implicit_pivoting:
45 |             pivot_candidates = A.matrix[i:, i] * row_max_inverse[i
46 |             :]
47 |         else:
48 |             pivot_candidates = A.matrix[i:, i]
49 |
50 |         pivot_idx = i + np.argmax(np.abs(pivot_candidates))
51 |         imax_ar[i] = pivot_idx
52 |         A.swap_rows(i, pivot_idx)
53 |
54 |     for i in range(A.num_columns):
55 |         # A.matrix[i:, i] selects all elements on or below the
56 |         diagonal
```

```

49         diag_element = A.matrix[i, i] # Use to scale alpha factors
50
51         for j in range(i + 1, A.num_rows): # This leaves a zero at
the end, not the best fix this!
52             A.matrix[j, i] /= diag_element
53             for k in range(i + 1, A.num_rows): # j+1):
54                 A.matrix[j, k] -= A.matrix[j, i] * A.matrix[i, k]
55
56     return A
57
58
59 def solve_lineqs_lu(LU, b):
60     """Performs the steps to solve a system of linear equations
after a matrix A has been LU decomposed. It
61     does this by first applying forward substitution to solve Ly =
b, and then applies backward substitution
62     to solve Ux = y.
63
64     Inputs:
65         LU: The decomposed L and U matrices, stored in a single
Matrix instance
66         b: The constraints of the linear equations, ndarray
67
68     Outputs:
69         x: Matrix instance containing the solution such that Ax = b
70     """
71     if type(b) == np.ndarray:
72         x = Matrix(values=b)
73     else:
74         x = b
75     # Begin by swapping the x's in the right order
76     x.matrix = x.matrix[LU.row_order]
77
78     # Forward Substitutions. Solves Ly = b
79     for i in range(0, x.num_rows):
80         x.matrix[i] -= np.sum(LU.matrix[i, :i] * x.matrix[:i])
81
82     # Backward Substitutions. Solves Ux = y
83     for i in range(x.num_rows-1, -1, -1):
84         x.matrix[i] = (1./LU.matrix[i, i])*(x.matrix[i] - np.sum(LU.
matrix[i, i+1:]*x.matrix[i+1:]))
85
86     return x
87
88 def outer_product(v, w):
89     """Compute the outer product of two vectors. This is a matrix A
with
90         A_ij = v_i * w_j
91     NOTE: This function doesn't assume the vectors are of the same
size, and
92     this function is not symmetric (outer(v,w) != outer(w,v))
93     """
94     A = np.zeros((v.shape[0], w.shape[0]))
95     for i in range(v.shape[0]):
96         A[i] = v[i] * w
97     return A
98
99
100 class Matrix():
101     """Matrix Class for linear algebra"""
102
103     def __init__(self, values=None, num_rows=None, num_columns=None

```

```

, dtype=np.float64):
104     """Check inputs and create a corresponding matrix or vector
    """
105     if values is not None:
106         self.num_rows = values.shape[0]
107         try:
108             self.num_columns = values.shape[1]
109         except IndexError:
110             self.num_columns = 1
111             #print(f'Warning! Values has dim=1. Making vector
with shape ({self.num_rows}, {self.num_columns})')
112         if type(values) == np.ndarray:
113             self.matrix = np.array(values, dtype=dtype)
114         else:
115             print(f'Datatype of values {type(values)} not
recognized. Initializing matrix with zeros.')
116             self.matrix = np.zeros((num_rows, num_columns),
dtype=dtype)
117         else:
118             self.num_rows = num_rows
119             self.num_columns = num_columns
120             self.matrix = np.zeros((num_rows, num_columns))
121
122         # Use row order to track rows that have been shuffled
123         self.row_order = np.arange(self.num_rows)
124
125     def swap_rows(self, idx1, idx2):
126         """Extract rows from a matrix, and switch them. Track the
change in row_order"""
127         self.matrix[[idx1, idx2]] = self.matrix[[idx2, idx1]]
128         self.row_order[[idx1, idx2]] = self.row_order[[idx2, idx1]]
129
130     def scale_row(self, idx, scalar):
131         """Multiply all elements of row {idx} by a factor {scalar}
    """
132         self.matrix[idx] *= scalar
133
134     def add_rows(self, idx1, idx2, scalar):
135         """Add row {idx2} multiplied by scalar to row {idx1}"""
136         self.matrix[idx1] += scalar * self.matrix[idx2]
137
138
139     def make_param_func(params, i):
140         """Given a list of parameters and an index i, return a function
with
141         p_i as the variable for use in differentiation algorithms"""
142         # should be a better way to do this right
143         first_half_p = params[:i]
144         if not i == len(params)-1: # Avoid indexing errors
145             second_half_p = params[i+1:]
146         else:
147             second_half_p = []
148         return lambda p: [*first_half_p, p, *second_half_p]
149
150
151     def make_alpha_matrix(xdata, sigma, func, params,
152                           h_start=0.1, dec_factor=2, target_acc=1e-10):
153         #derivative params
154         """Make a Matrix object containing the sum of N products of
derivatives
where the element i,j is the product of df/dxi and df/dxj. Each
value i

```

