Stats Week 3

November 6, 2017

1 Week 3 Stats Assignment

```
In [2]: import numpy as np
        import scipy as sci
        %matplotlib inline
        import matplotlib.pyplot as plt
        import itertools
```

1.1 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.

1.2 Question 2

Done on separate sheet.

1.3 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 $C = 0.080$ 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
```

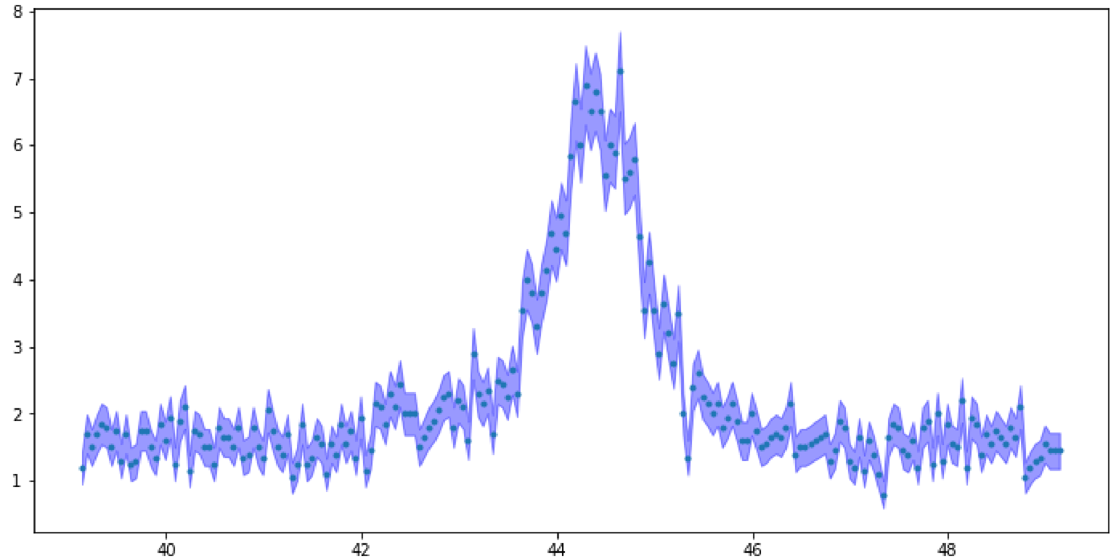
iii) What is the concentration given a measured rotation of $\theta = 70.3°$, and what is the uncertainty?
Invert fit function: $C = \theta/m - c/m$.
For the second term, from Table 7.2: $(\alpha_C/C)^2 = (\alpha_m/m)^2 + (\alpha_c/c)^2 - 2(\alpha_{mc}/mc)$
