Week 3 Stats Assignment

In [2]:

```
import numpy as np
import scipy as sci
%matplotlib inline
import matplotlib.pyplot as plt
import itertools
```

Question 1

In [3]:

```
freqs = np.linspace(10, 110, 11)
voltages = np.array((16, 45, 64, 75, 70, 115, 142, 167, 183, 160, 221),
                        dtype='f') * 1e-3
errors = np.array((5, 5, 5, 5, 30, 5, 5, 5, 5, 30, 5), dtype='f') * 1e-3
```

i) Calculate the 4 elements of the curvature matrix.

From last week we know a linear fit works for this data, so we can use the analytical results for the curvature matrix.

In [4]:

```
A_cc = sum(1. / errors**2, 0.)
A_cm = sum(freqs / errors**2, 0.)
A_mc = A_cm
A_mm = sum(freqs**2 / errors**2, 0.)
A = np.matrix([[A_cc, A_cm], [A_mc, A_mm]])
print('Curvature matrix is:\n', A)
```

```
Curvature matrix is:
 [[  3.62222187e+05   2.05666642e+07]
 [  2.05666642e+07   1.53788870e+09]]
```

ii) Invert this to give the error matrix.

Inverting A gives the error matrix C.

In [5]:

```
C = A.I
print('Error matrix is:\n', C)
```

```
Error matrix is:
 [[  1.14708120e-05  -1.53402738e-07]
 [ -1.53402738e-07   2.70174466e-09]]
```

iii) What are the uncertainties in the slope and intercept?

To get the uncertainties in m and c, we take the square root of the diagonal terms of C.

In [6]:

```
alphas = np.sqrt(C.diagonal())

print('Uncertainty in m is: {:.1g} mV/Hz'.format(alphas[0,1]*1e3))
print('Uncertainty in c is: {:.1g} mV'.format(alphas[0,0]*1e3))
```

```
Uncertainty in m is: 0.05 mV/Hz
Uncertainty in c is: 3 mV
```

iv) Comment on your answer.

These values are identical to those otained last week from doing a weighted least-squares fit.

Question 2

Done on separate sheet.

Question 3

In [7]:

```
concentrations = np.linspace(0.025, 0.175, 7)
thetas = np.array([10.7, 21.6, 32.4, 43.1, 53.9, 64.9, 75.4])
errors = np.full(7, 0.1)

# Straight line fit parameters
m = 431.7 # deg cm^3 / g
c = -0.03 # deg
```

Show that the curvature matrix is given by...

In [8]:

```
A_cc = sum(1. / errors**2, 0.)
A_cm = sum(concentrations / errors**2, 0.)
A_mc = A_cm
A_mm = sum(concentrations**2/errors**2, 0.)
A = np.matrix([[A_cc, A_cm], [A_mc, A_mm]])
print('Curvature matrix is:\n', A)
```

```
Curvature matrix is:
 [[ 700.     70.  ]
 [  70.      8.75]]
```

...and that the error matrix is...

In [9]:

```
C = A.I
print('Error matrix is:\n', C)
```

```
Error matrix is:
 [[ 0.00714286 -0.05714286]
 [-0.05714286  0.57142857]]
```

Calculate the associated correlation matrix.

Entries are given by $\rho_{AB} = \frac{C_{AB}}{\sqrt{C_{AA}C_{BB}}}$

In [10]:

```
def rho_ab(a, b, cov):
    a = int(a)
    b = int(b)
    return cov[a, b] / np.sqrt(cov[a, a] * cov[b, b])

# makes this function work with np.vectorize
vrho = np.vectorize(rho_ab, excluded={'cov'})

corr = np.fromfunction(vrho, (2,2),cov=C)
corr = np.matrix(corr)

print('Correlation matrix is:\n',corr)
```

```
Correlation matrix is:
 [[ 1.         -0.89442719]
 [-0.89442719  1.        ]]
```

i) What are the uncertainties in the best-fit intercept and gradient?

As before, these are given by the square roots of the diagonal elements of C.