```

155     can be weighted by its uncertainty sigma if desired. If this is
156     not
157     required one can set sigma = 1 to 'ignore' this step"""
158 N = len(xdata) # Number of data points
159 M = len(params) # Number of parameters
160 A = Matrix(num_columns=M, num_rows=M)
161
162 func_derivatives = np.zeros((M, N))
163
164 # Build up all M derivatives
165 for i in range(M):
166     param_func = make_param_func(params, i)
167     # Adjust Ridders method to do this in one go? Big speed
168     upgrade.
169     for j in range(N):
170         yp = lambda p: func([xdata[j]], *param_func(p))
171         dy_dpi, _ = ridders_method(yp, [params[i]], h_start,
172         dec_factor, target_acc)
173         func_derivatives[i][j] = dy_dpi
174
175 # Build up A-matrix
176 for i in range(M):
177     A.matrix[i][i] = alpha_kl(func_derivatives[i],
178     func_derivatives[i], sigma)
179     for j in range(i):
180         A.matrix[i][j] = alpha_kl(func_derivatives[i],
181         func_derivatives[j], sigma)
182     A.matrix[j][i] = A.matrix[i][j]
183
184 return A
185
186 def compute_chi_sq(x, y, sigma, func, params):
187     """Compute the chi squared value between N points x, y with
188     y uncertainty sigma and a function func with parameters params
189     Setting sigma = 1 reduces this to just lesat squares"""
190     return np.sum(((y - func(x, *params))**2)/(sigma*sigma))
191
192 def compute_chi_sq_likepoisson(x, y, func, params):
193     """Compute the chi squared value between N points x, y with
194     y uncertainty sigma and a function func with parameters params
195     under a Poisson distribution assumption, i.e. \sigma = \mu"""
196     mean = func(x, *params)
197     return np.sum(((y - mean)**2) / (mean))
198
199 def make_nabla_chi2(xdata, ydata, sigma, func, params,
200     h_start=0.1, dec_factor=2, target_acc=1e-5,
201     chisq_like_poisson=False):
202     """
203     M = len(params)
204     chisq_derivatives = np.zeros(M)
205     for i in range(M):
206         param_func = make_param_func(params, i)
207         if chisq_like_poisson:
208             chi2_func_p = lambda p: compute_chi_sq_likepoisson(
209             xdata, ydata, func, param_func(p))
210         else:
211             chi2_func_p = lambda p: compute_chi_sq(xdata, ydata,
212             sigma, func, param_func(p))
213         dchi_dpi, _ = ridders_method(chi2_func_p, [params[i]],
214         h_start, dec_factor, target_acc)

```

