Minimization and Curve Fitting with SciPy

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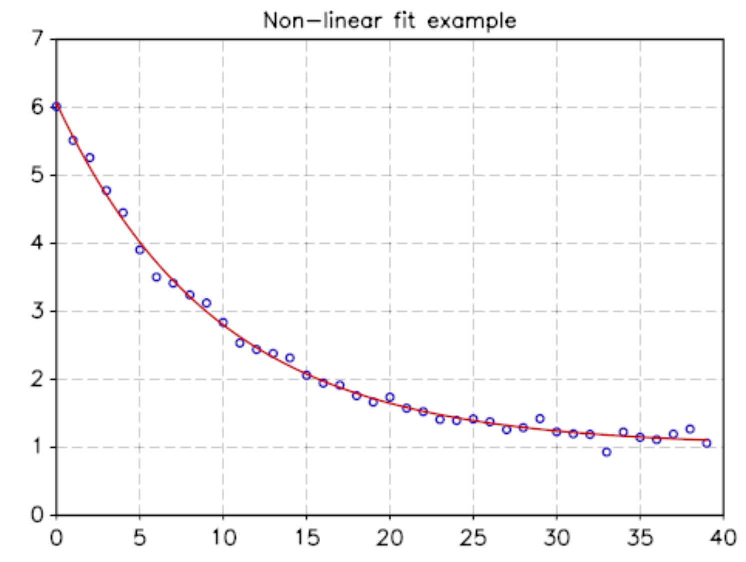
Why is this important

- Mathematical optimization underlies many machine learning algorithms
  - Need to know how to do deal with exceptionally circumstances
- Provides techniques for data exploration

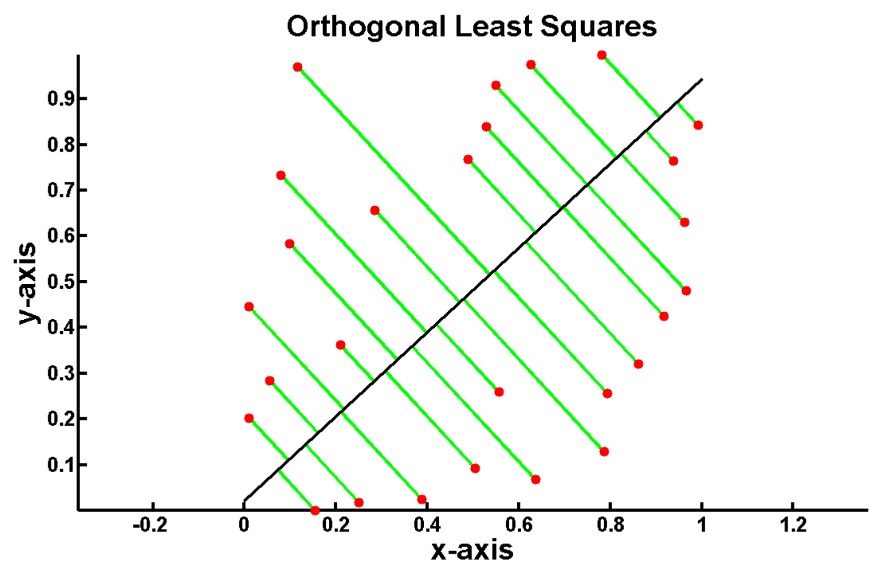
Curve Fitting

- Want to construct a curve (mathematical function) that best fits a series of data points
  - First, need to select a model: what type of curve?
  - Then, need to determine how we measure fit
    - Examples:
      - y-values:



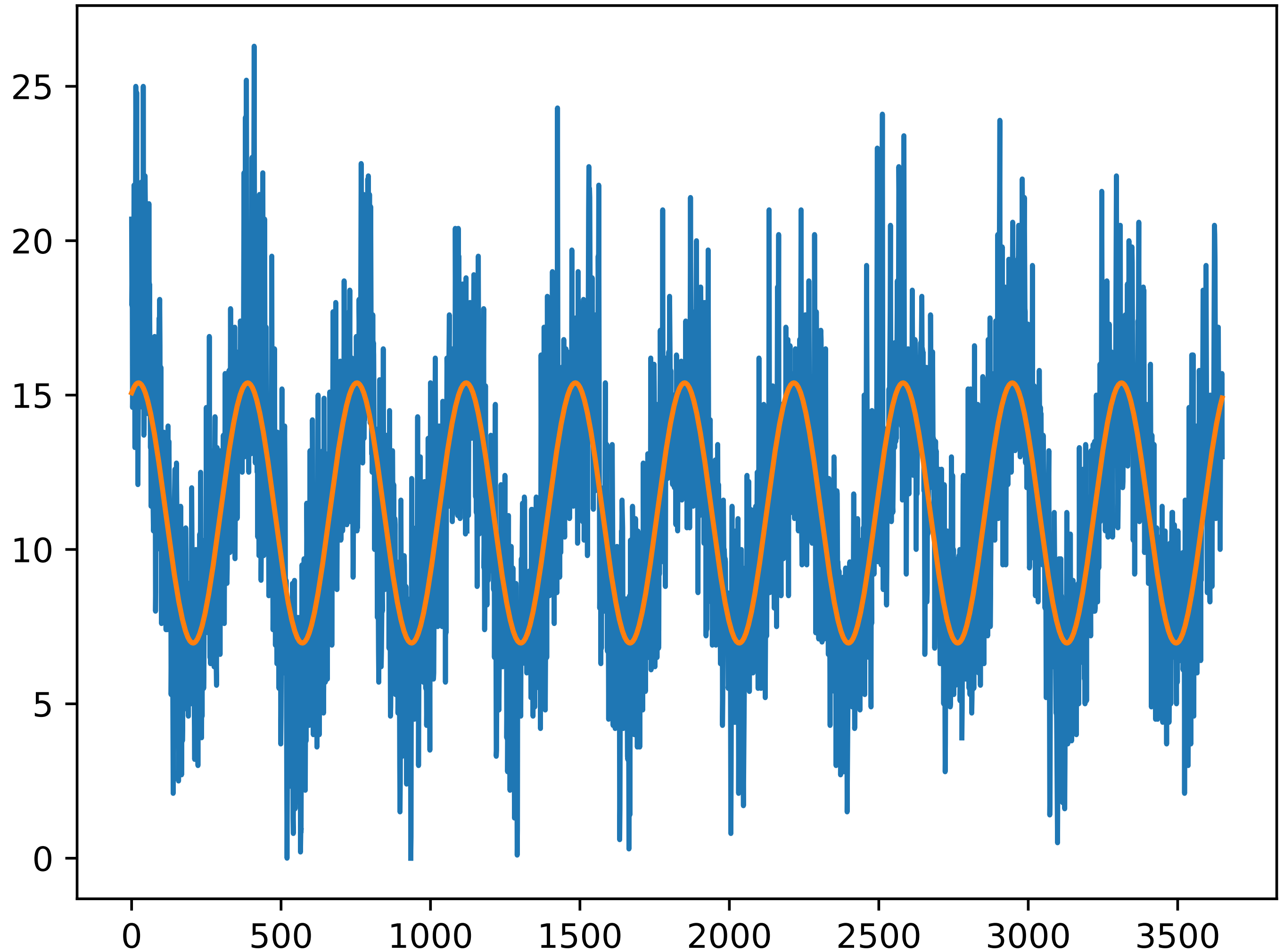
$$L(y, \hat{y}) = \sum_{\nu=1}^{n} (y_i - \hat{y}(i))^2 \rightarrow \min$$

      - orthogonal least squares



Curve Fitting

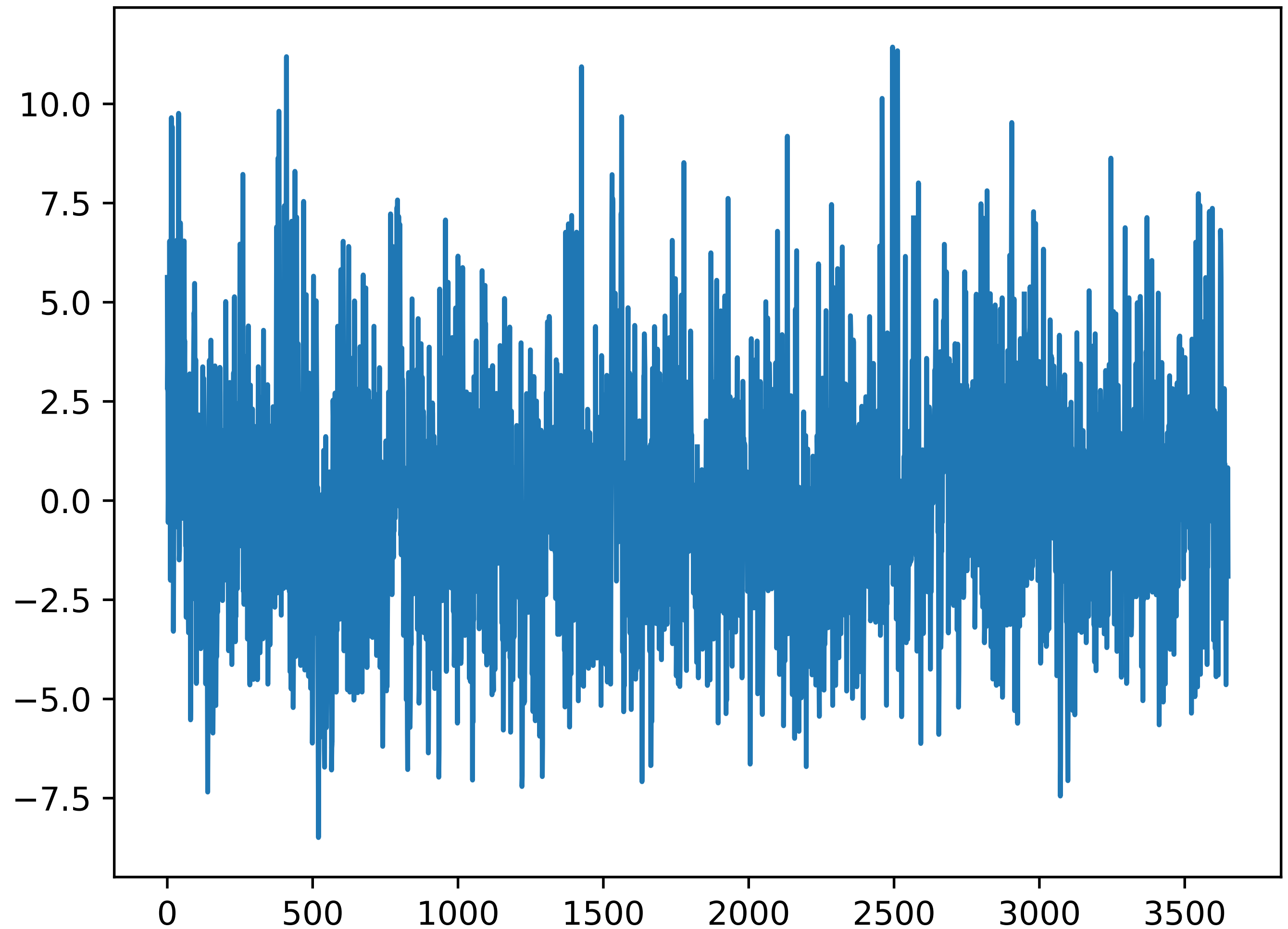
- Example: Fit a sine curve to meteorological data
  - Minimum daily temperatures in Melbourne