In [11]:

```
alphas = np.sqrt(C.diagonal())
alpha_m = alphas[0,1]
alpha_c = alphas[0,0]

print('Uncertainty in m is: {:.1g} deg cm^3 / g'.format(alpha_m))
print('Uncertainty in c is: {:.1g} deg'.format(alpha_c))
```

```
Uncertainty in m is: 0.8 deg cm^3 / g
Uncertainty in c is: 0.08 deg
```

ii) What optical rotation is expected for a known concentration of $C = 0.080 \text{ g cm}^{-3}$, and what is the uncertainty?

Fit is $\theta = mC + c$. The nonzero correlation coefficients found above need to be taken into account to calculate the uncertainty. The required expression (from Table 7.2 in the book) is:
$\alpha_\theta^2 = C^2\alpha_m^2 + \alpha_c^2 + 2C\alpha_{mc}$

In [12]:

```
conc = 0.080
expected_rotation = m * conc + c
uncertainty = np.sqrt(conc**2 * C[0,0] + C[1,1] + 2 * conc * C[0,1])

print('Result: expected rotation is ({:.3g} +- {:.1g}) deg'
      .format(expected_rotation, uncertainty))
```

```
Result: expected rotation is (34.5 +- 0.7) deg
```

iii) What is the concentration given a measured rotation of $\theta = 70.3^{\circ}$, and what is the uncertainty?

Invert fit function: $C = \theta/m - c/m$.

For the second term, from Table 7.2: $(\alpha_C/C)^2 = (\alpha_m/m)^2 + (\alpha_c/c)^2 - 2(\alpha_{mc}/mc)$

The first term contributes an additional factor α_m/m.

In [13]:

```
theta = 70.3
expected_conc = (theta - c) / m
alpha_1 = (theta / m) * (alpha_m / m)
alpha_2 = (c / m) * np.sqrt((alpha_c / c)**2 + (alpha_m / m)**2
                            - 2 * C[0, 1] / (m * c))
uncertainty = np.sqrt(alpha_1**2 + alpha_2**2)
print('Result: expected concentration is ({:.4g} +- {:.1g}) g/cm^3'
      .format(expected_conc, uncertainty))
```

```
Result: expected concentration is (0.1629 +- 0.0003) g/cm^3
```