```

209         chisq_derivatives[i] = dchi_dpi
210
211     return beta_k(chisq_derivatives)
212
213
214 def weigh_A_diagonals(A, lmda):
215     """Weigh the diagonal elements of a square matrix A by a
216     factor (1+lmda)"""
217     if not A.matrix.shape[0] == A.matrix.shape[1]:
218         raise ValueError(f"This Matrix object is not square: {A.
219         matrix}")
220     for i in range(A.matrix.shape[0]):
221         A.matrix[i][i] *= (1. + lmda)
222     return A
223
224 def alpha_kl(dydp1, dydp2, sigma):
225     """
226     return np.sum((1./(sigma**2.)) * dydp1 * dydp2)
227
228 def beta_k(dchi_dp):
229     """
230     return -0.5 * dchi_dp
231
232 def levenberg_marquardt(xdata, ydata, sigma, func, guess, linear=
233     True,
234     w=10, lmda=1e-3, chi_acc=1e-3, max_iter=int
235     (1e2),
236     epsilon = 1e-13, # fit procedure params
237     chisq_like_poisson=False,
238     h_start=0.1, dec_factor=2, target_acc=1e
239     -13): # derivative params
240     """
241     if chisq_like_poisson:
242         # sqrt becaues it computes the mean
243         sigma = np.sqrt(func(xdata, *guess))
244         if np.isnan(sigma).any():
245             raise ValueError(f'NaN in sigma {sigma}')
246         chi2 = compute_chi_sq_likepoisson(xdata, ydata, func, guess
247         )
248     else:
249         chi2 = compute_chi_sq(xdata, ydata, sigma, func, guess)
250
251     N = len(xdata) # Number of data points
252     M = len(guess) # Number of parameters
253     b = Matrix(num_columns=1, num_rows=M)
254     params = guess
255
256     # Can do this beforehand because the derivatives never change
257     # if the functions depend linearly on the parameters
258     if linear:
259         A = make_alpha_matrix(xdata, sigma, func, params, h_start,
260         dec_factor, target_acc)
261
262     for iteration in range(max_iter):
263         if linear:
264             A_weighted = copy.deepcopy(A) # ensure no pointing goes
265             towards A
266             A_weighted = weigh_A_diagonals(A_weighted, lmda) # Make
267             \alpha_prime

```

```

262         else:
263             A = make_alpha_matrix(xdata, sigma, func, params,
264                                   h_start, dec_factor, target_acc)
265             # Combat round-off errors and divisions by zero
266             A.matrix[np.abs(A.matrix)<epsilon] = epsilon
267             A_weighted = weigh_A_diagonals(A, lmda)
268
269             b.matrix = make_nabla_chi2(xdata, ydata, sigma, func,
270                                       params, h_start, dec_factor, target_acc)
271
272             # Solve the set of linear equations for \delta p with LU
273             decomposition
274             LU = lu_decomposition(A_weighted, implicit_pivoting=True)
275             delta_p = solve_lineqs_lu(LU, b).matrix
276
277             # Evaluate new chi^2
278             new_params = params + delta_p.flatten()
279
280             if chisq_like_poisson:
281                 new_sigma = np.sqrt(func(xdata, *new_params))
282                 new_chi2 = compute_chi_sq_like_poisson(xdata, ydata,
283                                                         func, new_params)
284             else:
285                 new_chi2 = compute_chi_sq(xdata, ydata, sigma, func,
286                                           new_params)
287
288             delta_chi2 = new_chi2 - chi2
289
290             if delta_chi2 >= 0 or not np.isfinite(new_chi2): # reject
291                 the solution
292                 lmda = w*lmda
293                 #print(f'delta = {delta_chi2}. Reject. lambda = {lmda
294                       :.2E} chi2 = {chi2}')
295                 continue
296
297             if np.abs(delta_chi2) < chi_acc:
298                 return params, new_chi2, iteration+1 # converged!
299
300             # accept the step and make it
301             params = new_params
302             chi2 = new_chi2
303             lmda = lmda/w
304             if chisq_like_poisson:
305                 sigma = new_sigma
306             #print(f'delta = {delta_chi2}. Accept. lambda = {lmda:.2E}
307                   chi2 = {chi2}')
308
309         print("Max Iterations Reached")
310         return params, new_chi2, iteration+1

```

Listing 9: Code for the Marquardt-Levenberg algorithm

1.2.2 Poisson

For the Poisson fit we have two options: we can either use the same binned data as is used for the χ^2 fit, or we can opt to not use bins at all. In this latter case we pretend as though we did bin the data, however with bin size sufficiently small such that each bin contains either 0 or 1 objects. Doing this allows us to make better use of the data at the cost of more computational load. In the

worst case, namely the first dataset, this difference is a factor on the order of 10^4 . Unfortunately while implemented, we have been unable to use this binless fitting as computing time exceeds the maximum allotted time of ten minutes. Therefore we opt to fit the data here using the same bins as in the previous section. The log-likelihood of a Poisson distribution is given as

$$-\ln \mathcal{L}(\mathbf{p}) = - \sum_{i=0}^{N-1} (y_i \ln [\mu(x_i|\mathbf{p})] - \mu(x_i|\mathbf{p}) - \ln(y_i!)). \quad (5)$$

When minimizing this equation we can ignore the last term, $\ln(y_i!)$ because it is independent of the parameters we are fitting and therefore constant. We are then left with only the first two terms in the sum. For the minimization we will make use of the downhill simplex method where we initialize one of the vertices of the first simplex using the same parameters as before ($a = 2.4$, $b = 0.25$, $c = 1.6$). We initialize the other three vertices by adding one to parameter i for vertex i .

We also attempted to implement the Quasi-Newton method to minimize the log likelihood function, however this also has proven unsuccessful due to extremely steep gradients which often led the line minimization algorithm to regions in parameter space where the likelihood function is not defined. This only led to NaN values as a result for the parameters. While not used, the code is still included at the end of this report.

