Introduction to High Performance Computing

Autumn, 2018

Lecture 5

Git/Bitbucket notes

- After modifying files in your local repo, remember to *add*, *commit*, and *push* your changes
- Before starting work which will modify files in your local repo, remember to sync your fork and *pull* any changes into your local repo.
- This will help you avoid merging problems which occur when your fork and local repo are both being updated independently
- There is a link to a nice, short online tutorial on using git in the supplementary reading section of the course webpage.

Python notes

Main differences between arrays and lists:

Lists are *flexible*: heterogeneous data, can grow or shrink, numerical calculations can be slow/cumbersome

Arrays: calculations are generally faster, but elements must be homogeneous, difficult to adjust size

- **Lists can be grown/shrunk more efficiently than arrays**

- L.append() **for a list,** L**, is more efficient than** np.append(A) **for an array,** A**. The numpy command will make a new copy of the array, the list will grow *in place***

Python notes

Getting comfortable with python:

- **Have command of *all* of the material in online lectures –use exercises for self-assessment (solutions are online)**
- **Understand structure and purpose of functions (lecture 3 slides)**
- **Choose an editor + terminal combination for developing code. Can be *spyder* (distributed w/ anaconda), *canopy*, or *atom* + *jupyter qtconsole*. Use python3.x (e.g. python3.6)**
- **Understand *mysqrt.py* and *brown.py* (provided in lecture 4 and 5 directories of course repo)**
- **Further help: list of supplementary material on course webpage, office hours**

Today

- Improving Brownian motion code
- Basics of optimization
- Using *scipy.minimize* package in python

Code development

- **Use built-in functions whenever possible (*e.g.* sqrt instead of mysqrt.sqrt2)**