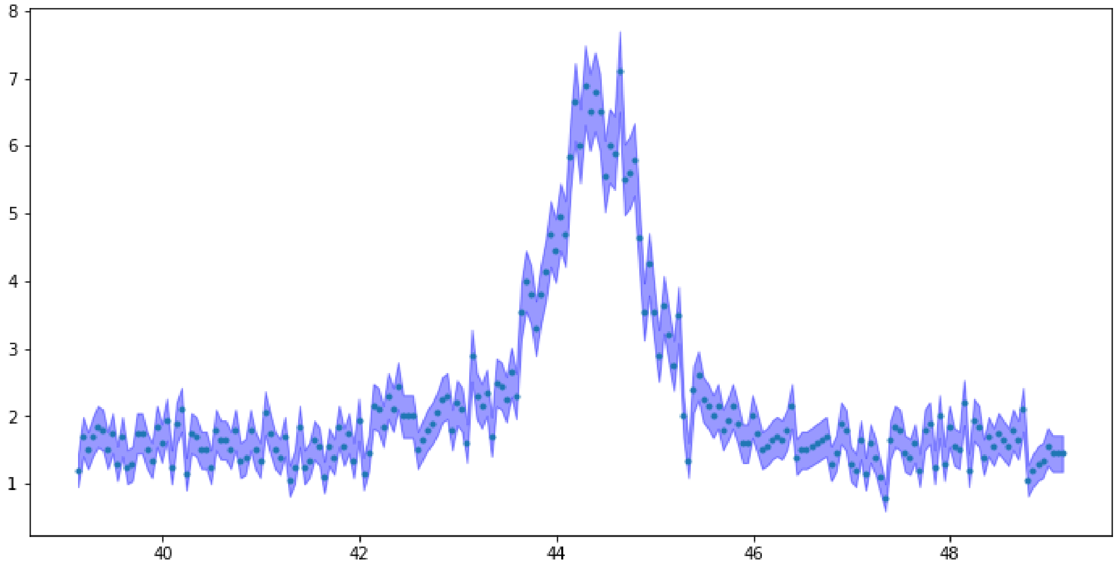
Question 4

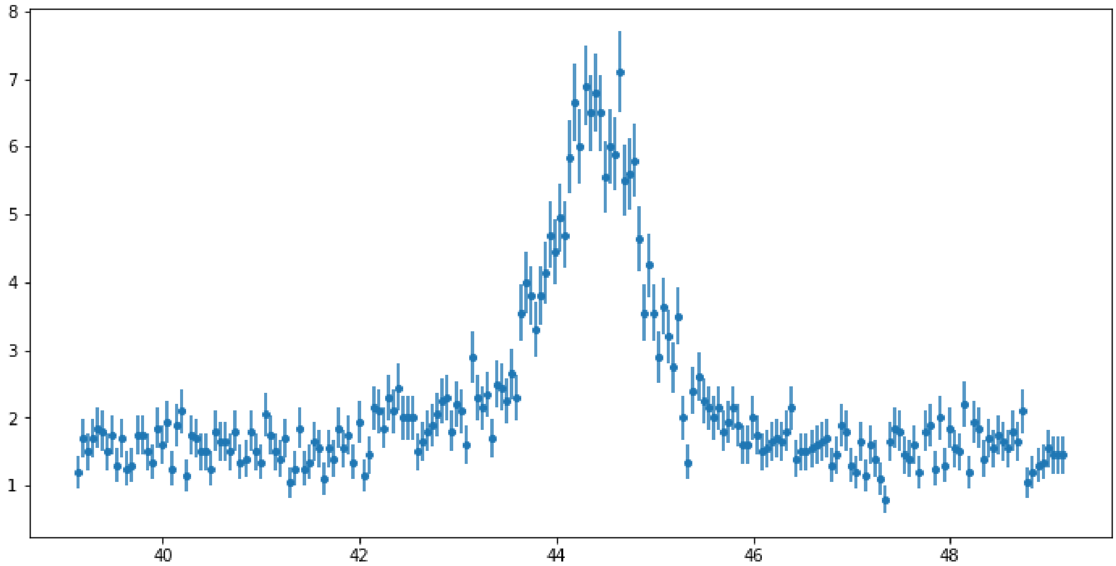
In [14]:

```
data = np.loadtxt('LorentzianData.csv', skiprows=3,
                  dtype = [('angle', 'f'), ('cps', 'f'), ('err', 'f')])

plt.figure(figsize=(12, 6))
plt.fill_between(data['angle'], data['cps'] + data['err'],  data['cps'] - data[
'err'],
                 alpha=0.4, color='b')
plt.plot(data['angle'], data['cps'], 'o', ms=3)

plt.figure(figsize=(12, 6))
plt.errorbar(data['angle'], data['cps'], data['err'], fmt='o', ms=4)
```

Out[14]:

<Container object of 3 artists>





i) Explain how the error in the count rate was calculated.

The counts measured per second should follow a Poisson distribution, for which the error in the counts is given by $\sqrt{\bar{x}}$. Since the results have been measured in 20-second bins, the count rate should first be divided by 20.

In [15]:

```
# tests whether the statement above is right
print(np.isclose(data['err'], np.sqrt(data['cps'] / 20)).all())
```

True

ii) Perform a χ^2 minimisation. What are the best-fit parameters?

In [16]:

```
# The form of the fitting function
def S(theta, S_bgd, S_0, theta_0, delta_theta):
    return S_bgd + S_0 / (1 + 4 * ((theta - theta_0) / delta_theta)**2)

#  The gradient vector for the fitting function
def dS(theta, S_bgd, S_0, theta_0, delta_theta):
    dSdS_0 = 1 / (1 + 4 * ((theta - theta_0) / delta_theta)**2)
    dSdS_bgd = np.ones_like(theta)
    dSdtheta_0 = ((8 * delta_theta **2 * S_0 * (theta - theta_0))/
                  (4 * (theta - theta_0)**2 + delta_theta**2)**2)
    dSddelta_theta = ((8 * delta_theta * S_0 * (theta - theta_0)**2)/
                      (4*(theta - theta_0)**2 + delta_theta**2)**2)
    return (dSdS_bgd,dSdS_0, dSdtheta_0, dSddelta_theta)

# Definition of chi squared
def chi2(x):
    return sum((data['cps'] - S(data['angle'], *x))**2 / data['err']**2)

# Gradient vector/Jacobian for chi squared
def dchi2(x):
    diff = dS(data['angle'], *x)
    return np.array([sum((data['cps'] - S(data['angle'], *x)) / data['err']**2
                     * -2. * diff[i]) for i in range(4)])
```

SciPy has the `optimize` library which can do the minimisation for us. Specifically the `minimize` function takes the (multi-variable) function to minimise and a vector of initial guesses for the parameters.