$$f_{\alpha,\beta,\gamma,\delta}(t) = \alpha + \beta \sin(\gamma t + \delta)$$

Curve Fitting

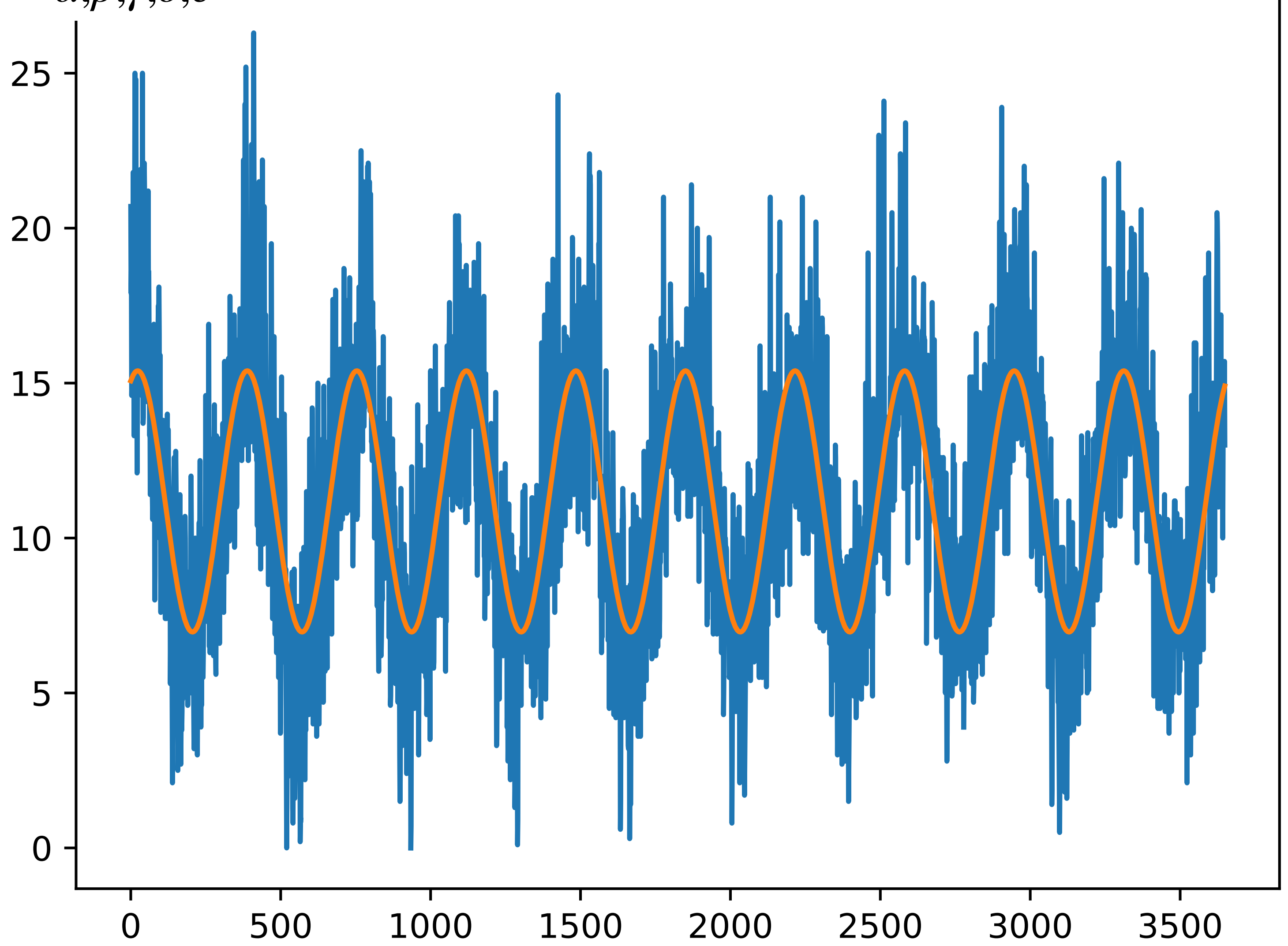
- The data after removing the sine curve shows a seemingly random time series with just a little bit of seasonality



Curve Fitting

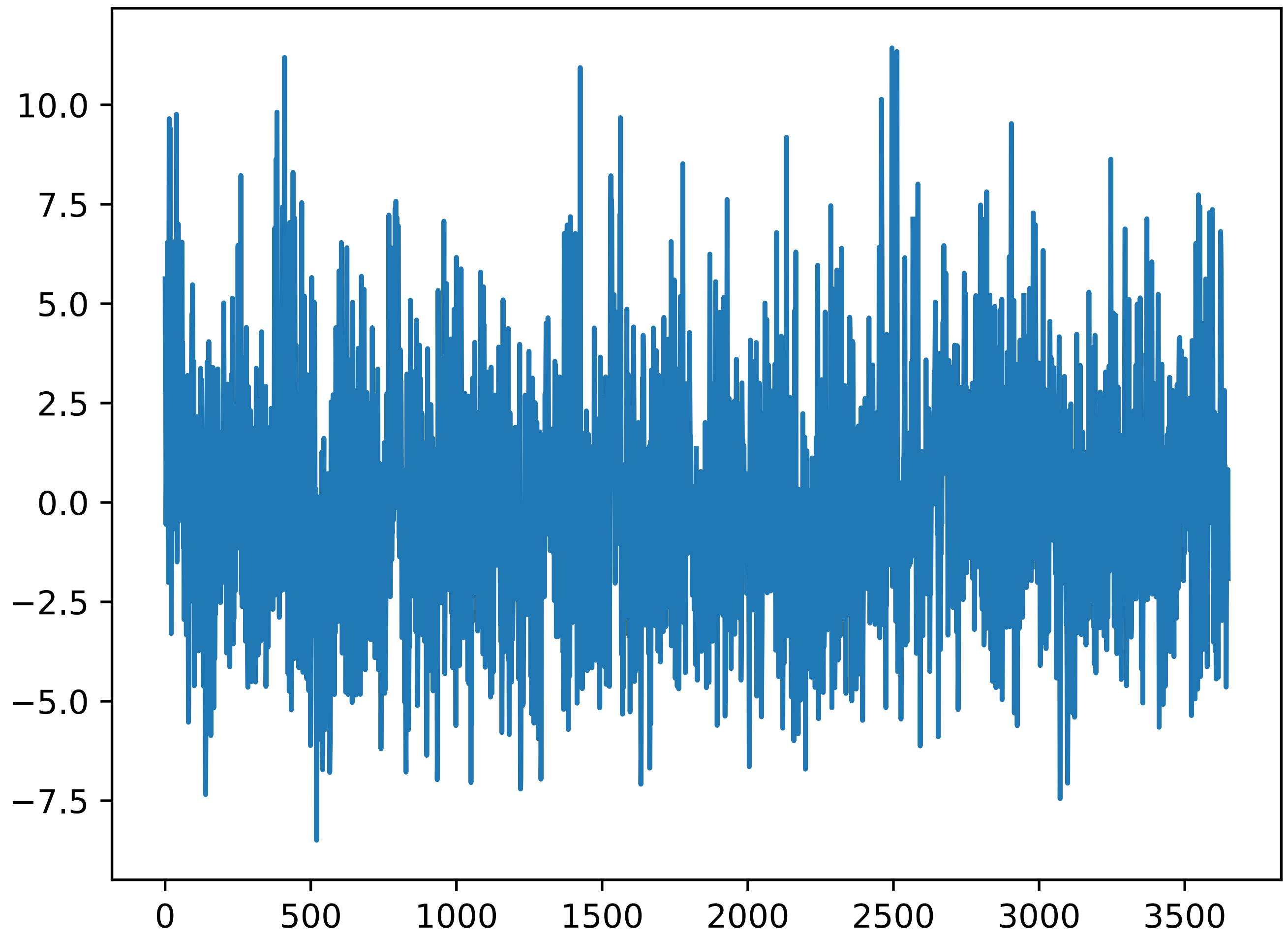
- We can do better by including a cos (which is just a second sine)

$$f_{\alpha,\beta,\gamma,\delta,\epsilon}(t) = \alpha + \beta \sin(\gamma t + \delta) + \epsilon \cos(\gamma t + \delta)$$



Curve Fitting

- Residual:
  - Looks slightly better?



Curve Fitting

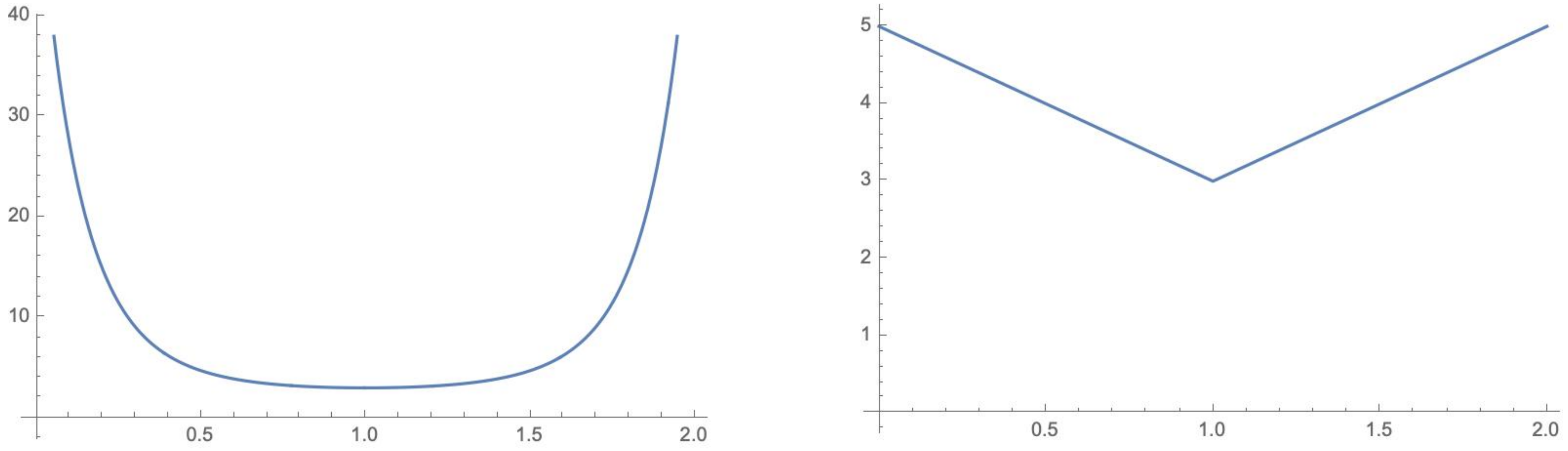
- Find the parameters that minimize the squared difference between function and model
  - This is a minimization problem
- Too general a model:
  - Optimization can be very difficult and lengthy
  - Overfit: The result matches the test set, but not the future
- Not general a model
  - Fit is not good, therefore no strong predictions either

Program

- Need to learn about minimization
  - One dimensional methods: Minimization along a line
  - Gradient Descent Methods
  - Minimization for Sums of Squares
  - Curve-fitting

