

BIG DATA COLOMBIA

11 al 15 de febrero 2019
Medellín - Colombia



Python for Data Science

Parameter Estimation

Anna Scaife

University of Manchester

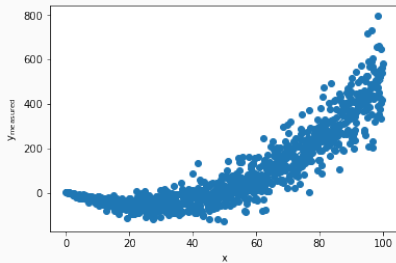
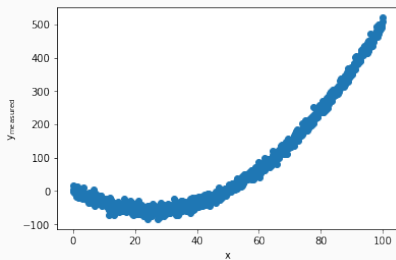


Science & Technology
Facilities Council

Parameter Estimation

Parameter estimation is one of the most common applications in numerical data science.

Parameter Estimation



We think that the model which describes the data has this form:

$$y = ax^2 - mx + c$$

and we know the value of the measurement noise for each data point, σ_i .

What we don't know is the value of the parameters a , m and c .

Cost Function

To fit the model to our data we need to specify a *cost function*. This is a function that evaluates the deviation of the model from the measurements.

The most commonly used cost function is chi-squared:

$$\chi^2 = \sum_i \frac{(d_i - m_i)^2}{\sigma_i^2}$$

The cost function that we specify expresses our *a priori* knowledge of the data.

Direct Optimisation

Import the library:

```
import scipy.optimize as op
```

Define the function you want to fit:

```
def model(p,x):  
  
    a,m,c = p  
    y = a*x**2 - m*x + c  
  
    return y
```

Direct Optimisation

Define the cost function. Here it is the Gaussian loglikelihood:

```
def ll(p,x,y,sigma):  
  
    y_try = model(p,x)  
    diff = y_try - y  
  
    ll = -0.5*np.sum(diff**2/sigma**2)  
  
    return ll
```

scipy optimisation requires the negative loglikelihood:

```
nll = lambda *args: -ll(*args)
```

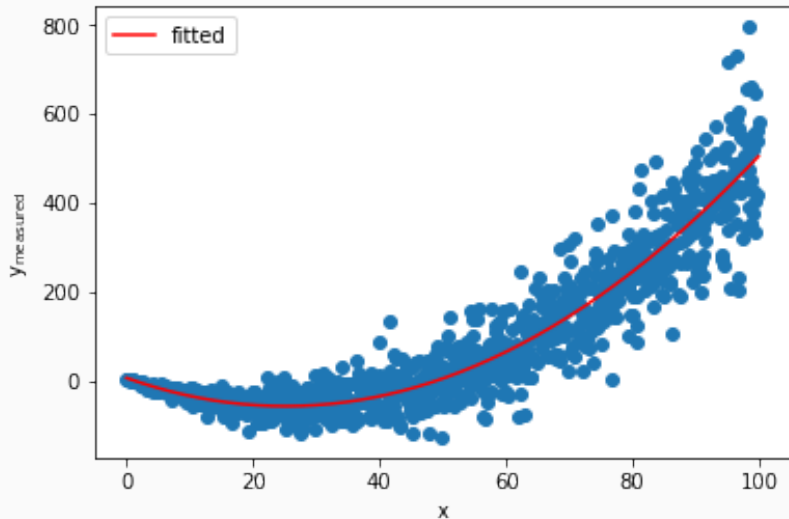
Direct Optimisation

```
initial = np.array([1.,1.,1.])
```

```
result = op.minimize(nll, initial, args=(x, y_meas, sigma))  
a, m, c = result["x"]
```

```
In [12]: print result  
  
      fun: 482.94548559080283  
      hess_inv: array([[1.80041525e-07, 1.79870092e-05, 2.99227436e-04],  
                       [1.79870092e-05, 1.91700675e-03, 3.58894926e-02],  
                       [2.99227436e-04, 3.58894926e-02, 8.96796830e-01]])  
      jac: array([-7.62939453e-06, 0.00000000e+00, -3.81469727e-06])  
      message: 'Optimization terminated successfully.'  
      nfev: 50  
      nit: 7  
      njev: 10  
      status: 0  
      success: True  
      x: array([0.10051117, 5.05231612, 5.89715686])
```


Direct Optimisation



Markov Chain Monte Carlo

Import the library:

```
import emcee
```

Set up the MCMC sampler:

```
ndim, nwalkers = len(initial), 10
p0 = initial + 1e-8 * np.random.randn(nwalkers, ndim)
sampler = emcee.EnsembleSampler(nwalkers, ndim, ll,
                                args=(x,y_meas,sigma))
```

Markov Chain Monte Carlo

```
print("Running burn-in...")  
p0,_,_ = sampler.run_mcmc(p0, 1000)  
sampler.reset()
```

```
print("Running production...")  
sampler.run_mcmc(p0, 3000)
```

```
import corner

tri_labels = [r"a", r"m", r"c"]
tri_truths = [0.1, 5., 5.]
tri_range = [(0, 1.), (0, 10), (0, 10)]
inds = np.array([0, 1, 2])
corner.corner(sampler.flatchain[:, inds], truths=tri_truths,
              labels=tri_labels)
```

Markov Chain Monte Carlo