The BFGS solver is ideal because it also calculates (approximately) the inverse of the Hessian matrix, which we can use to obtain the error matrix.

In [17]:

```
import scipy.optimize as optimize

# Initial guesses for the parameters
S_bgd = 1.5
S_0 = 5
theta_0 = 45
delta_theta = 1

# The initial guesses get passed in as a vector
x0 = np.array([S_bgd, S_0, theta_0, delta_theta])

res = optimize.minimize(chi2, x0, jac=dchi2, method='BFGS')
print('''Best-fit parameters are:
    S_bgd = {}
    S_0 = {}
    theta_0 = {}
    delta_theta = {}'''.format(*res.x))

S_bgd, S_0, theta_0, delta_theta = res.x
minimised_chi2 = res.fun

xs = data['angle']
ys = S(xs, *res.x)
residuals = (data['cps'] - ys) / data['err']

plt.figure(figsize=(12, 12))
plt.subplots_adjust(hspace=0.001)
ax1 = plt.subplot(211)
ax1.xaxis.set_visible(False)
ax1.set_ylabel('Count $(s^{-1})$')
plt.plot(xs, ys, 'orange')
plt.scatter(data['angle'], data['cps'], s=5)

ax2 = plt.subplot(212)
ax2.set_ylabel('Residual $(s^{-1})$')
ax2.set_xlabel('Angle (degrees)')
plt.scatter(data['angle'], residuals, s=5)
```

```
Best-fit parameters are:
    S_bgd = 1.404403699969694
    S_0 = 5.4263184427109055
    theta_0 = 44.390120690814236
    delta_theta = 0.9498836597699426
```

```
Out[17]:
```

```
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```
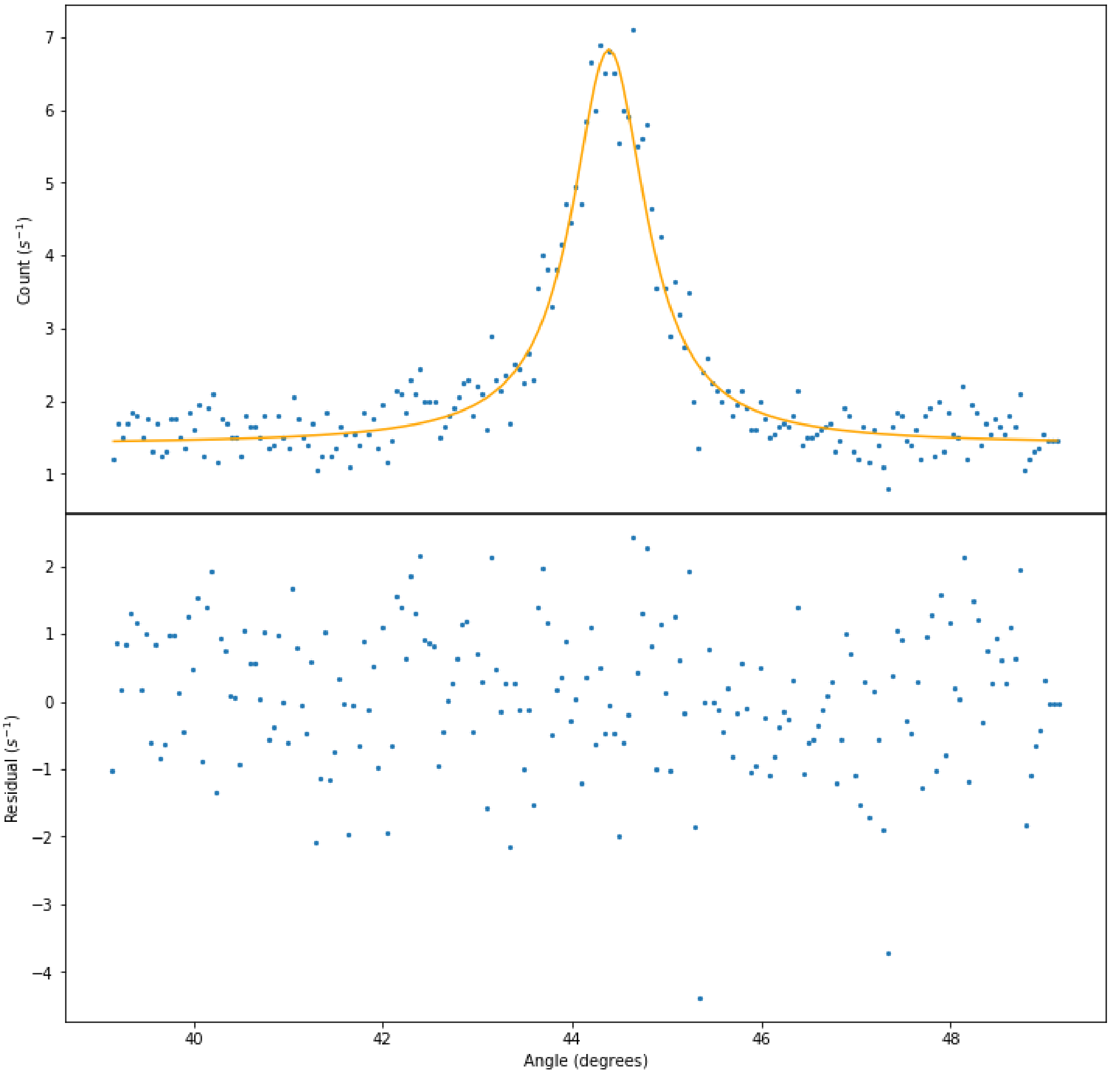



iii) Evaluate the error matrix.

Error matrix $C = A^{-1}$.
Curvature matrix $A = 0.5H$.
Hessain matrix H is matrix of partial differentials of χ^2.

In [18]:

```
# C = inverse(0.5 * H)
#   = inverse(H) * 2

C = 2 * res.hess_inv

print('Error matrix is:\n', C)
```

```
Error matrix is:
 [[  7.68169703e-04   1.71465082e-04   9.20430007e-08  -5.92329255e
-04]
 [  1.71465082e-04   3.75929645e-02   1.42361411e-04  -5.45041180e-
03]
 [  9.20430007e-08   1.42361411e-04   2.44137195e-04  -2.38469721e-
05]
 [ -5.92329255e-04  -5.45041180e-03  -2.38469721e-05   1.81134950e-
03]]
```

iv) Calculate the correlation matrix.

Same method as in Q3.

In [19]:

```
# S_bgd       S_0 theta_0 delta_theta
# S_0
# theta_0
# delta_theta
corr = np.fromfunction(vrho, (4, 4), cov=C)
corr = np.matrix(corr)
print('Correlation matrix is:\n', corr)
```

```
Correlation matrix is:
 [[  1.00000000e+00   3.19075763e-02   2.12542217e-04  -5.02150001e
-01]
 [  3.19075763e-02   1.00000000e+00   4.69917935e-02  -6.60503162e-
01]
 [  2.12542217e-04   4.69917935e-02   1.00000000e+00  -3.58604009e-
02]
 [ -5.02150001e-01  -6.60503162e-01  -3.58604009e-02   1.00000000e+
00]]
```

v) What are the uncertainties in the best-fit parameters?

As before, this is just the square root of the diagonal of the error matrix.

In [20]:

```
alphas = np.sqrt(C.diagonal())
print('''Uncertainties in best-fit parameters are:
    alpha_S_bgd = {}
    alpha_S_0 = {}
    alpha_theta_0 = {}
    alpha_delta_theta = {}'''.format(*alphas))

print('''Hence results are:
    S_bgd = {:.2f} +- {:.1g}
    S_0 = {:.3g} +- {:.2g}
    theta_0 = {:.4g} +- {:.1g}
    delta_theta = {:.2g} +- {:.1g}'''.format(*itertools.chain(*zip(res.x, alphas
))))
```