- **When working with arrays, *vectorize* code whenever possible:**

```
In [8]: def sinx(x):
   ...: y = np.zeros_like(x)
   ...: for i,xi in enumerate(x):
   ...: y[i] = sin(xi)
   ...: return y
   ...:
In [9]: x = np.random.randn(10000)

In [10]: timeit y1=sin(x) #vectorized
159 µs ± 989 ns per loop (mean ± std. dev. of 7 runs, 10000 loops each)

In [11]: timeit y2 = sinx(x)
18.6 ms ± 140 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

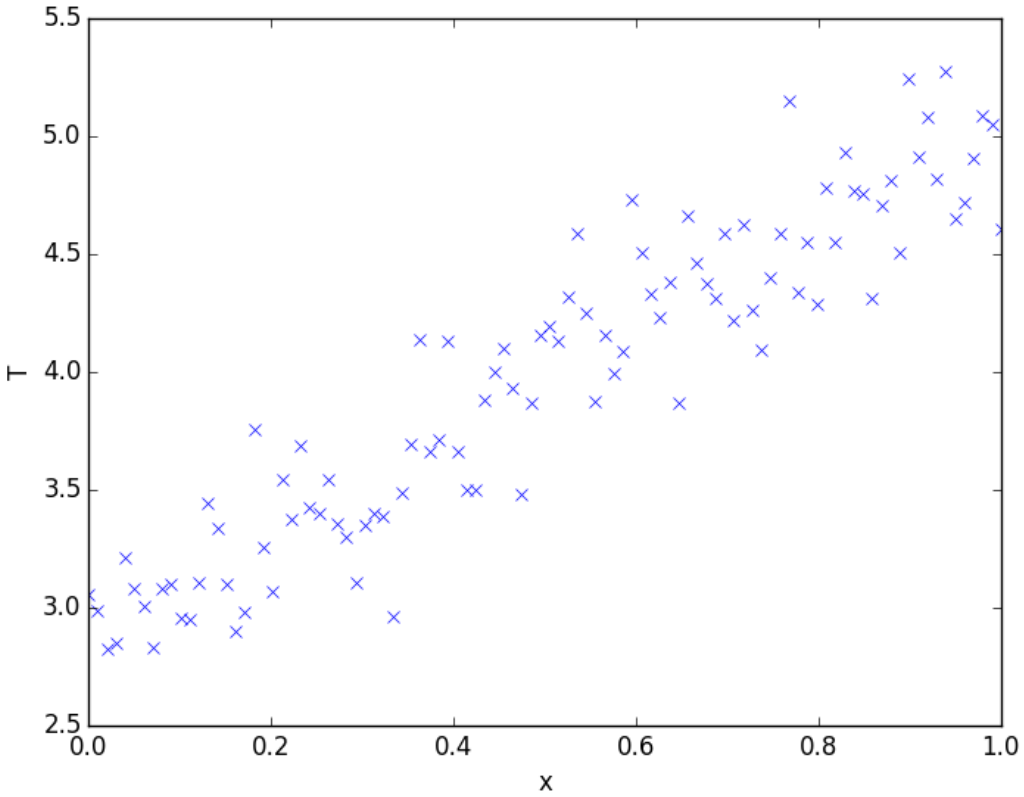
Optimization with Python

We will focus almost entirely on the scipy.optimize **package**

- optimize **contains all standard methods for unconstrained optimization**
- **Choices for constrained optimization are more limited**
  - **Other packages are available (*e.g.*** pyopt**)**

Getting started – finding trends in data

Consider the noisy data:



Getting started – finding trends in data

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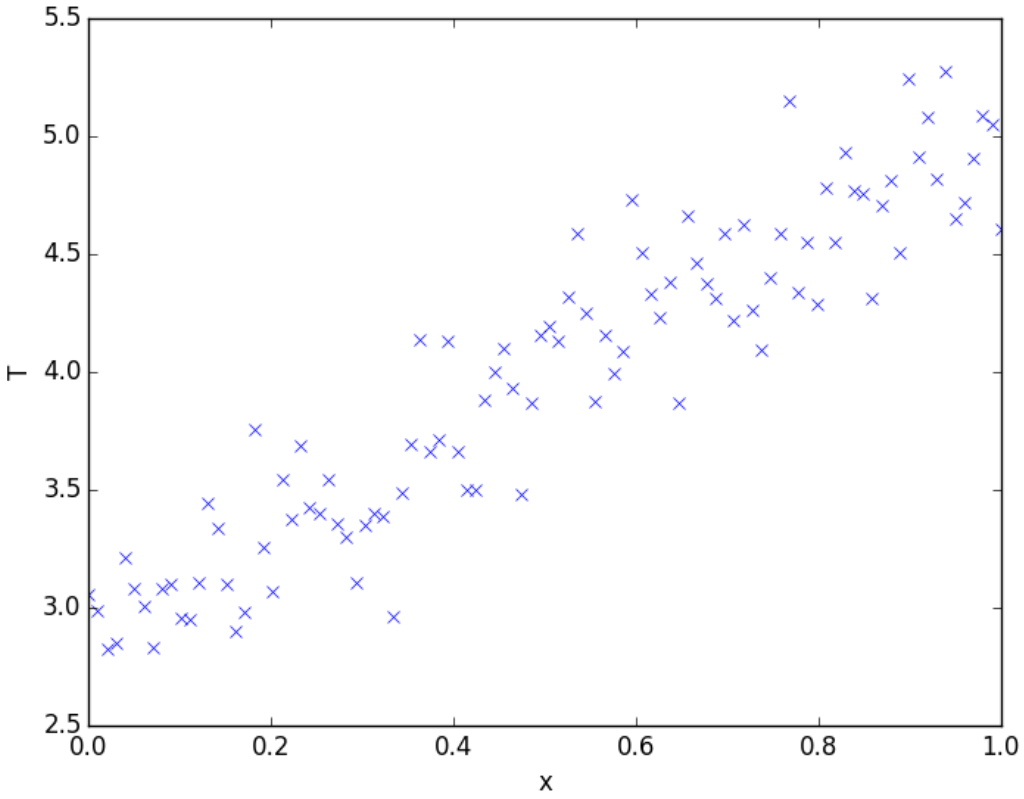


- **How can we construct a linear fit?**
  ***i.e.* find c_1 and c_2 such that**
  $T = c_1 x + c_2$
- **Python provides several options:**
  - scipy.stats
  - numpy.linalg.lstsq
  - scipy.optimize.curve_fit
  - numpy.polyfit
  - Pandas, statsmodel, **probably quite a few more!**
- **As a start, let's use** polyfit

Getting started – finding trends in data

x and T are simple arrays:

```
In [8]: x = np.linspace(0,1,100)

In [9]: T = 2*x + 3 + 0.25*np.random.randn(100)
```

Getting started – finding trends in data

x and T are simple arrays:

```
In [8]: x = np.linspace(0,1,100)

In [9]: T = 2*x + 3 + 0.25*np.random.randn(100)
```

And we use polyfit to fit a 1st order polynomial (i.e. a line) to the data:

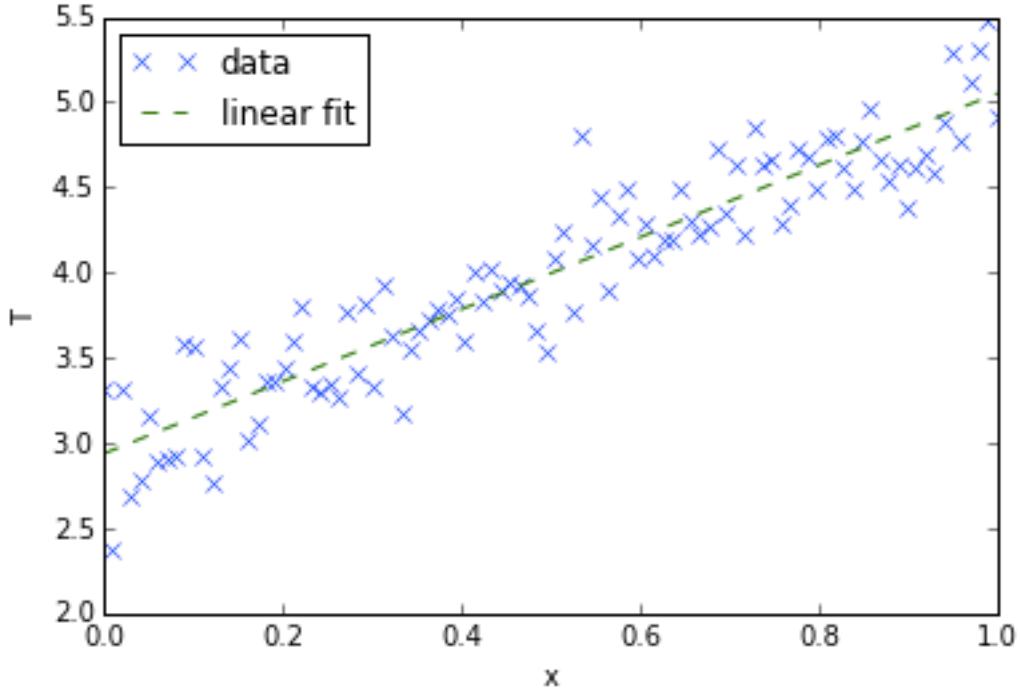
```
In [10]: C = np.polyfit(x,T,1)