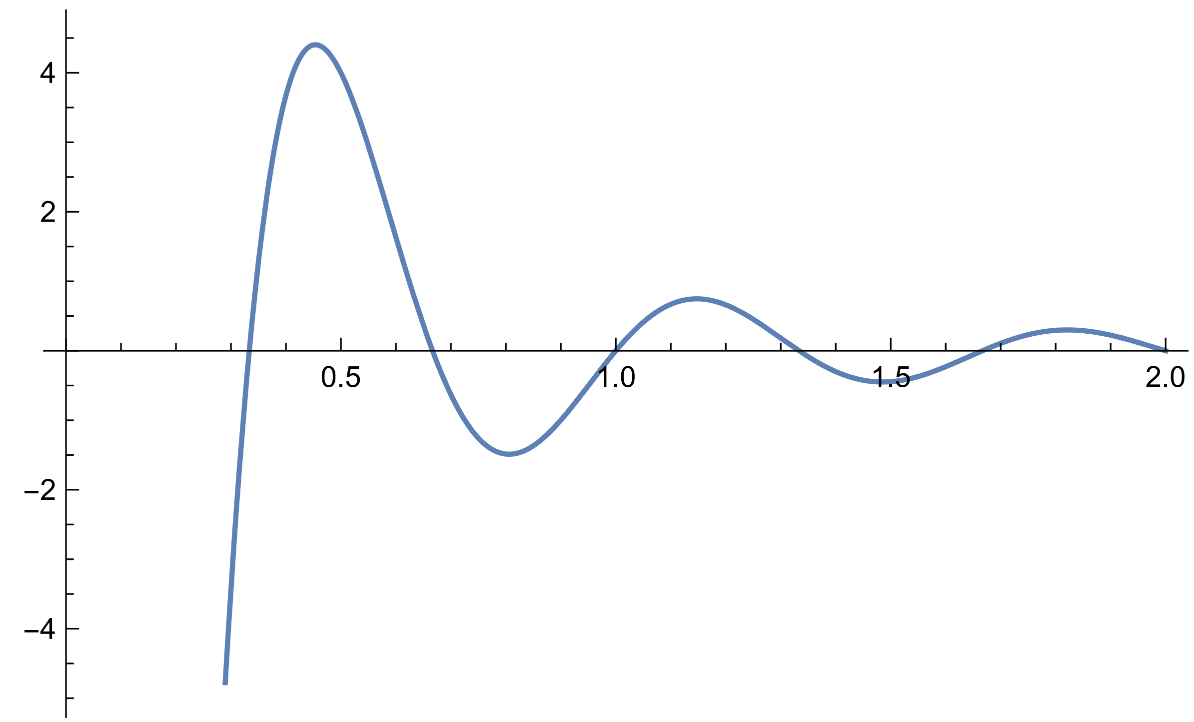
Minimization

- Functions can be smooth and non-smooth



Minimization

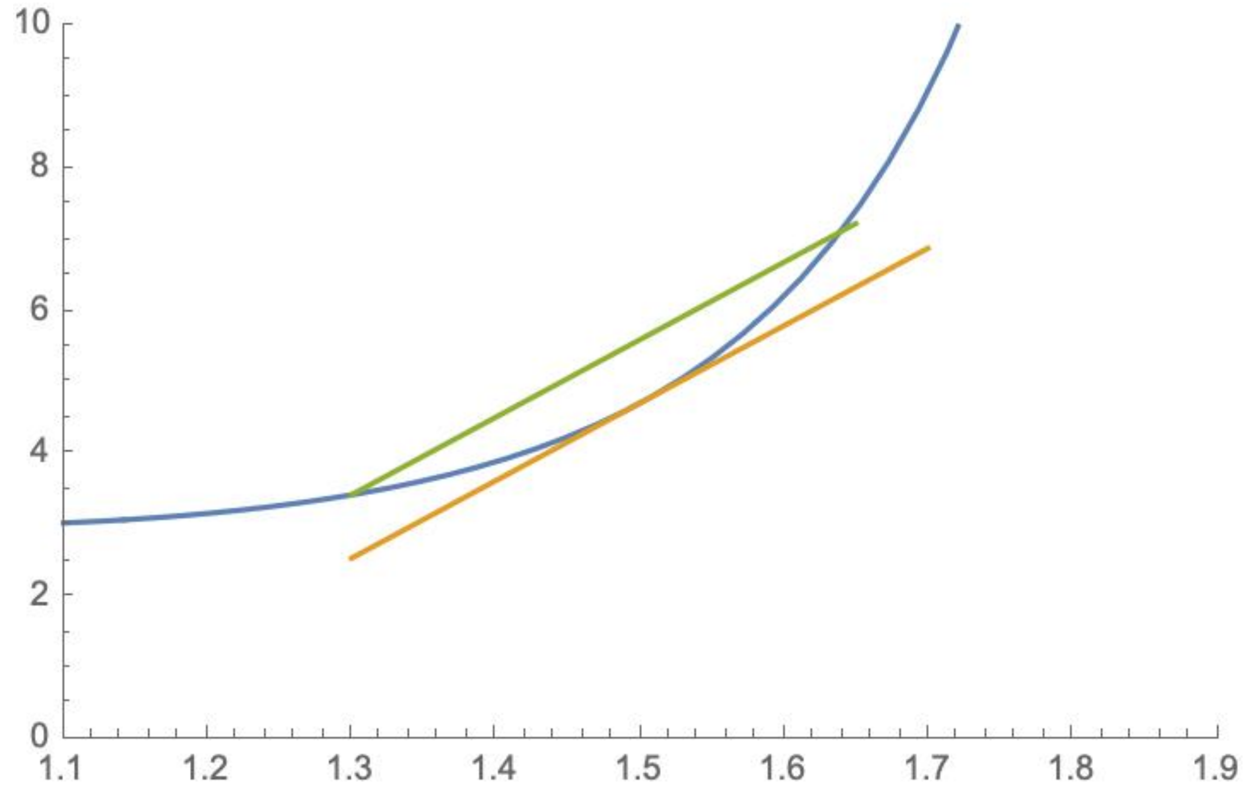
- Given a function $\mathscr{R}^n \rightarrow \mathscr{R}$
    - Find a minimum



- Potential problems:
    - Minimum might not exist
    - Minimum might be local

Minimization

- Convex functions: For $t \in [0,1]$:
  - $f(\overrightarrow{a} + t(\overrightarrow{b} - \overrightarrow{a})) \leq f(\overrightarrow{a}) + t(f(\overrightarrow{b}) - f(\overrightarrow{a}))$
  - Tends to be easy
  - Relative minimum is unique



Scalar Minimization

- Minimum implies derivatives vanish
  - Can use the derivatives to guide us to the minimum
  - Can be done by using bisection:
    - Find two points a, b such that $f(a)$ and $f(b)$ have different signs
    - Then there is a zero between a, b
    - Can evaluate function at $\frac{a+b}{2}$
  - Can be done using the secant method
    - Find two points a, b such that $f(a) \neq f(b)$, but both values have the same sign
    - Use the slope in order to guess a zero
  - Brent's method combines both with quadratic interpolation

Scalar Minimization

- Brent's method is the default for scipy:
  - Optimizing a curvy function

```
from scipy import optimize
import numpy as np
from matplotlib import pyplot as plt

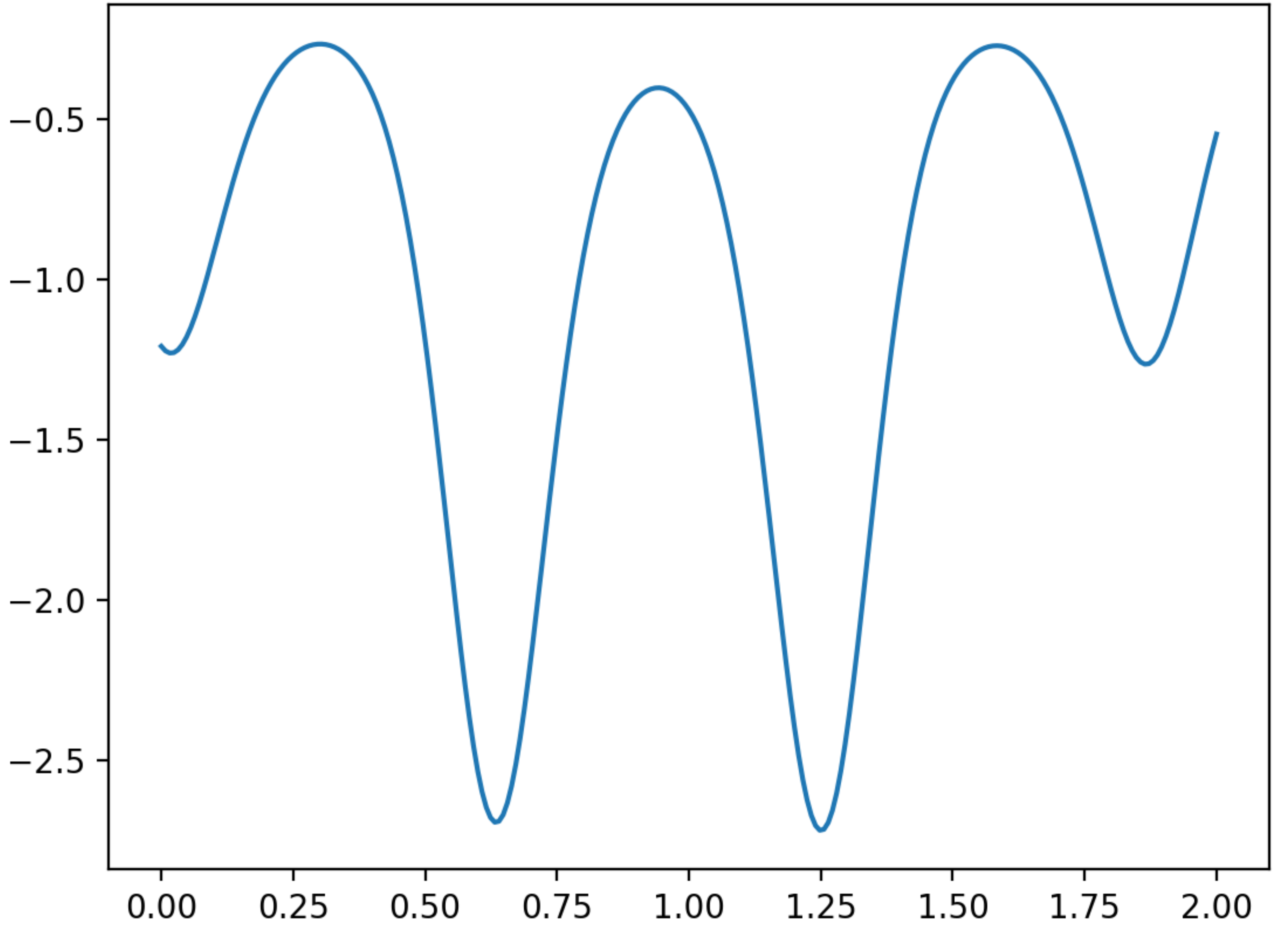

def f2(x):
    return -np.exp(-(x-.9)**2+0.1*x+np.cos(10*x))
```

Scalar Minimization

- Show:

```
def show(f):
    x = np.linspace(0,2,251)
    y = f(x)
    plt.plot(x,y)
    plt.show()
```

Scalar Minimization



Scalar Minimization

- Brent's method is the default

```
from scipy import optimize

result = optimize.minimize_scalar(f2)


>>> result>>> result
     fun: -2.7191461357325406
 message: 'Solution found.'
    nfev: 12
  status: 0
 success: True
       x: 1.2506211193351628
```

Scalar Minimization

- Bounded Brent method

```
result = optimize.minimize_scalar(f2, bounds=(0,2),
method='bounded')
```