```

1  ## POISSON FITTING ##
2  def poisson_fit_func(x, y, delta_x, bin_edges, Nsat, params, xmin,
3     xmax, no_bins):
4     """Procedure to be iteratively called in quasi_newton to fit a
5     Poisson
6     distribution to the satellite galaxy data. Adjusted from the
7     chi^2 fit
8     for optimization reasons. delta_x is the smallest non-zero
9     difference
10    between two x used as a proxy for bin size"""
11    # Start by computing A corresponding to these a, b, c like
12    handin 2
13
14    N_fit = lambda x: N(x, 1, Nsat, *params)
15    integral = romberg_integration(N_fit, xmin, xmax, 8)
16    A = Nsat/integral
17    N_fit = lambda x: N(x, A, Nsat, *params)
18
19    mean_ar = np.zeros(len(x))
20    for i in range(len(mean_ar)):
21        if no_bins:
22            int_min, int_max = x[i] - delta_x, x[i]+delta_x
23        else:
24            int_min, int_max = bin_edges[i], bin_edges[i+1]
25
26        mean_ar[i] = romberg_integration(N_fit, int_min, int_max,
27            8)
28
29    if no_bins:
30        ll = -1.*np.sum(np.log(mean_ar)) # plus an integral we take
31        as constant
32    else:
33        ll = -1.*np.sum(y*np.log(mean_ar) - mean_ar) # plus a
34        factor of y! which is constant

```

```

28     return ll
29
30 def fit_satellite_data_poisson(x, y, Nsat, guess, bin_edges,
31                               no_bins):
32     """Computes the Poisson likelihood of a function in the limit
33     where the data is essentially unbinned. This function
34     automatically
35     computes the binsize required to obtain this.
36     mean_func should be the function that computes the mean of the
37     distribution, which should of course be linked to the fit
38     function"""
39
40     if no_bins:
41         # Find the smallest difference between two x neighbouring x
42         . Need to sort the
43         # array first to find this. Sorting immediately gives us
44         max(x) and min(x) as well
45         # NOTE the below could have been done a lot quicker with
46         numpy!
47         x_sorted = merge_sort(x)
48         diff_x = x_sorted[1:] - x_sorted[:-1]
49         diff_sorted = merge_sort(diff_x)
50         smallest_diff = diff_sorted[diff_sorted > 0][0] # smallest
51         non-zero element
52         # This smallest difference sets the "bin size"
53     else:
54         smallest_diff = None
55
56     # Fitting function and procedure
57     fit_func = lambda p: poisson_fit_func(x, y, smallest_diff,
58     bin_edges, Nsat, p, bin_edges[0], bin_edges[-1], no_bins)
59     #fit_params, n_iter = quasi_newton(fit_func, guess)
60     fit_params, n_iter = downhill_simplex(fit_func, guess)
61     logL = fit_func(fit_params)
62     return fit_params, logL, n_iter

```

Listing 10: Code to compute the Poisson likelihood, and to call the minimization functions

```

1 # CODE FOR THE N-DIMENSIONAL DOWNHILL SIMPLEX
2 def compute_centroid(A):
3     """Compute the centroid of N points in N dimensional space. x
4     should
5     be an NxN array of N vectors with N dimensions (in that order).
6     The function
7     then returns one ndarray of length N with the centroid
8     coordinates."""
9     return (1./A.shape[1]) * np.sum(A, axis=0)
10
11 def downhill_simplex(func, start, shift_func=lambda x: x+1,
12                     max_iter=int(1e5), target_acc=1e-10):
13     """Finds the minimum of a function using the downhill simplex
14     method
15     INPUT:
16         func: A function taking only one variable as input with
17         dimension N
18         start: N-Dimensional numpy array where the function starts
19         searching for a minimum
20         shift_func: A function taking only one float as input
21         dictating how to mutate the
22         initial simplex vertices

```