In [11]: print "C1=",C[0],", C2=",C[1]
C1= 1.99587384666 , C2= 2.9703841544

In [13]: Tf = C[0]*x + C[1]
```

So the constants are close to what we expect, let's now display the fit:

Getting started – finding trends in data



- polyfit **constructs a linear least-squares fit to a nth-order polynomial:**

$$f(x) \approx c_1 x + c_2 x^2 + c_3 x^3 + ... + c_n x^n$$

so, it is only the fitting parameters that must be linear

- **The functional form for least-squares fits can be arbitrary (polynomial, trigonometric, etc…)**

General linear least squares

- Let's say you have data T_1, T_2, …, T_n at the points x_1, x_2, … x_n and expect the data to fit a function of the form:

$$T = c_a + c_b g_b(x) + c_c g_c(x) + ...$$

- Here, g_b, g_c ,… can be any "well-behaved" functions. For polyfit, they have to be of the form x^n (with n an integer)

- As needed for *linear* least squares, the parameters c_a, c_b, … appear in a linear form

- Substituting each of the data points into the functional form (for the case with three parameters), we expect:

$$\begin{bmatrix} 1 & g_b(x_1) & g_c(x_2) \\ 1 & g_b(x_2) & g_c(x_2) \\ \vdots & \vdots & \vdots \\ 1 & g_b(x_n) & g_c(x_n) \end{bmatrix} \begin{bmatrix} c_a \\ c_b \\ c_c \end{bmatrix} \approx \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_n \end{bmatrix}$$

- And we can use linear least-square to find the "best" c_a, c_b, and c_c.

General linear least squares

$$\begin{bmatrix} 1 & g_b(x_1) & g_c(x_2) \\ 1 & g_b(x_2) & g_c(x_2) \\ \vdots & \vdots & \vdots \\ 1 & g_b(x_n) & g_c(x_n) \end{bmatrix} \begin{bmatrix} c_a \\ c_b \\ c_c \end{bmatrix} \approx \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_n \end{bmatrix}$$

- np.linalg.lstsq **requires the** n x 3 **matrix on the left and the** n x 1 **column vector on the right as input**

General linear least squares

- **What does linear least-squares have to do with optimization?**
- **Rewrite matrix "equation" on previous slide as:** $M\mathbf{c} \approx \mathbf{t}$
- **Least-squares problem is:** $\text{Find } \mathbf{c} \text{ such that } \epsilon = (M\mathbf{c} - \mathbf{t})^2 \text{ is } \textit{minimized}$
- **How do we minimize this?**

General linear least squares

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- Rewrite matrix "equation" on previous slide as: $M\mathbf{c} \approx \mathbf{t}$
- Least-squares problem is: Find $\mathbf{c}$ such that $\epsilon = (M\mathbf{c} - \mathbf{t})^2$ is *minimized*
- How do we minimize this?
- Single-variable calculus: set derivative with respect to c to zero, and check that the second derivative at the minimum is positive
- Generalizing to n-dimensions:

$$\begin{aligned} \epsilon &= (M\mathbf{c} - \mathbf{t})^T (M\mathbf{c} - \mathbf{t}) \\ &= \mathbf{c}^T M^T M\mathbf{c} - 2\mathbf{c}^T M^T \mathbf{t} + \mathbf{t}^T \mathbf{t} \\ \frac{\partial \epsilon}{\partial \mathbf{c}^T} &= 2M^T M\mathbf{c} - 2M^T \mathbf{t} \end{aligned}$$

General linear least squares

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- Now setting the derivative to zero, c must satisfy: $M^T M\mathbf{c} = M^T \mathbf{t}$