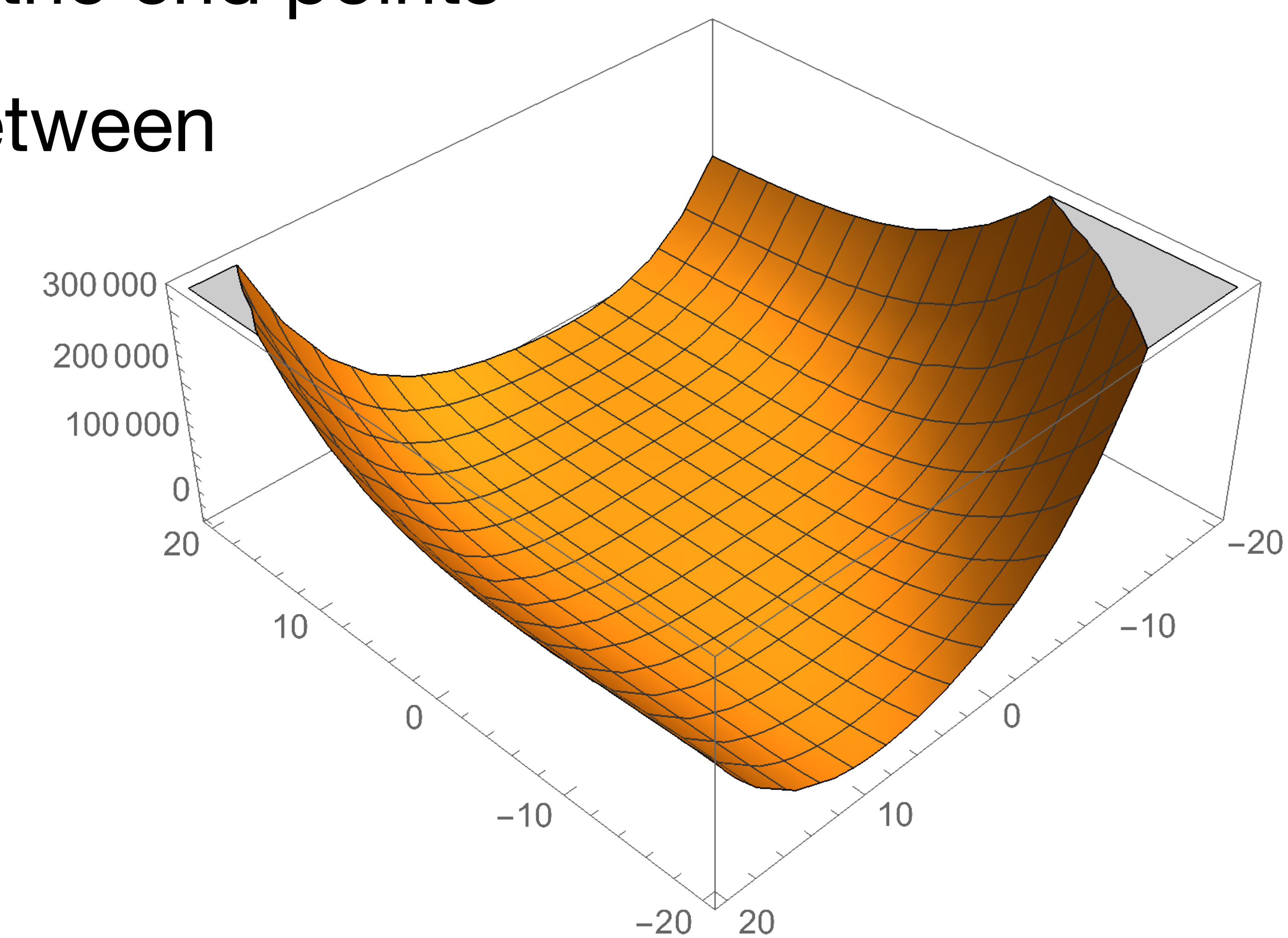
```
>>> result
     fun: -2.7191461357325406
 message: 'Solution found.'
    nfev: 12
  status: 0
 success: True
       x: 1.2506211193351628
```

Minimization

- Smooth functions are (usually) easier than non-smooth functions
  - Exception: Linear systems with constraints —> Linear Programming

Minimization

- Minimization is easier for convex functions
  - Take a line segment $[a, b]$
  - Values are higher on the end points
  - Than on points in between

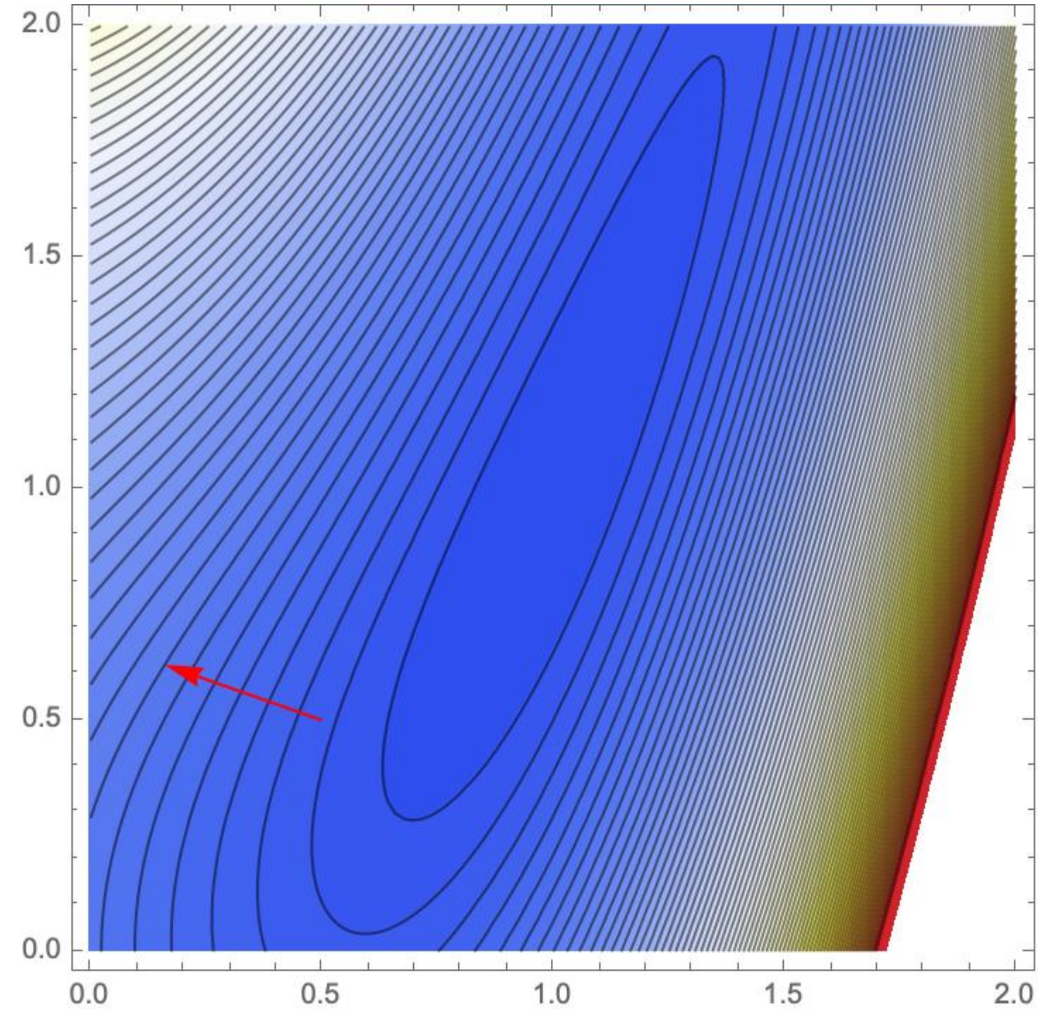


Minimization

- Gradient $\nabla f = (\frac{df}{dx_1}, \frac{df}{dx_2}, \frac{df}{dx_3}, \ldots, \frac{df}{dx_n})$ is always in the direction of greatest increase of a function

Minimization

- Example: Rosenbrock Function
  - $f(x, y) = 1.2(y - x^2)^2 + 1.1(1 - x)^2$
  - Gradient is $(-2.2(1 - x) - 4.8x(-x^2 + y), 2.4(-x^2 + y))$
  - Contour graph is



Minimization

- Descent Methods:

1. Choose a starting point $x_0 \in \mathscr{R}^n$
2. If $\|\nabla f(x_k)\| < \epsilon$ declare victory and return x_k
3. Pick a search direction $d_k \in \mathscr{R}^n$ s.t. $\nabla f(x_k) \cdot d_k < 0$
4. Choose a step size $\alpha_k > 0$ s.t. $f(x_k + \alpha_k d_k) < f(x_k)$
5. Set $x_{k+1} = x_k + \alpha_k d_k$. Go to 2

Minimization

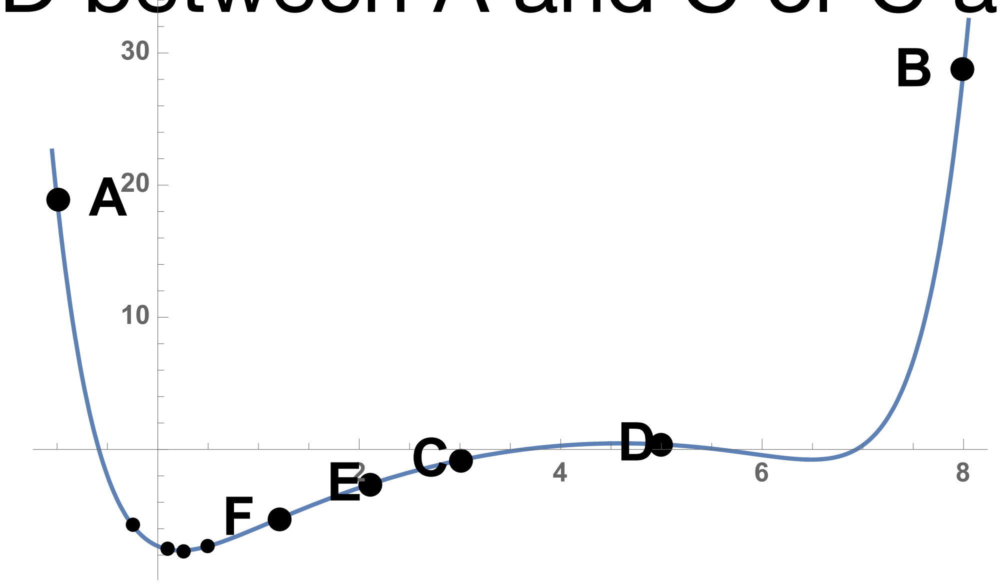
- This algorithm leaves two things open:
  - Selecting the step length α_k
  - Selecting the search direction d_k

Minimization

- Finding minimum along line:
  - Finding minimum of function $t \mapsto f(x_k + td_k)$
  - Use derivative is usually dangerous:
    - Often function too flat
    - Better bracketing