```

16 """
17 dim = start.shape[0] # = N
18 # Store N+1 vertex vectors in this matrix. This ordering fails
19 # if we feed it directly to func,
20 # but it allows us to choose a vertex as vertices[i]. The
21 # function problem we solve by just
22 # transposing this matrix.
23 vertices = np.zeros((dim+1, dim))
24 func_vals = np.zeros(dim+1) # Store the f(X) values in here
25
26 # Create the simplex, add slight variation to each vector
27 # except the first using 'shift_func'
28 vertices[0] = start
29 func_vals[0] = func(vertices[0])
30
31 for i in range(dim):
32     vertices[i+1] = vertices[0]
33     vertices[i+1][i] = shift_func(vertices[i+1][i])
34     func_vals[i+1] = func(vertices[i+1])
35
36 # Start algorithm
37 for i in range(1, max_iter+1):
38     # Sort everything by function value
39     sort_idx = merge_sort(key=func_vals)
40     vertices = vertices[sort_idx]
41     func_vals = func_vals[sort_idx]
42     #print(f'Current best logL = {func_vals[0]} at ', vertices
43     [0])
44
45     # Check if we have reached our accuracy level by comparing
46     # the best and worst function evals.
47     accuracy = (np.abs(func_vals[-1] - func_vals[0]) / np.abs
48     (0.5*(func_vals[-1] + func_vals[0])))
49     if accuracy < target_acc:
50         return vertices[0], i # corresponds to func_vals[0], so
51         the best point
52
53     # Compute the centroid of all but the last (worst) point
54     centroid = compute_centroid(vertices[:-1])
55
56     # Try out a new points
57     x_try = 2.* centroid - vertices[-1]
58     f_try = func(x_try)
59
60     if f_try < func_vals[-1]:
61         # There is improvement in this step
62         if f_try < func_vals[0]:
63             # We are the best point. Try expanding
64             x_exp = 2*x_try - centroid
65             f_exp = func(x_exp)
66             if f_exp < f_try:
67                 # expanded point is even better. Replace x_N
68                 vertices[-1] = x_exp
69                 func_vals[-1] = f_exp
70             else:
71                 # x_try was good, x_exp is not better
72                 vertices[-1] = x_try
73                 func_vals[-1] = f_try
74         else:
75             # Better than x_N, not better than x_0. Just accept
76             the point
77             vertices[-1] = x_try

```