- All linear least-squares routines are solving this system of equations.
  - Routines for nonlinear least squares are also available

Optimization: basic ideas

- For linear least squares, we don't need to check the second derivative (due to the general "shape" of norms like ε).
- For more general functions it is (often) useful to look at the second derivative
- Consider "general" optimization problem:

Find $\mathbf{x}$ so that $f(\mathbf{x})$ is minimized

- To start, consider behavior near minimizing point, x*
  - In 1-D: $f(x^* + h) = f(x^*) + \frac{df}{dx}|_{x^*} h + \frac{d^2 f}{dx^2}|_{x^*} \frac{h^2}{2} + O(h^3)$

  and since the derivative is zero at a minimum:

$$f(x^* + h) = f(x^*) + \frac{d^2 f}{dx^2}|_{x^*} \frac{h^2}{2} + O(h^3)$$

  So, the second derivative must be positive at a minimum (otherwise f is smaller at x*+h than it is at x*)

Optimization: basic ideas

- To start, consider behavior near minimizing point, x*
  - In 1-D: $f(x^* + h) = f(x^*) + \frac{d^2 f}{dx^2}|_{x^*} \frac{h^2}{2} + O(h^3)$
  - Now in n-dimensions:

$$f(x_i^* + h_i) = f(x_i^*) + \sum_{j=1}^{n} \frac{\partial f}{\partial x_j}|_{x_i^*} h_j + \sum_{j=1}^{n} \sum_{k=1}^{n} \frac{\partial^2 f}{\partial x_j x_k}|_{x_i^*} \frac{h_j h_k}{2} + O(|h|^3)$$

or in vector notation:

$$f(\mathbf{x}^* + \mathbf{h}) = f(\mathbf{x}^*) + \mathbf{h}^T \nabla f|_{\mathbf{x}^*} + \frac{1}{2}\mathbf{h}^T H|_{\mathbf{x}^*}\mathbf{h} + O(|h|^3)$$

Here, H is the ***Hessian***, $H_{j,k} = \frac{\partial^2 f}{\partial x_j x_k}$, a n x n symmetric matrix.

- At the minimum, the ***gradient***, is zero, so we have:

$$f(\mathbf{x}^* + \mathbf{h}) = f(\mathbf{x}^*) + \frac{1}{2}\mathbf{h}^T H|_{\mathbf{x}^*}\mathbf{h} + O(|h|^3)$$

- The Hessian must be positive for any (small) h

Optimization: basic ideas

- All optimization routines require the user to specify the function to be minimized (usually called the *cost* function or the *objective* function)
- Most optimization routines use the gradient to search for a minimum (starting from an user-specified “guess”)
- Some routines use the Hessian, some don’t.

Optimization: basic ideas

- All optimization routines require the user to specify the function to be minimized (usually called the *cost* function or the *objective* function)
- Most optimization routines use the gradient to search for a minimum (starting from an user-specified "guess")
- Some routines use the Hessian, some don't
- Today, we'll look at two methods:

  1. (Truncated) Newton's method: uses gradient and Hessian
  2. BFGS method: uses gradient

Newton's method

- **Classical method:**
  1. **Evaluate function, gradient and Hessian at a guess, x_0**
  2. **Use these values to fit a quadratic to the function:**

$$g(\mathbf{h}) = f(\mathbf{x}_0) + \mathbf{h}^T \nabla f|_{\mathbf{x}_0} + \tfrac{1}{2}\mathbf{h}^T H|_{\mathbf{x}_0}\mathbf{h}$$

  3. **Setting** $\frac{\partial g}{\partial \mathbf{h}} = 0$ **:**

$$H|_{\mathbf{x}_0}\mathbf{h} = -\nabla f|_{\mathbf{x}_0}$$