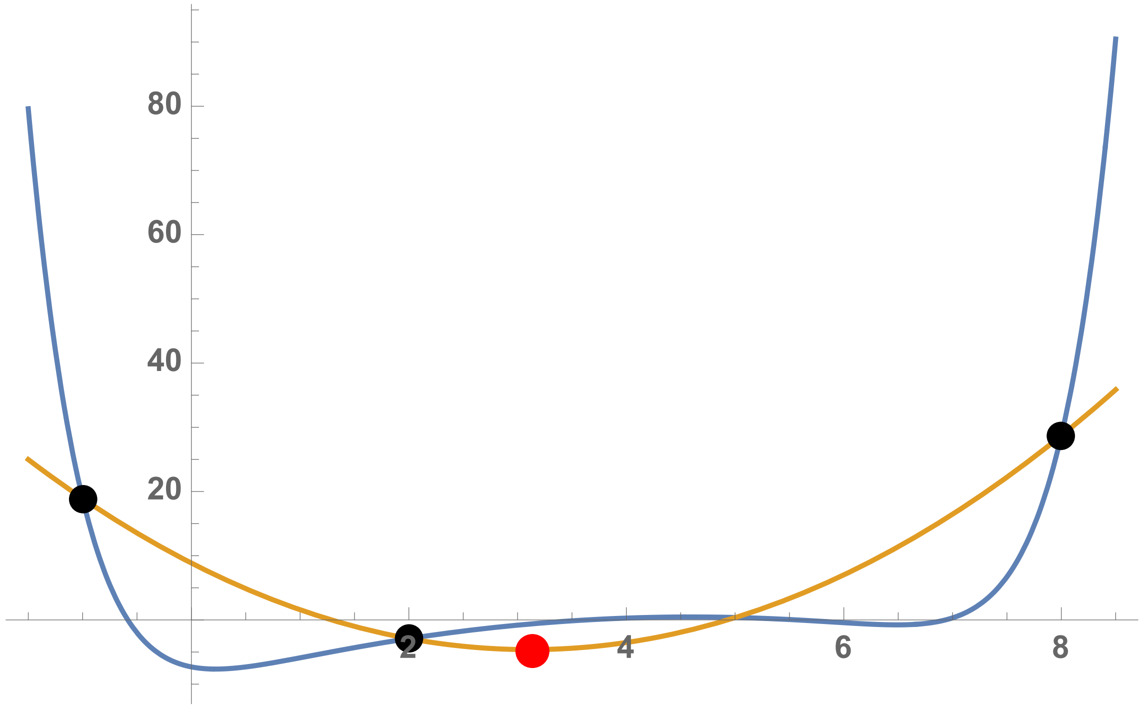
Minimization

- Can use bracketing
  - Three points A < C < B such that $f(A) > f(C) < f(B)$
    - Thus, minimum guaranteed to exist
    - Now find another point D between A and C or C and B
    - Get a new bracket



Minimization

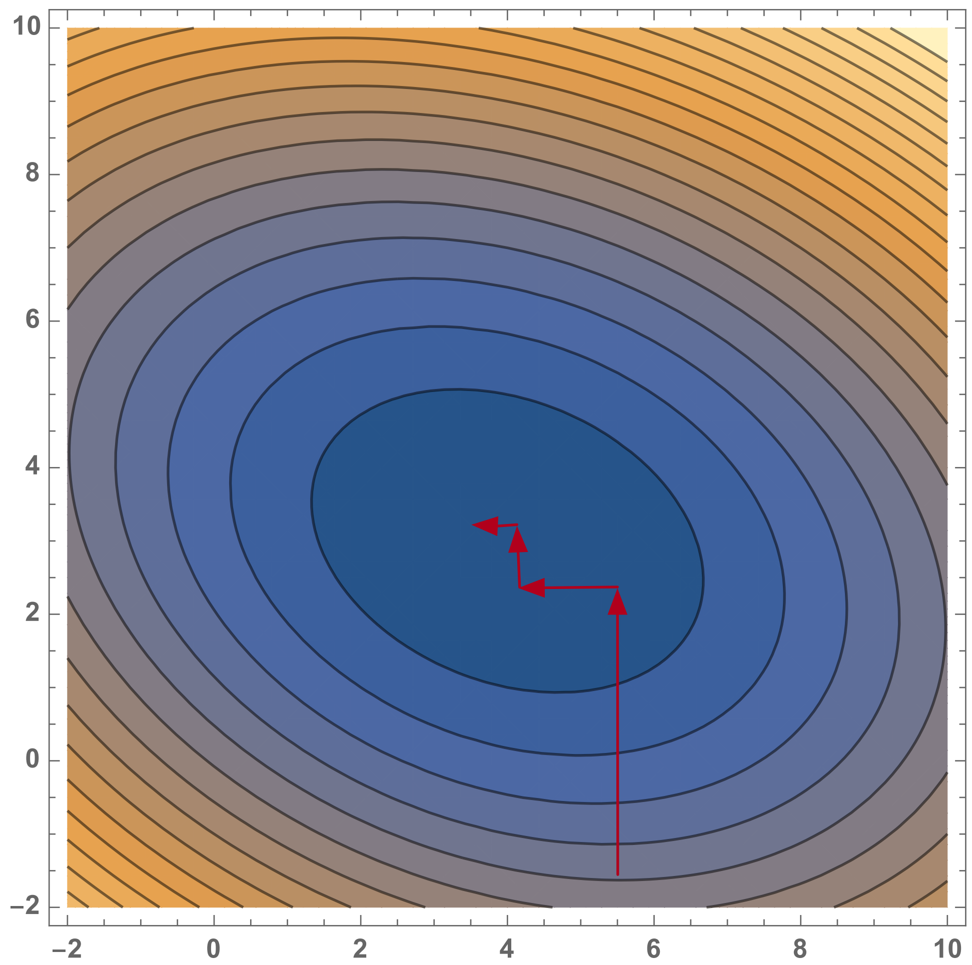
- One possibility: golden ratio: $\dfrac{|A-C|}{|A-B|} = \dfrac{|B-C|}{|A-C|}$
- Other possibility: parabolic approximation
- Or a combination of both

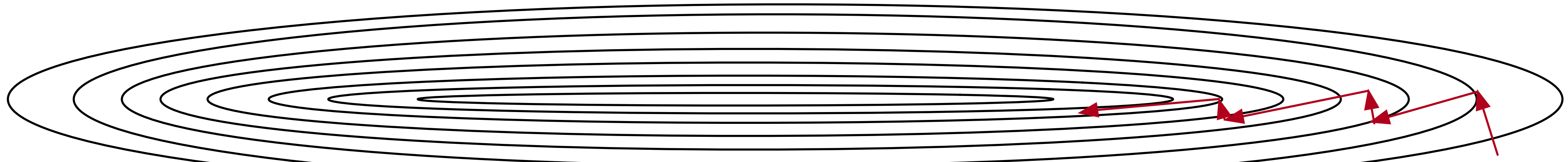


Minimization

- Determining direction:
  - Can use coordinates

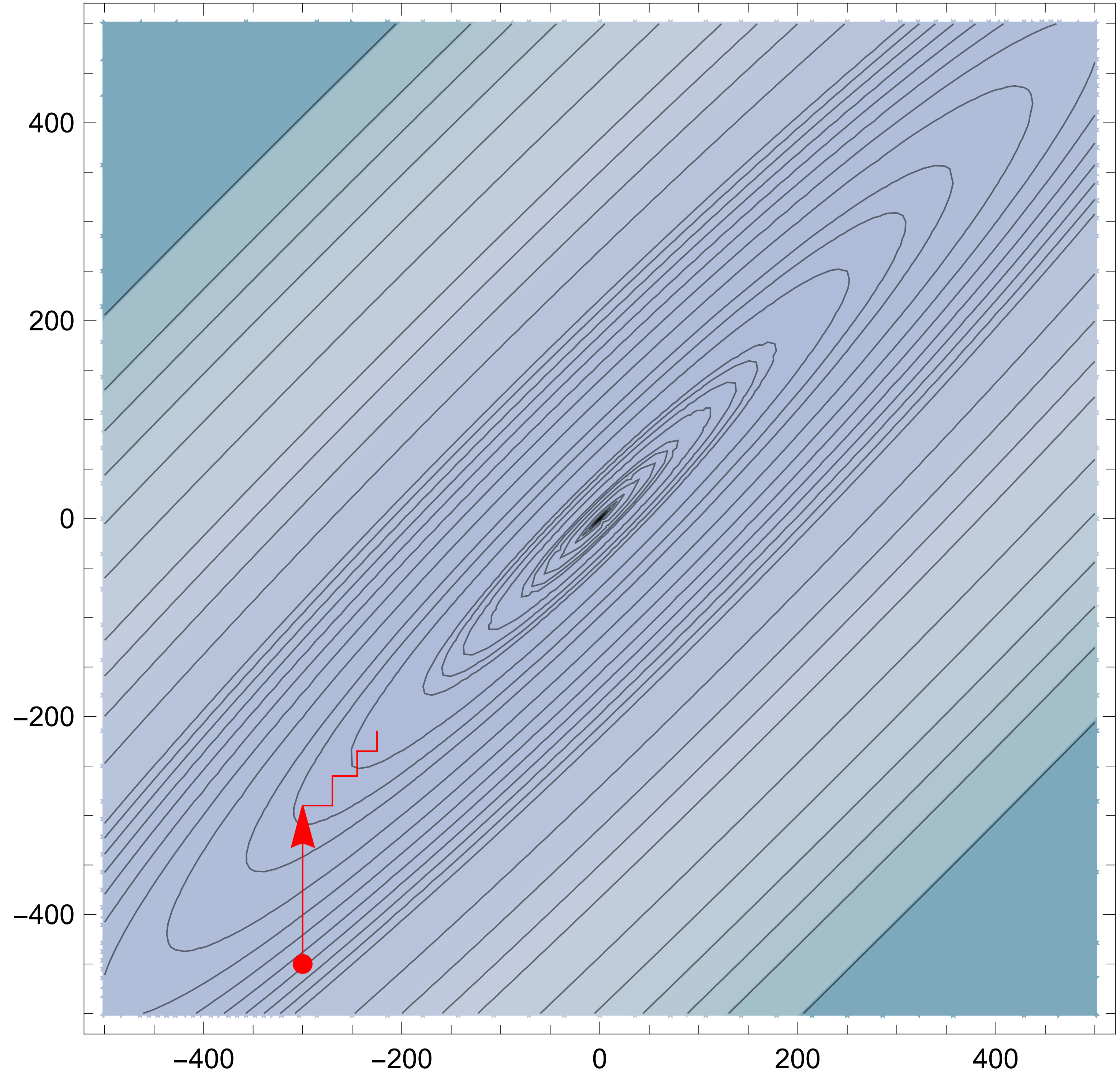
Minimization





Minimization

- Using coordinates
  - Make little progress per iteration



Minimization

- Better use orthogonal directions:
  - otherwise we partially undo the previous steps
- Possibilities
  - Canonical Directions
  - Steepest Descent (Cauchy)
    - badly affected by round-off errors and subject to zigzagging
  - Powell: Change set of directions every so often

Minimization

- Selecting the step length
  - Finding the best step length is laborious
  - Often do better by guessing
  - Many machine learning algorithms use a steadily declining α
    - Trying out several guesses

Minimization

- Newton Methods:
  - Repeatedly replace condition $\nabla f(x) = 0$ by a sequence of linear problems
  - Newton-Raphson:
    - apply **exact** Newton steps
- possibly does not converge
- works best for convex functions
  - Use linear-search descent, then switch to Newton

Minimization

- Numerical minimization of a cost function of the parameters
  - Various minimization methods
    - Line methods
      - Minimize along a particular line

Minimization

- Instead of line searches: **Trust Region Methods**
  - **Idea:** for each iteration: replace f with a **quadratic model function**
    - Quadratic model function approximates f in the "trust region"
    - And quadratic model functions are easy to minimize!
    - The proposed solution can or cannot have a smaller value for f
    - Many different ways of defining the model