```

70         func_vals[-1] = f_try
71
72     else:
73         # This point is worse than what we had. First try
74         contracting, new x_try
75         x_try = 0.5*(centroid+vertices[-1])
76         f_try = func(x_try)
77         if f_try < func_vals[-1]:
78             # contracting improved x
79             vertices[-1] = x_try
80             func_vals[-1] = f_try
81         else:
82             # Nothing worked, just contract all points towards
83             the best points
84             vertices = 0.5*(vertices[0] + vertices) # x0 doesnt
85             shift here: 0.5(x0 + x0) = x0
86             # need to evaluate all but x0 because they shifted
87             for i in range(dim):
88                 func_vals[i+1] = func(vertices[i+1])
89
90     print('Maximum Number of Evaluations Reached')
91     return vertices[0], i

```

Listing 11: Downhill simplex code

1.3 Fit Results

We apply the fitting methods described in the previous sections to each of the datasets `satgals_m1i.txt` with $i \in [1, 5]$, and present the results in Figure 3. We also include the parameters and χ^2 or $\ln \mathcal{L}$ values in Table 1

M	$\langle N_{sat} \rangle$	a	b	c	χ^2	$\ln \mathcal{L}$
10^{11}	1.37E-02	2.40	0.27	1.01	6.64E+12	
		1.18	1.20	3.64		1.67E+06
10^{12}	2.51E-01	2.40	0.26	1.03	9.92E+11	
		1.55	0.94	3.63		1.40E+06
10^{13}	4.37E+00	2.40	0.26	1.11	2.20E+09	
		0.44	1.22	3.92		-7.97E+05
10^{14}	2.91E+01	2.42	0.31	1.30	1.50E+06	
		1.93	0.61	2.55		-1.22E+04
10^{15}	3.30E+02	0.12	0.06	0.08	NAN	
		2.00	0.69	1.98		-2.47E+03

Table 1: Numerical results of both fitting procedures. For each of the five datasets we first present the results of the χ^2 fit, and the results of the Poisson fit, this is clearly visible through which field out of χ^2 or $\ln \mathcal{L}$ is filled in. The values provided here are rounded to only 2 significant digits to let them fit on the page. However the full values are given at the end of this report.

In the figure we can see that the χ^2 fits appear to have performed quite badly for all datasets, underestimating the amount of satellite galaxies at low x and extremely overestimating this in the highest x bin in the first three datasets. In the last two sets this pattern appears reversed and the peaks of the data- and model distributions do not match anymore. This is possibly caused by the fact

Fit Results

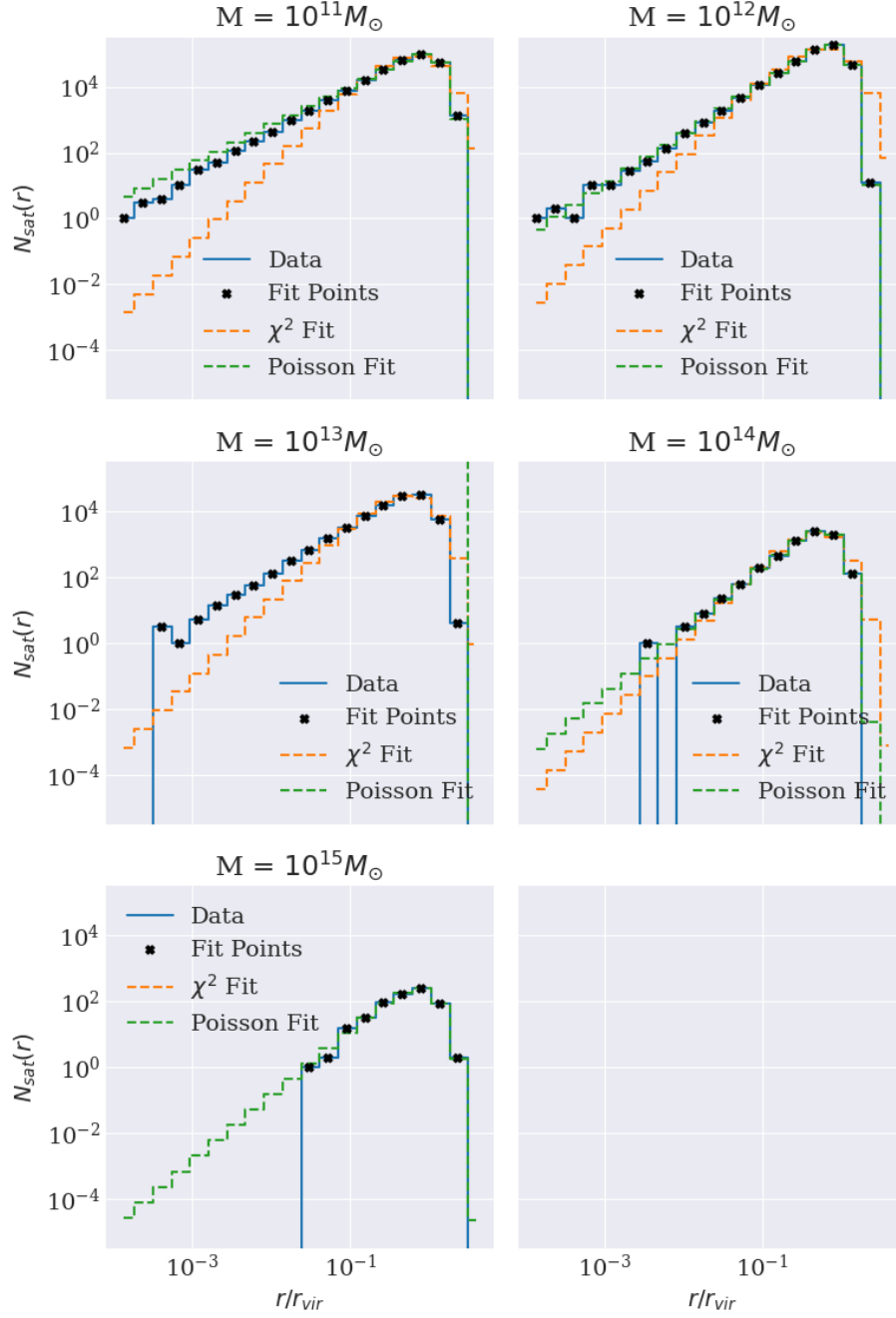


Figure 3:

that there is almost no data below $x \sim 10^{-2}$ which confuses the χ^2 statistic. The Poisson fits on the other hand appear to fit quite well to the data. In most of the plots the Poisson fit appears to at most be off by a few from the real data which could just be due to noise. Only in the $10^{11} M_{\odot}$ fit can we see that the Poisson fit appears to be biased towards higher values in the low x end, and appears to be 'off' by a few hundred to a thousand in the highest x bin.

But to draw some quantitative conclusions about these fits we have to perform some statistical test. We will do a G-test on the binned fit results and binned data. This G statistic is defined as