  4. **This can be solved for h and the new guess for the minimum is then:** $x_1 = x_0 + h$

- **Classical method only works well if guess is good**

- **In practice, a quadratic fit may be inaccurate or inappropriate**
  - **Truncated-Newton and BFGS methods both address this**

Truncated Newton's method

- **Classical method:**
  1. **Evaluate function, gradient and Hessian at a guess, x_0**
  2. **Use these values to fit a quadratic to the function:**

$$g(\mathbf{h}) = f(\mathbf{x}_0) + \mathbf{h}^T \nabla f|_{\mathbf{x}_0} + \tfrac{1}{2}\mathbf{h}^T H|_{\mathbf{x}_0}\mathbf{h}$$

  3. **Setting** $\frac{\partial g}{\partial \mathbf{h}} = 0$ **:**

$$H|_{\mathbf{x}_0}\mathbf{h} = -\nabla f|_{\mathbf{x}_0}$$

  4. **This can be solved for h and the new guess for the minimum is then:**

$x_1 = x_0 + h$

Truncated approach:

1. **Iteratively solve for h as in the classical approach (but truncate iterations if local curvature is negative)**
2. **Then search in the direction of h for the minimum along this direction**

- **Step 2 is called a *line search*, idea is similar to finding the zero of a 1-d function (e.g. Newton-Rhapson, secant, Brent methods)**

Optimizers in Scipy

- **We will use the** scipy.optimize **package**
- **And particularly, the function,** scipy.optimize.minimize
- **The optimization *method* can be specified when calling this function, e.g.:**

  method = 'Newton-CG'

- **This will use truncated Newton's method**
- **The CG indicates the conjugate gradient method is used to solve for** h
- **There is a separate CG method for optimization**

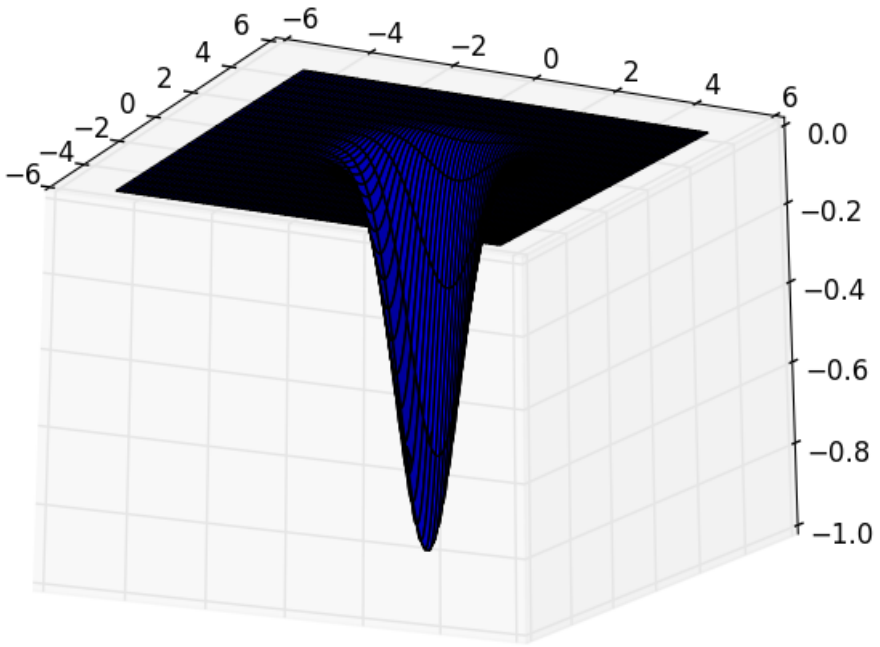
Optimizers in Scipy

- Newton-CG **requires the user to specify:**
  - **A python function which computes the cost function**
  - **A function for computing the gradient**
  - **A function for computing the Hessian (or instruct the optimizer to approximate it)**
  - **A guess,** x0**, where the optimizer starts its search for a minimum**

Simple example

- **Simple illustrative example:**

Find x and y that minimize $f = -exp(-\alpha(x - x_0)^2 - \beta(y - y_0)^2)$



Simple example

The code, *gauss2d.py*, applies a few different approaches to this problem

- **It has three functions:** gauss2d, gauss2d_grad, gauss2d_hess
- gauss2d_grad **returns the two components of the gradient:**

$$\nabla f = (\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}) = (-2\alpha(x - x_0)f, -2\beta(y - y_0)f)$$

- gauss2d_hess **returns the 2 x 2 Hessian matrix:**

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y \partial y} \end{bmatrix} = \begin{bmatrix} -2\alpha(f + (x - x_0)\frac{\partial f}{\partial x}) & 4\alpha\beta(x - x_0)(y - y_0)f \\ 4\alpha\beta(x - x_0)(y - y_0)f & -2\beta(f + (y - y_0)\frac{\partial f}{\partial y}) \end{bmatrix}$$

- **The minimizer is called near the bottom with different inputs**

Simple example

- **The code, *gauss2d.py*, applies a few different approaches**
- **Let's first look at the Newton-CG, approximate gradient case (ncg1=True)**
- **The call to the minimizer is:**