Minimization with SciPy

- Can use a number of method for finding a local minimum
  - Some need the Jacobian and some need in addition the Hessian
  - Can be calculated numerically but results are better with exact functions
  - Jacobian $\mathbf{J}(f) = \frac{df}{dx} = (\frac{\delta f}{\delta x_1}, \frac{\delta f}{\delta x_2}, \ldots, \frac{\delta f}{\delta x_n})$
  - Hessian $\mathbf{H}(f) = \left(\frac{\delta^2 f}{\delta x_i \delta x_j}\right)_{i,j}$

Minimization with SciPy

- Use scipy.optimize.minimize
  - Needs a function that is a one-dimensional np.array
  - Specify a starting point, options, and method

Minimization with SciPy

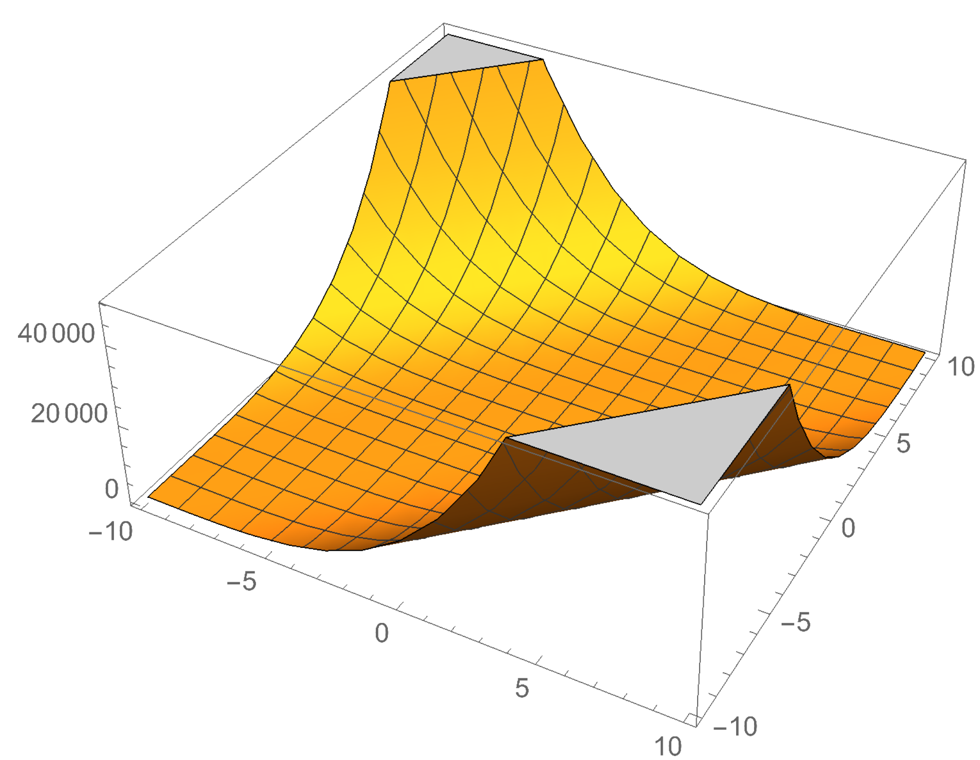
- Importing the optimizer:

```
import numpy as np
from scipy.optimize import minimize
```

Minimization with SciPy

- Defining a function to be minimized
  - Needs to be in "standard form", i.e. numpy array of one dimension

```
def func(x):
    return np.sin(x[0]*x[1])+(x[0]+x[1]-1)**2+(x[0]-x[1]+1)**4
```



Minimization with SciPy

- Sometimes need to give Jacobian
- ```
  def jacob(x):
      return np.array(
        (4*(1+x[0]-x[1])**3 +
         2*(x[0]+x[1]-1)+
         x[1]*np.cos(x[0]*x[1]),
         -4*(1+x[0]-x[1])**3 +
         2*(x[0]+x[1]-1)+
         x[0]*np.cos(x[0]*x[1])) )
  ```
  ```

Minimization with SciPy

- We pick (5,5) as the starting point

```
res = minimize(func,
               [5,5],
               method = 'nelder-mead',
               options = {'xatol': 1e-9, 'disp':True}
               )

print(res.x)
```

Minimization with SciPy

- Success: (but with lots of function evaluations)

```
Optimization terminated successfully.
         Current function value: -0.295490
         Iterations: 84
         Function evaluations: 164
[-0.37249737  1.18821832]
```

Minimization with SciPy

```
res = minimize(func,
               [5,5],
               method = 'Newton-CG',
               jac = jacob,
               options = {'disp':True}
               )
print(res.x)
```

Minimization with SciPy

```
Optimization terminated successfully.
         Current function value: -0.295490
         Iterations: 10
         Function evaluations: 12
         Gradient evaluations: 47
         Hessian evaluations: 0
[-0.37249737  1.18821832]
```

Minimization with SciPy

```
res = minimize(func,
               [5,5],
               method = 'Powell',
               options = {'disp':True}
               )
print(res.x)
```

Minimization with SciPy

```
Optimization terminated successfully.
         Current function value: -0.295490
         Iterations: 5
         Function evaluations: 139
[-0.37249969  1.18821518]
```

Minimization with SciPy

```
res = minimize(func,
               [5,5],
               method = 'BFGS',
               options = {'disp':True}
               )
print(res.x)
```

Minimization with SciPy

```
Optimization terminated successfully.
         Current function value: -0.295490
         Iterations: 15
         Function evaluations: 84
         Gradient evaluations: 21
[-0.37249848  1.18821848]
```

Least Square Optimization

- For curve fitting, we want to optimize polynomials of degree 2 in several variables
    - Allows using special methods

Least Square Optimization

- Want to minimize a sum of squares
  - $f : \mathscr{R}^n \rightarrow \mathscr{R}^m$

$$f(\overrightarrow{x}) = \frac{1}{2} \sum_{j=1}^{m} r_j^2(\overrightarrow{x})$$

  - (Factor of 1/2 to make derivatives look nicer)

Least Square Optimization

- With this special form, we can calculate the Jacobian of $(r_1(\overrightarrow{x}), r_2(\overrightarrow{x}), \ldots, r_m(\overrightarrow{x}))^T$ more easily

$$\mathbf{J}^T = \begin{pmatrix} \frac{\delta r_1}{\delta x_1} & \frac{\delta r_2}{\delta x_1} & \cdots & \frac{\delta r_m}{\delta x_1} \\ \frac{\delta r_1}{\delta x_2} & \frac{\delta r_2}{\delta x_2} & \cdots & \frac{\delta r_m}{\delta x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\delta r_1}{\delta x_n} & \frac{\delta r_2}{\delta x_n} & \cdots & \frac{\delta r_m}{\delta x_n} \end{pmatrix} = \left(\frac{\delta r_j}{\delta x_i} \right)$$

Least Square Optimization

- Then

$$\nabla f(\overrightarrow{x}) = \mathbf{J}(\overrightarrow{x})^T \mathbf{r}(x)$$

$$\nabla^2 f(\overrightarrow{x}) = \mathbf{J}(\overrightarrow{x})^T \mathbf{J}(\overrightarrow{x}) + \sum_{j=1}^{m} r_j(\overrightarrow{x}) \nabla^2 r_j(\overrightarrow{x})$$

Least Square Optimization

- Now we assume that $||\mathbf{r}(\overrightarrow{x})||$ is linear
  - Then $\mathbf{J}$ is a constant
  - $\nabla^2(r_j)(\overrightarrow{x}) = 0$
  - Taylor expansion is

$$f(\overrightarrow{x}) = f(x_0) + \mathbf{J}(f(x))|_{\overrightarrow{x}_0}(\overrightarrow{x} - \overrightarrow{x}_0) + \frac{1}{2}(\overrightarrow{x} - \overrightarrow{x}_0)^T\mathbf{H}(f(\overrightarrow{x})|_{\overrightarrow{x}_0}(\overrightarrow{x} - \overrightarrow{x}_0) + \dots$$

  - Taking derivatives gives
  - $\nabla f(\overrightarrow{x}) = \mathbf{J}^T(\mathbf{J}\overrightarrow{x} + \vec{r}) = 0$
  - at a minimum

Least Square Optimization

- This means we can solve for the minimum since then $\mathbf{J}^T\mathbf{J}\overrightarrow{x} = -\mathbf{J}^T\mathbf{r}(\overrightarrow{x})$
- and so we could solve $\overrightarrow{x} = (\mathbf{J}^T\mathbf{J})^{-1}\mathbf{J}^T\mathbf{r}$

Least Square Optimization

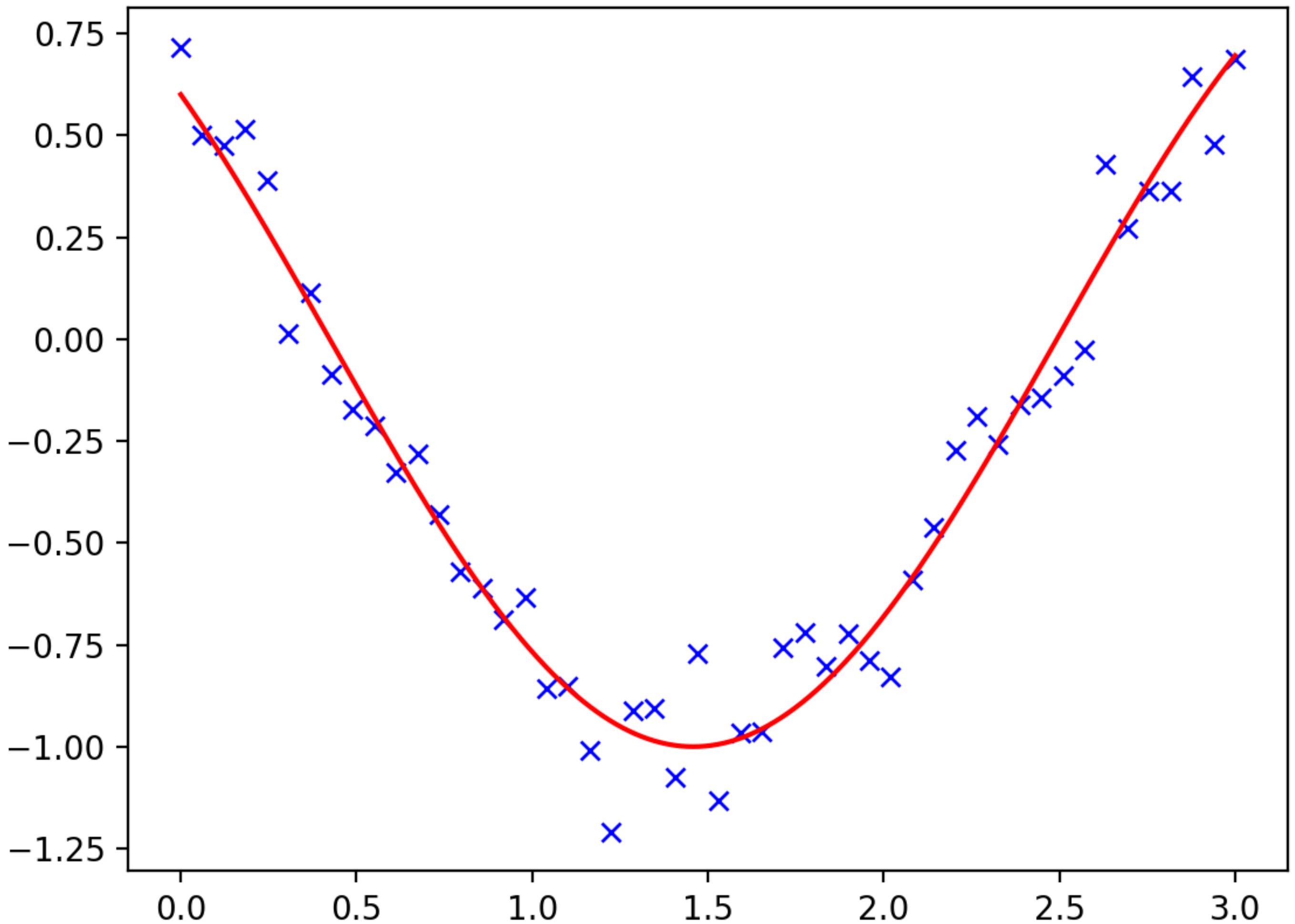
- However, calculating the inverse is
  - computationally expensive
  - numerically unstable

Least Square Optimization

- Can use
  - Cholesky factorization
  - QR factorisation
  - Singular value decomposition of
    - $\mathbf{J}^T\mathbf{J}$
  - which are all implemented in np.linalg

Curve Fitting

- Number of numerical methods for minimization problems
- Curve fitting:
  - Given a number of points, find a smooth curve going through it



Curve Fitting

- Use a cosine as the test function