$$G = 2 \sum_i^N O_i \ln \left(\frac{O_i}{E_i} \right). \quad (6)$$

Where O_i is the observed number of instances in a bin, which should always be an integer, and E_i is the expected number of observations in a bin. This latter value is the expected model value in a given bin, and therefore is not limited to being an integer. We can use this G statistic in a goodness of fit test for χ^2 to compute the Q-value, which is equivalent to the p-value. This Q is defined as

$$Q = 1 - \frac{\gamma\left(\frac{k}{2}, \frac{x}{2}\right)}{\Gamma\left(\frac{k}{2}\right)} \quad (7)$$

With

$$\gamma(s, x) = \int_0^x t^{s-1} e^{-t} dt \quad (8)$$

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt \quad (9)$$

the lower incomplete gamma function, and the gamma function respectively which we compute using `scipy.special.gammainc` and `scipy.special.gamma`. k is the number of degrees of freedom in the data, which is given by $N - M$ where N is the number of data points and M is the number of free parameters. In our case N is the number of data bins which we have set to 20, and M is the number of parameters we fit, 3, but also $\langle N_{sat} \rangle$ which sets the area under the curve. This means $M = 4$ and therefore the total number of degrees of freedom $k = 16$. We compute the G and Q values for each fit on each dataset, and present the results in Table 2.¹

A Q value lower than ~ 0.1 would indicate that our fit is bad. Unfortunately, this appears to be the case for all of the fits computed in this report. Most of the Q-values reported here take on the exact same value, which is an indication that our G values are extremely high and therefore also statistically extremely bad fits. We see one negative value in the G value for one of the Poisson fits, this in principle should never happen. Especially not a negative number that is as large as this is. This is another strong indication that there is most likely something wrong with the fit for that particular dataset.

¹The code for this section was already given in Section 1.2 because it is done in the same loop as all the fitting procedures.

M	Method	G	Q
10^{11}	χ^2	28175.43917756349	0.0001984126984126984
10^{11}	Poisson	1087.0882149857707	0.0001984126984126984
10^{12}	χ^2	47702.887489199704	0.0001984126984126984
10^{12}	Poisson	5418.609065069538	0.0001984126984126984
10^{13}	χ^2	6250.032384770378	0.0001984126984126984
10^{13}	Poisson	-1811729.4716788493	nan
10^{14}	χ^2	344.76724586865157	0.0001984126984126984
10^{14}	Poisson	92.53161867435563	0.00019841269841252922
10^{15}	χ^2	nan	nan
10^{15}	Poisson	15.368470301292744	9.963597234230879e-05

Table 2: G-test values for each dataset and each fitting method.

The only thing one might be able to conclude from these statistics is the fact that, while the fits look reasonably good when inspected visually, when analyzing them quantitatively, with the G-statistic, they are actually quite bad. Although it is also important to note here that another statistic might have yielded better, or at least different, results than what is presented here.

Listing 12: Unrounded numerical values for the fitting parameters presented in Table 1.