```
minimize(gauss2d,xguess,args=parameters,method='Newton-CG',jac=gauss2d_grad)
```

Note: since the name of the Hessian function is not specified, it is approximated from the gradient

Simple example

- **Running the code:**

```
In [44]: run gauss2d
Gauss2d, Newton-CG, approximate Hessian
optimum: [ 0.5   0.25]
info:    status: 0
 success: True
    njev: 17
    nfev: 6
     fun: -1.0
       x: array([ 0.5 ,  0.25])
 message: 'Optimization terminated successfully.'
    nhev: 0
     jac: array([ -5.37315725e-09,  -2.68657863e-09])
```

Notes:

- gauss2d **sets (**x0,y0**) to (**0.5,0.25**) so the answer is correct**
- **17 gradient evaluations and 6 function evaluations were needed**
- **What happens if we now specify the exact Hessian (ncg2=True)?**

Simple example

Running the code with:

minimize(gauss2d,xguess,args=parameters,method='NewtonCG',
jac=gauss2d_grad,hess=gauss2d_hess)

```
Gauss2d, Newton-CG, exact Hessian
optimum: [ 0.5   0.25]
info:    status: 0
 success: True
    njev: 9
    nfev: 6
     fun: -1.0
       x: array([ 0.5 ,  0.25])
 message: 'Optimization terminated successfully.'
    nhev: 4
     jac: array([ -2.28865316e-09,  -1.14432658e-09])
```

Notes:

- **The number of gradient evaluations reduced from 17 to 9**
- gauss2d **also has options for BFGS and Nelder-Mead methods – how do these work?**

Overview of BFGS

- BFGS is generally the method-of-choice for unconstrained optimization problems involving smooth functions
- Works surprisingly well for non-smooth/noisy functions as well
- Can be memory-intensive, use L-BFGS-B for large problems
- Motivating idea:
  - Computing and inverting the Hessian can be very expensive
  - Instead, approximate the (inverse) Hessian, and update this approximation at each step (quasi-Newtonian methods)

Overview of BFGS

- **Motivating idea:**
  - **Computing and inverting the Hessian can be very expensive**
  - **Instead, approximate the (inverse) Hessian, and update this approximation at each step (quasi-Newtonian methods)**
- **Newton-CG:**

1. **Solve for** h: $H|_{\mathbf{x}_0}\mathbf{h} = -\nabla f|_{\mathbf{x}_0}$
2. **Search along direction of** h **for minimum →** x_1 **and repeat step 1**

- **BFGS:**

1. **Approximate inverse Hessian and solve for** h: $M^i \approx H^{-1}$, $\mathbf{h} = -M^i \nabla f|_{\mathbf{x}_i}$
2. **Similar to Newton-CG**
3. **Update** M: $M^{i+1} = f(M^i, h)$

- **The update should result in a positive-definite (approximate) Hessian, and the BFGS update formula produces particularly good results**

- **Now back to** *gauss2d*

Simple example -- BFGS

Results for BFGS with approximate gradient

minimize(gauss2d,xguess,args=parameters,method='BFGS',jac=False)

```
Gauss2d, BFGS, approximate gradient
optimum: [ 0.49999556  0.24999778]
info:     status: 0
  success: True
     njev: 5
     nfev: 20
 hess_inv: array([[ 0.60077592, -0.19961208],
       [-0.19961208,  0.90019394]])
      fun: -0.9999999999753861
        x: array([ 0.49999556,  0.24999778])
  message: 'Optimization terminated successfully.'
      jac: array([ -8.85874033e-06,  -4.43309546e-06])
```

Simple example -- BFGS

Results for BFGS with exact gradient

minimize(gauss2d,xguess,args=parameters,method='BFGS',jac=gauss2d_grad)

```
Gauss2d, BFGS, exact gradient
optimum: [ 0.49999557  0.24999779]
info:     status: 0
  success: True
     njev: 5
     nfev: 5
 hess_inv: array([[ 0.60077589, -0.19961205],
       [-0.19961205,  0.90019397]])
      fun: -0.9999999999754784
        x: array([ 0.49999557,  0.24999779])
  message: 'Optimization terminated successfully.'
      jac: array([ -8.85828506e-06,  -4.42914253e-06])
```

Notes:

1. **BFGS requires less function, gradient evaluations than Newton-CG**
2. **For large (slow) problems, specifying the gradient (and Hessian if appropriate) can make a big difference**