```
def f(t, omega, phi):
    return np.cos(omega * t + phi)
```

Fitting with scipy

- Create sample data

```
x = np.linspace(0, 3, 50)
y = f(x, 1.5, 1) + .1*np.random.normal(size=50)
```

Fitting with scipy

- Now fit using scipy.optimize

```
params, params_cov = optimize.curve_fit(f, x, y)
print(params)
```

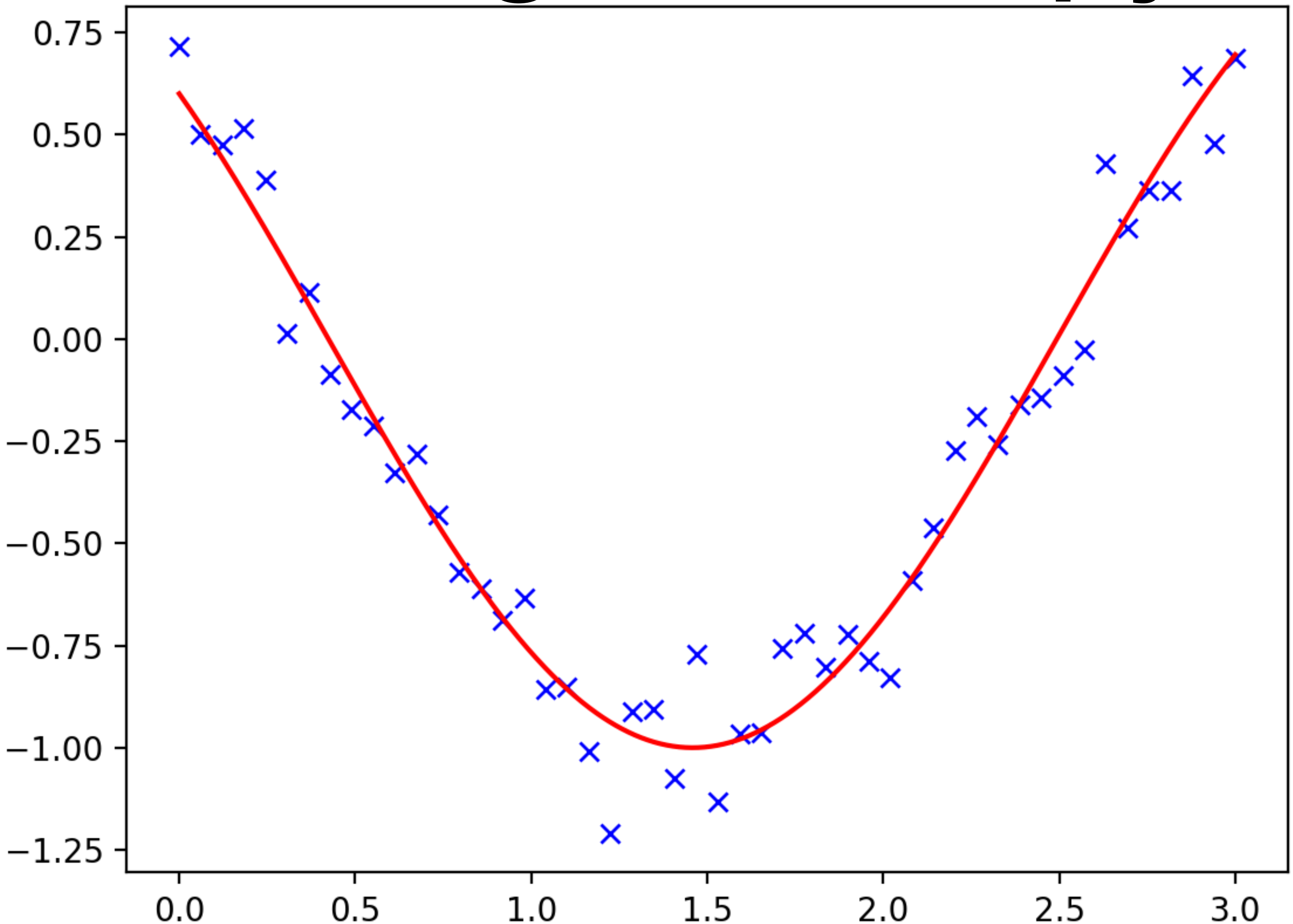
Fitting with scipy

- Can almost recover parameters

```
y = f(x, 1.5, 1) + .1*np.random.normal(size=50)
```

```
[1.51854577 0.92665541]
```

Fitting with scipy



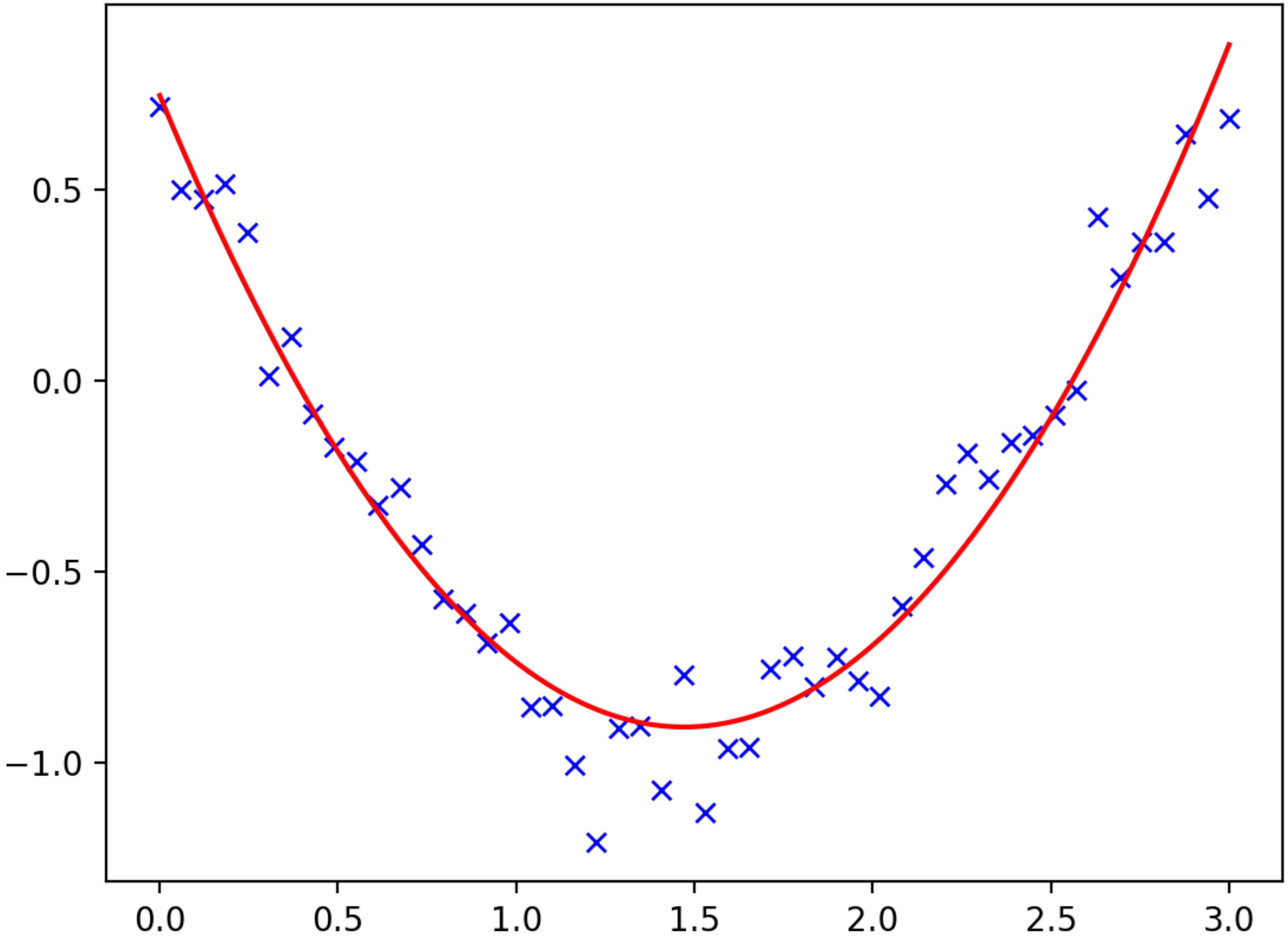
Fitting with scipy

- Could also fit with a quadratic

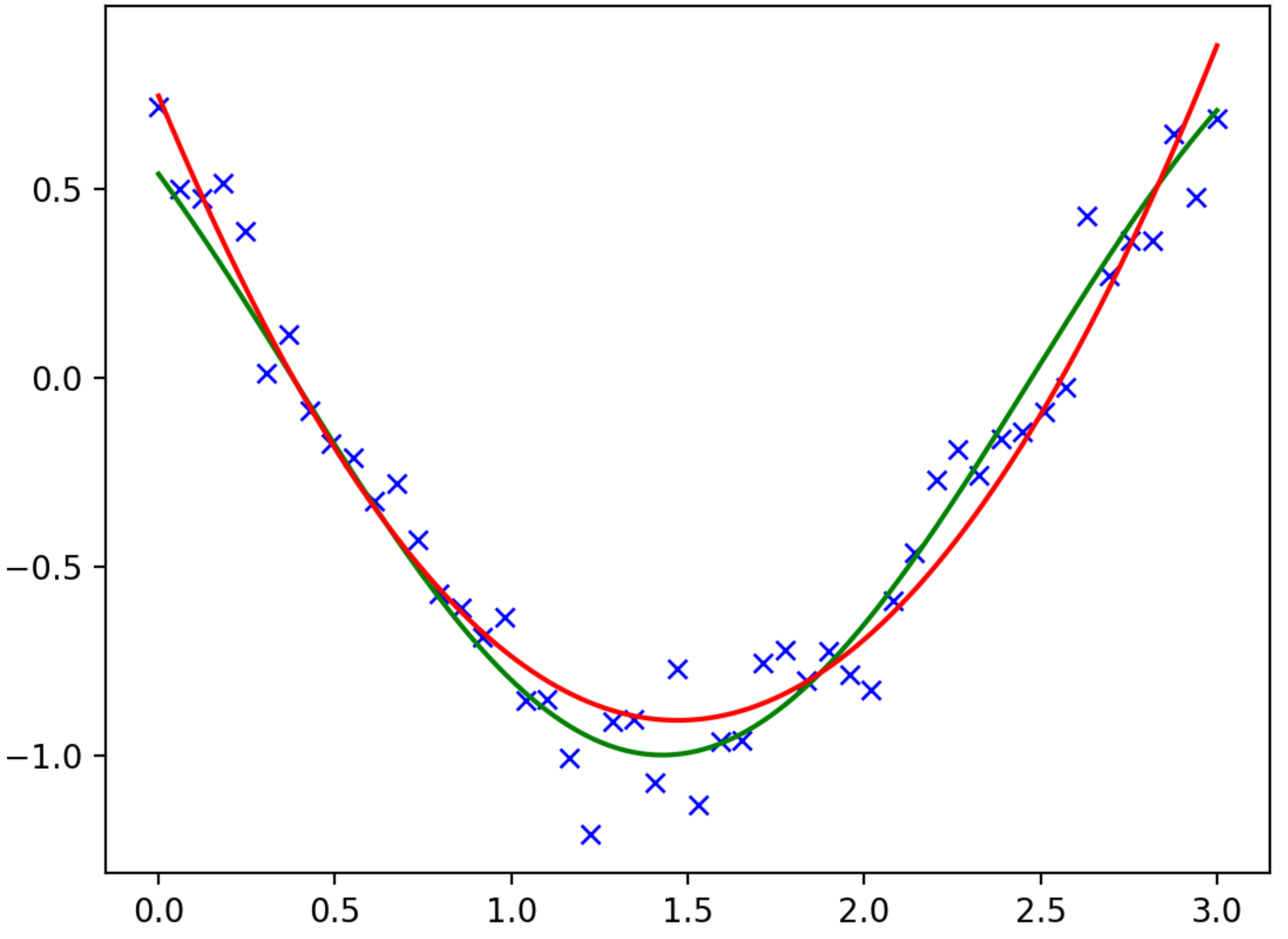
```
def g(t, a, b, c):
    return a*t**2+b*t+c