```
Uncertainties in best-fit parameters are:
    alpha_S_bgd = 0.02771587456322677
    alpha_S_0 = 0.1938890520891835
    alpha_theta_0 = 0.015624890238459057
    alpha_delta_theta = 0.042559951844800416
Hence results are:
    S_bgd = 1.40 +- 0.03
    S_0 = 5.43 +- 0.19
    theta_0 = 44.39 +- 0.02
    delta_theta = 0.95 +- 0.04
```

vi) Make χ^2 contour plots for (a) S_{bgd} against θ_0, (b) S_{bgd} against $\Delta\theta$

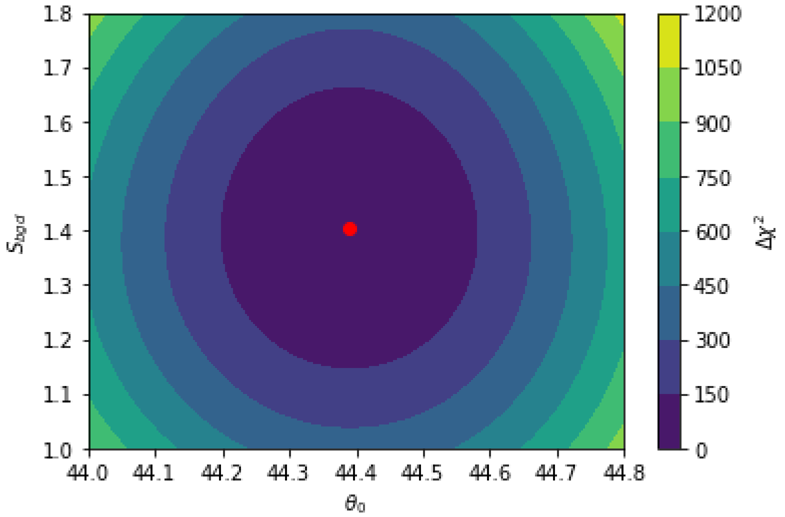
Comment on the shape of the contours.

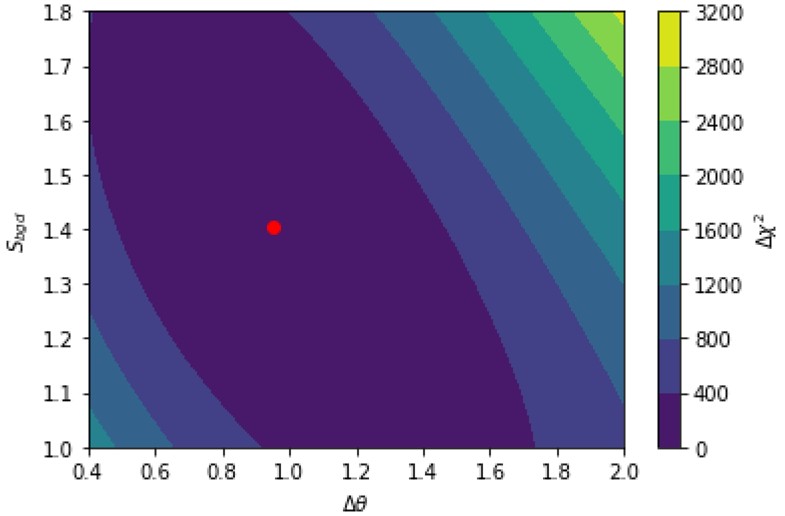
In [21]:

```
# S_bgd - theta_0
N = 100
rge_S_bgd = np.linspace(1.0, 1.8, N)
rge_theta_0 = np.linspace(44, 44.8, N)

chisqs = np.zeros((N, N))
for x in range(N):
        for y in range(N):
            chisqs[y, x] = chi2((rge_S_bgd[y], S_0, rge_theta_0[x], delta_theta
)) - minimised_chi2

plt.figure()
ax = plt.gca()
ax.set_ylabel('$S_{bgd}$')
ax.set_xlabel(r'$\theta_0$')
plt.contourf(rge_theta_0, rge_S_bgd, chisqs)
cb = plt.colorbar()
cb.set_label('$\Delta\chi^2$')
plt.scatter(theta_0, S_bgd, c='r')