The first term contributes an additional factor α_m/m.

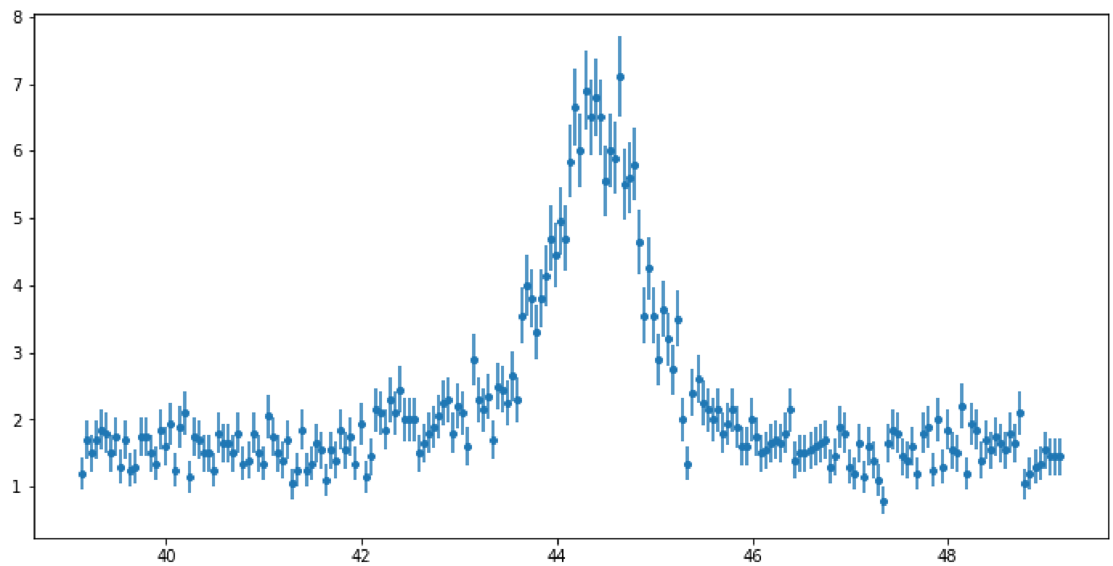
```
In [13]: theta = 70.3
         expected_conc = (theta - c) / m
         alpha_1 = (theta / m) * (alpha_m / m)
         alpha_2 = (c / m) * np.sqrt((alpha_c / c)**2 + (alpha_m / m)**2
                                     - 2 * C[0, 1] / (m * c))
         uncertainty = np.sqrt(alpha_1**2 + alpha_2**2)
         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
```

1.4 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.

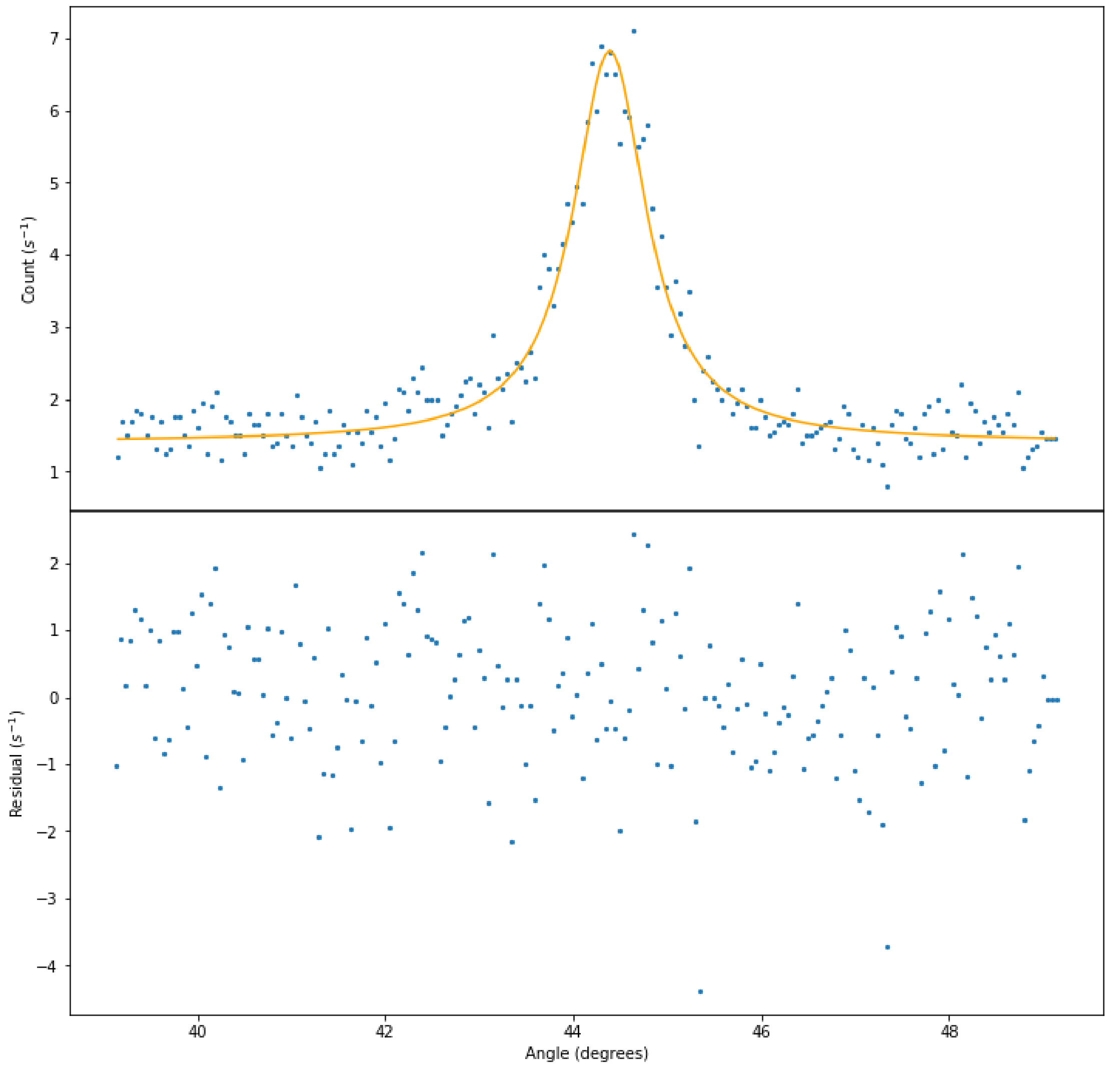
The `BFGS` solver is ideal because it also calculates (approximately) the inverse of the Hessian matrix, which we can use to obtain the error matrix.