```

1 # QUASI-NEWTON
2 def line_minimization(func, x_vec, step_direction, method=
  golden_section_search, minimum_acc=0.1):
3     """
4     # Make a function f(x+lmda*n)
5     minim_func = lambda lmda: func(x_vec + lmda * step_direction)
6
7     # The parameter landscape is very prone to diverging, and the
8     gradients are very steep. Attempt to keep steps small!
9     inv_stepdirection = np.abs(1./np.sum(step_direction)) # roughly
    equal to 1
10    bracket_edge_guess = [0, 1]#inv_stepdirection] # keeps the
    steps realatively small to combat divergence
11    bracket, _ = make_bracket(minim_func, bracket_edge_guess) #
    make a 3-point bracket surrounding a minimum
12
13    # Use a 1-D minimization method to find the 'best' lmda
14    minimum, _ = method(minim_func, bracket, target_acc=minimum_acc
15    )
16    return minimum
17
18 def compute_gradient(func, x_vec):
19    """Computes the gradient of a multi-dimensional function by
20    applying
21    Ridder's method on each dimension separately"""
22    dim = x_vec.shape[0]
23    nabla_f = np.zeros(dim)
24
25    for i in range(dim):
26        # The function below transforms the multi-dimensional
27        function func
28        # into a function that only varies along dimension i
29        func_1d = lambda xi: func([*x_vec[:i], xi, *x_vec[i+1:]])
30        nabla_f[i] = ridders_method(func_1d, [x_vec[i]], target_acc
31        =1e-5)[0][0] # we don't store the uncertainty now
32    return nabla_f
33
34 def bfgs_update(H, delta, D):
35    """Updates the approximated Hessian using the Broyden-Fletcher-
36    Goldfarb-Shannon
37    algorithm, used for optimization with the quasi-Newton method.
38    INPUTS:
39        H: NxN ndarray, approximation of the Hessian
40        delta: N ndarray, last taken optimization step in x_vec
41        D: N ndarray, difference between new and old gradients
42    OUTPUTS:
43        H': NXN ndarray, updated approximation of the Hessian
44    """
45    # Pre-compute some values for efficiency and clarity
46    deltaD = delta @ D
47    HD = H @ D
48    DHD = D @ HD
49
50    u = (delta/deltaD) - (HD/DHD)
51
52    H_update1 = outer_product(delta, delta)/deltaD
53    H_update2 = outer_product(HD, HD)/DHD
54    H_update3 = DHD * outer_product(u, u)
55    return H + H_update1 - H_update2 + H_update3

```



```

53
54
55 def quasi_newton(func, start, target_step_acc=1e-3, target_grad_acc
56                 =1e-3, max_iter=int(1e3)):
57     """
58     # SETUP
59     dim = start.shape[0]
60     H = np.eye(dim)
61     x_vec = start
62     # Do this before the loop because we compute the gradient at
63     # x_i+1 in loop i
64
65     gradient = compute_gradient(func, x_vec)
66
67     for i in range(max_iter):
68         step_direction = -H @ gradient
69         step_size = line_minimization(func, x_vec, step_direction)
70         # Make the step
71         delta = step_size * step_direction
72         x_vec += delta
73         #print(step_direction, step_size)
74         # Check if we are going to make a small step
75         if np.abs(np.max(delta/x_vec)) < target_step_acc:
76             return x_vec, i
77         #print(gradient)
78         # Compute the gradient at the new point, and check relative
79         # convergence
80         new_gradient = compute_gradient(func, x_vec)
81         if np.abs(np.max((new_gradient - gradient)/(0.5*(
82         new_gradient+gradient)))) < target_grad_acc:
83             return x_vec, i
84
85         # If no accuracies are reached yet, sadly we have to
86         # continue
87         D = new_gradient - gradient
88         gradient = new_gradient
89         H = bfgs_update(H, delta, D)
90
91     return x_vec, i
92
93 def outer_product(v, w):
94     """Compute the outer product of two vectors. This is a matrix A
95     with
96     A_ij = v_i * w_j
97     NOTE: This function doesn't assume the vectors are of the same
98     size, and
99     this function is not symmetric (outer(v,w) != outer(w,v))
100     """
101     A = np.zeros((v.shape[0], w.shape[0]))
102     for i in range(v.shape[0]):
103         A[i] = v[i] * w
104     return A

```

Listing 13: Code for the Quasi-Newton algorithm which was too prone to divergence and is therefore sadly unused in this report