# S_bgd - delta_theta
rge_delta_theta = np.linspace(0.4, 2.0, N)

chisqs = np.zeros((N, N))
for x in range(N):
        for y in range(N):
            chisqs[y, x] = chi2((rge_S_bgd[y], S_0, theta_0, rge_delta_theta[x
])) - minimised_chi2

plt.figure()
ax = plt.gca()
ax.set_ylabel('$S_{bgd}$')
ax.set_xlabel(r'$\Delta \theta$')
plt.contourf(rge_delta_theta, rge_S_bgd, chisqs)
cb = plt.colorbar()
cb.set_label('$\Delta\chi^2$')
plt.scatter(delta_theta, S_bgd, c='r')
```

Out[21]:

<matplotlib.collections.PathCollection at 0x7f025a1e1358>





The contours for plot *(a)* are almost circular, indicating there is a low level of correlation between S_{bgd} and θ_0
.

Conversely, the contours in plot *(b)* have a considerable negative tilt, indicating negative correlation between S_{bgd} and $\Delta\theta$.

These conclusions are supported by the relevant entries of the correlation matrix: $\rho_{S_{bgd}\theta_0} = 0.0002$, whereas $\rho_{S_{bgd}\Delta\theta} = -0.5$.

vii? What is the area of the Lorentzian peak?

Integrate the curve between $\theta_0 \pm \Delta\theta$.

In [22]:

```
import scipy.integrate as integrate

ll = theta_0 - delta_theta
ul = theta_0 + delta_theta

peak_area, _ = integrate.quad(S, ll, ul, args=(S_bgd, S_0, theta_0, delta_theta
))

print('Area of peak: {:.3g}'.format(peak_area))
```

```
Area of peak: 8.37
```

viii) Evaluate the Durbin-Watson statistic for the fit to this data set.

In [23]:

```
dw = sum([(residuals[i] - residuals[i - 1])**2
          for i in range(1, len(residuals))]) / sum(residuals**2)

print('Durbin-Watson statistic: {:.3g}'.format(dw))
```

```
Durbin-Watson statistic: 1.82
```

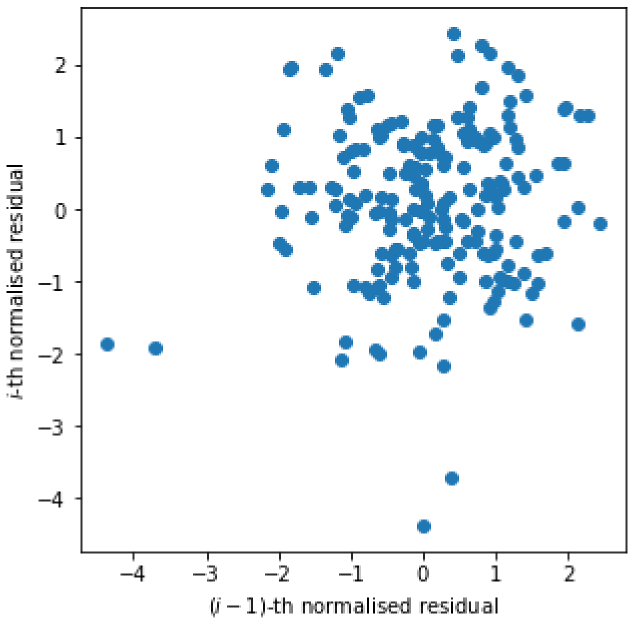
This is close to the value of 2 expected for randomly-distributed residuals. Can verify this by plotting lag plot: i th vs $(i-1)$th residuals.

In [24]:

```
plt.figure(figsize=(5,5))
ax = plt.gca()
ax.set_aspect('equal')
ax.set_ylabel('$i$-th normalised residual')
ax.set_xlabel('$(i-1)$-th normalised residual')
plt.scatter(residuals[1:], [residuals[i - 1] for i in range(1, len(residuals))])
```

Out[24]:

```
<matplotlib.collections.PathCollection at 0x7f026054d940>
```



Apart from a few weird outliers, this looks pretty good: the majority of the points lie within ± 2.