```
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]: <matplotlib.collections.PathCollection at 0x7f028ff6ee10>
```



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.

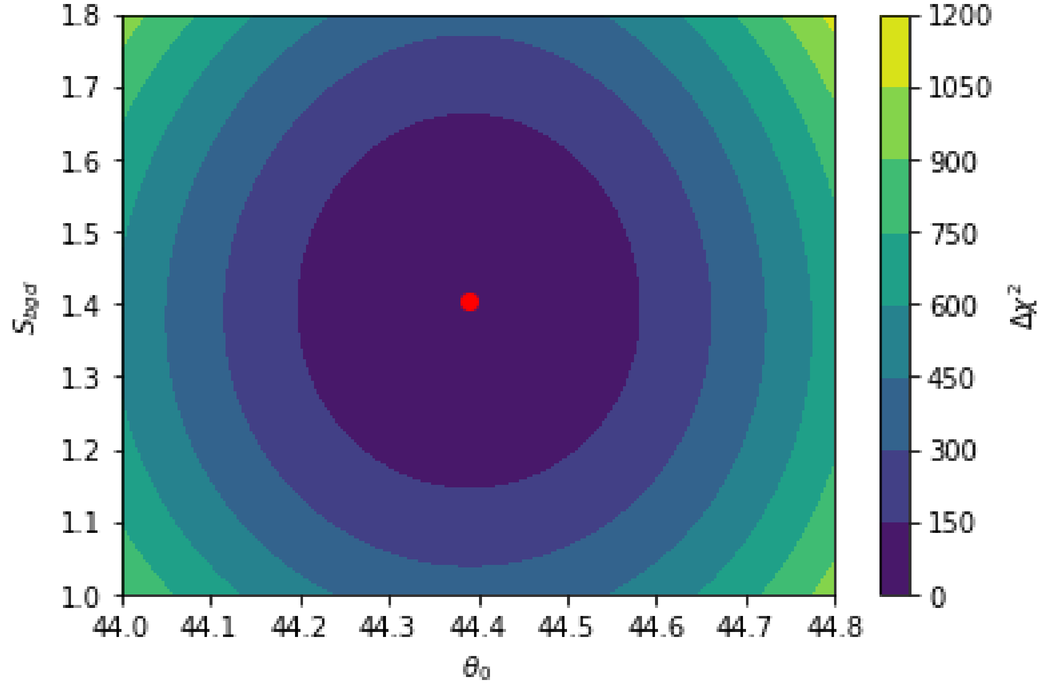
```
In [20]: alphas = np.sqrt(C.diagonal())
         print('''Uncertainties in best-fit parameters are:
             alpha_S_bgd = {}
             alpha_S_0 = {}
             alpha_theta_0 = {}
             alpha_delta_theta = {}'''.format(*alphas))

         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))))
```

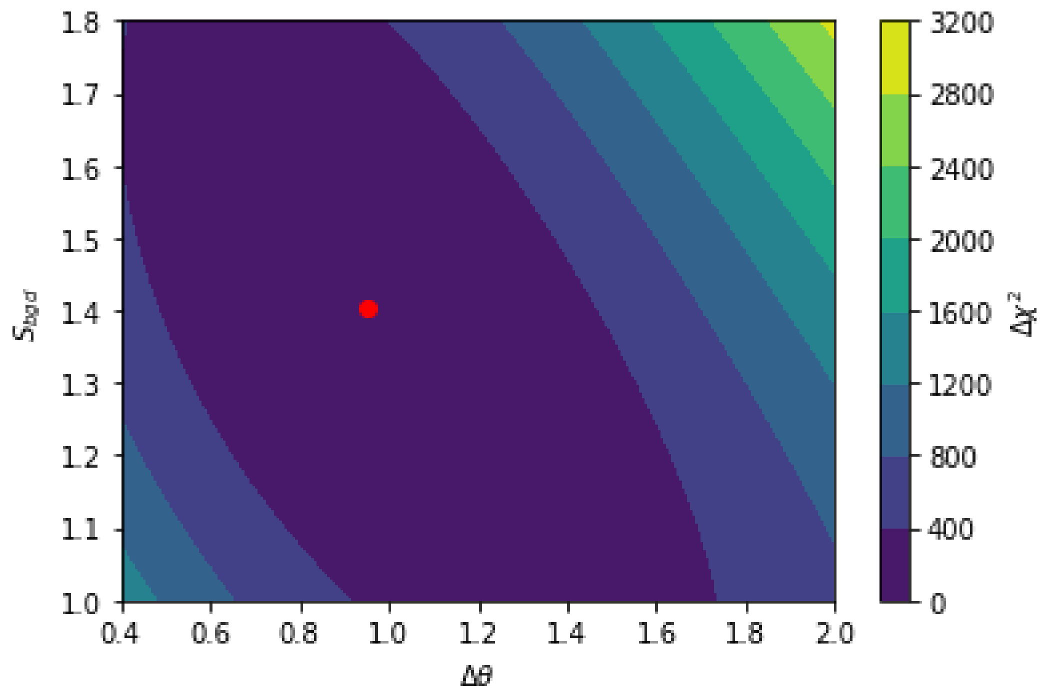
```
Uncertainties in best-fit parameters are:
    alpha_S_bgd = 0.02771587456322677
    alpha_S_0 = 0.1938890520891835
    alpha_theta_0 = 0.015624890238459057
    alpha_delta_theta = 0.042559951844800416
Hence results are:
    S_bgd = 1.40 +- 0.03
    S_0 = 5.43 +- 0.19
    theta_0 = 44.39 +- 0.02
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

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])) - min

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
```

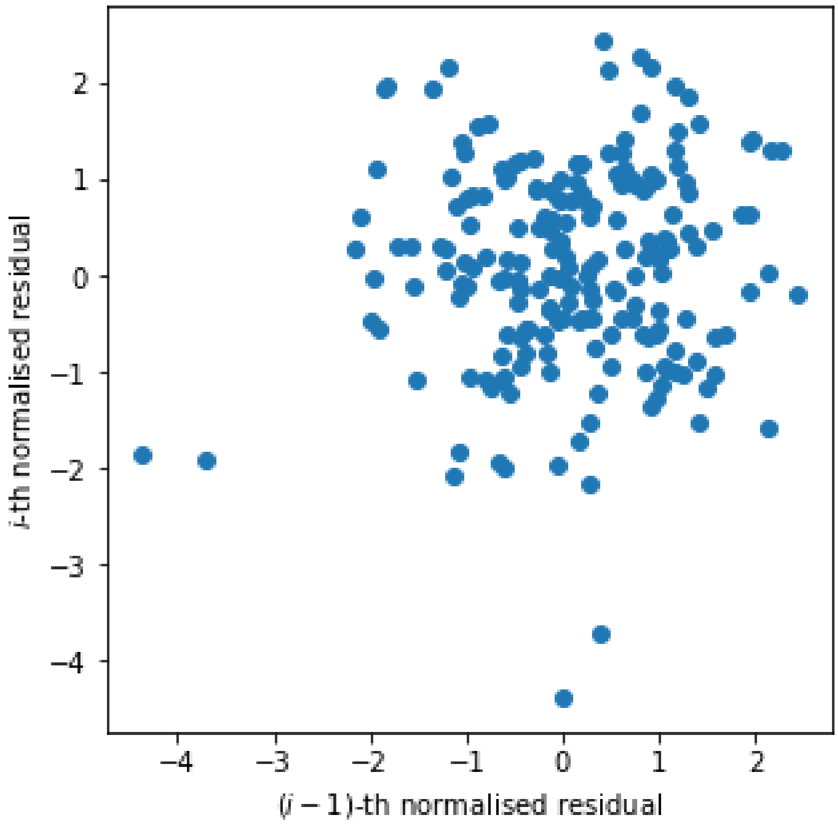
viii) Evaluate the Durbin-Watson statistic for the fit to this data set.

```
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: ith 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.