params, params_cov = optimize.curve_fit(g, x, y)
```

Fitting with scipy

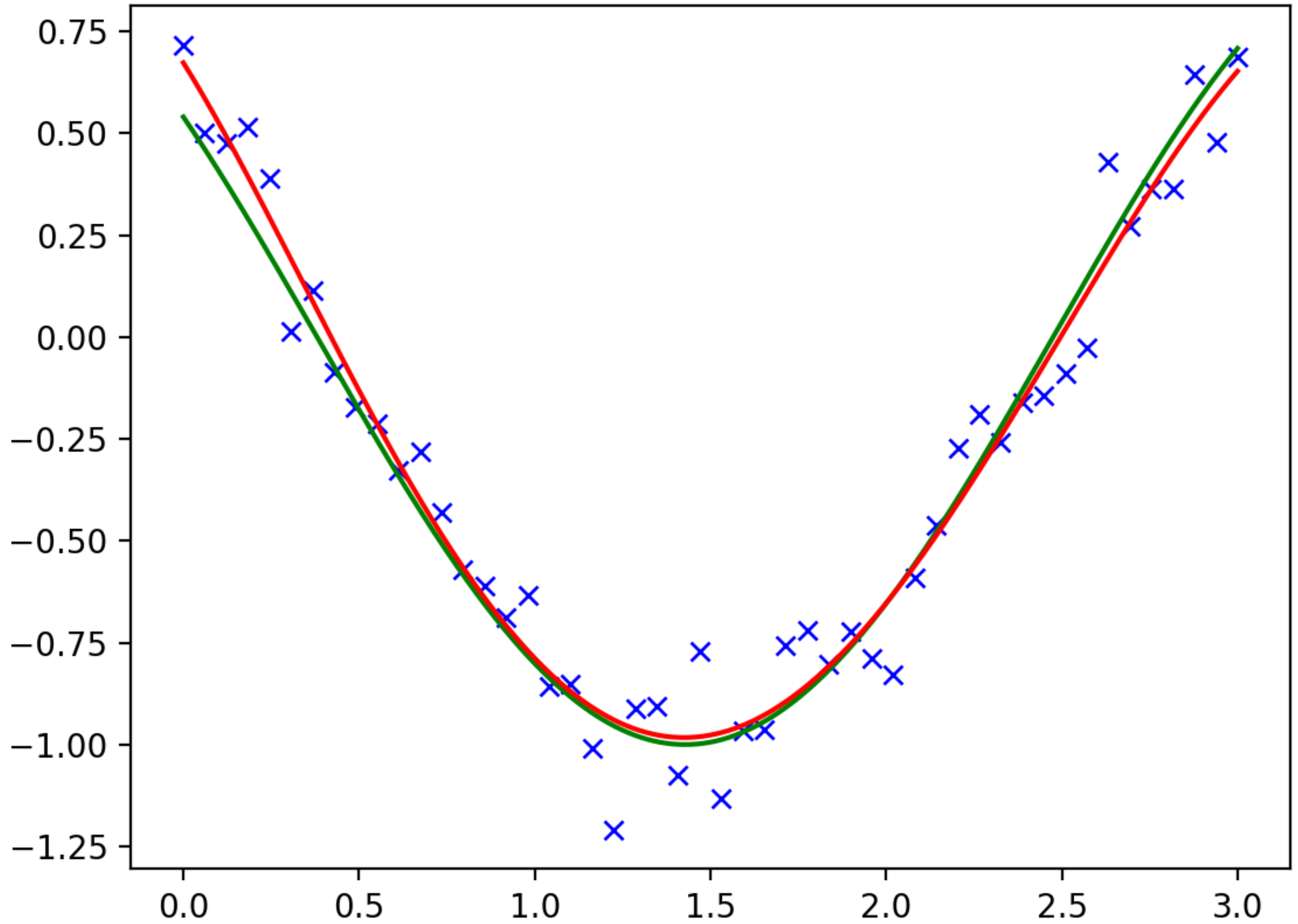


Fitting with scipy



Fitting with scipy

- Could also try a higher level polynomial



Fitting with scipy

- And if we try with a polynomial with as many degrees as there are points, we would get perfect fit
  - And absolutely no insights!

Example

- Macro-economic data from Longley
  - Can download from jbrownlee's github site
    - GNP.deflator: GNP implicit price deflator (1954=100)
    - GNP: Gross National Product.
    - Unemployed: number of unemployed.
    - Armed.Forces: number of people in the armed forces.
    - Population: ‘noninstitutionalized’ population $\geq$ 14 years of age.
    - Year: the year (time).
    - Employed: number of people employed.

Example

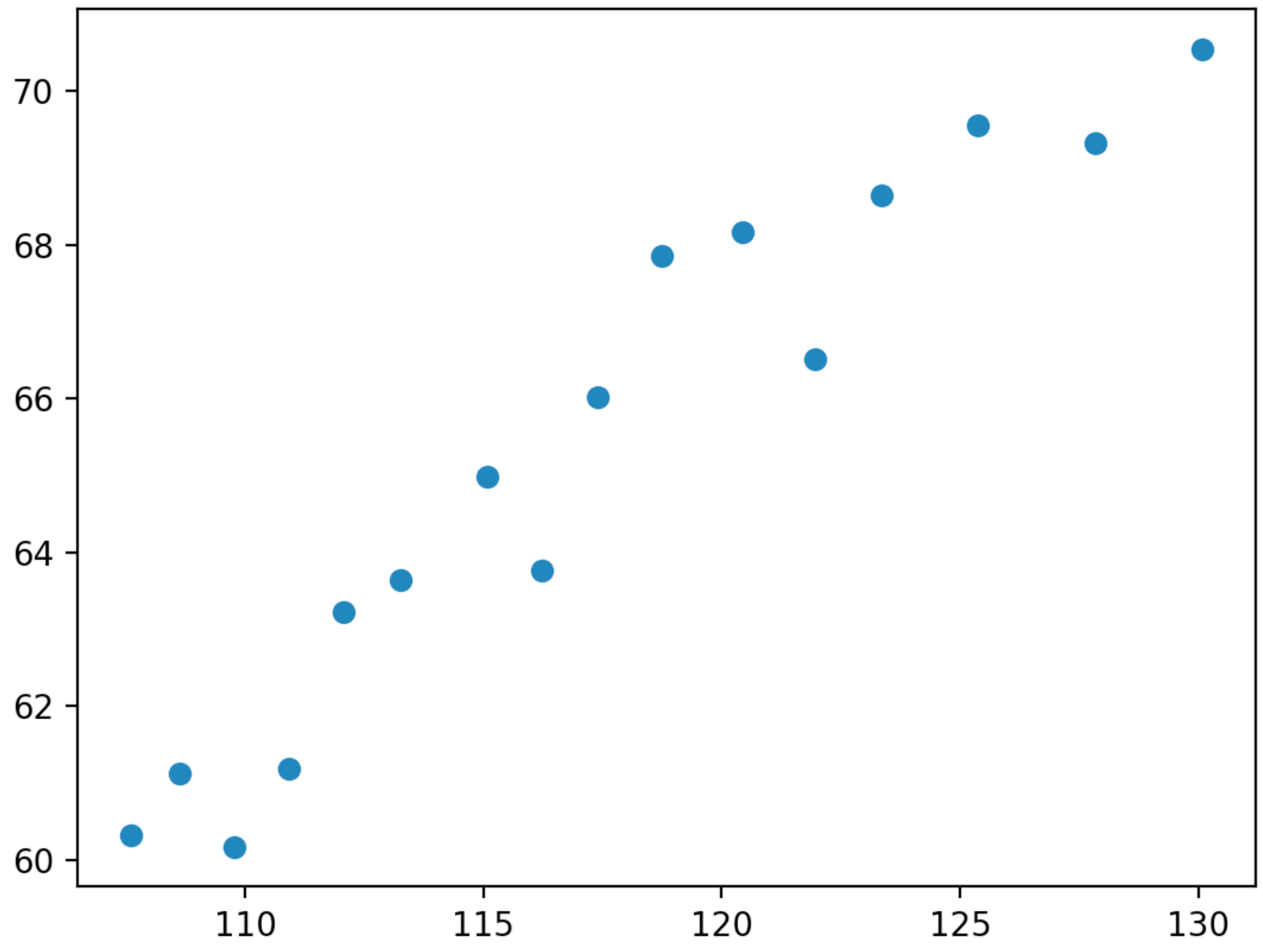
```
import scipy.optimize as opt
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

url = 'https://raw.githubusercontent.com/jbrownlee/
Datasets/master/longley.csv'
dataframe = pd.read_csv(url, header = None)
data = dataframe.values
```

Example

- Employment dependent on population

```
x, y = data[:,4], data[ :,-1]
plt.scatter(x,y)
plt.show()
```



Example

- Define a *model function*
  - What is the proposed dependence:
    - Linear Regression:
      - $\text{emp} = \alpha \cdot \text{pop} + \beta$

```
def model(x, alpha, beta):
    return alpha*x+beta
```

Example

- Now we can use curve-fitting
  - scipy.optimize.curve_fit(model, xvals, yvals) returns
    - popt: optimal parameters
    - pcov: covariance matrix

Example

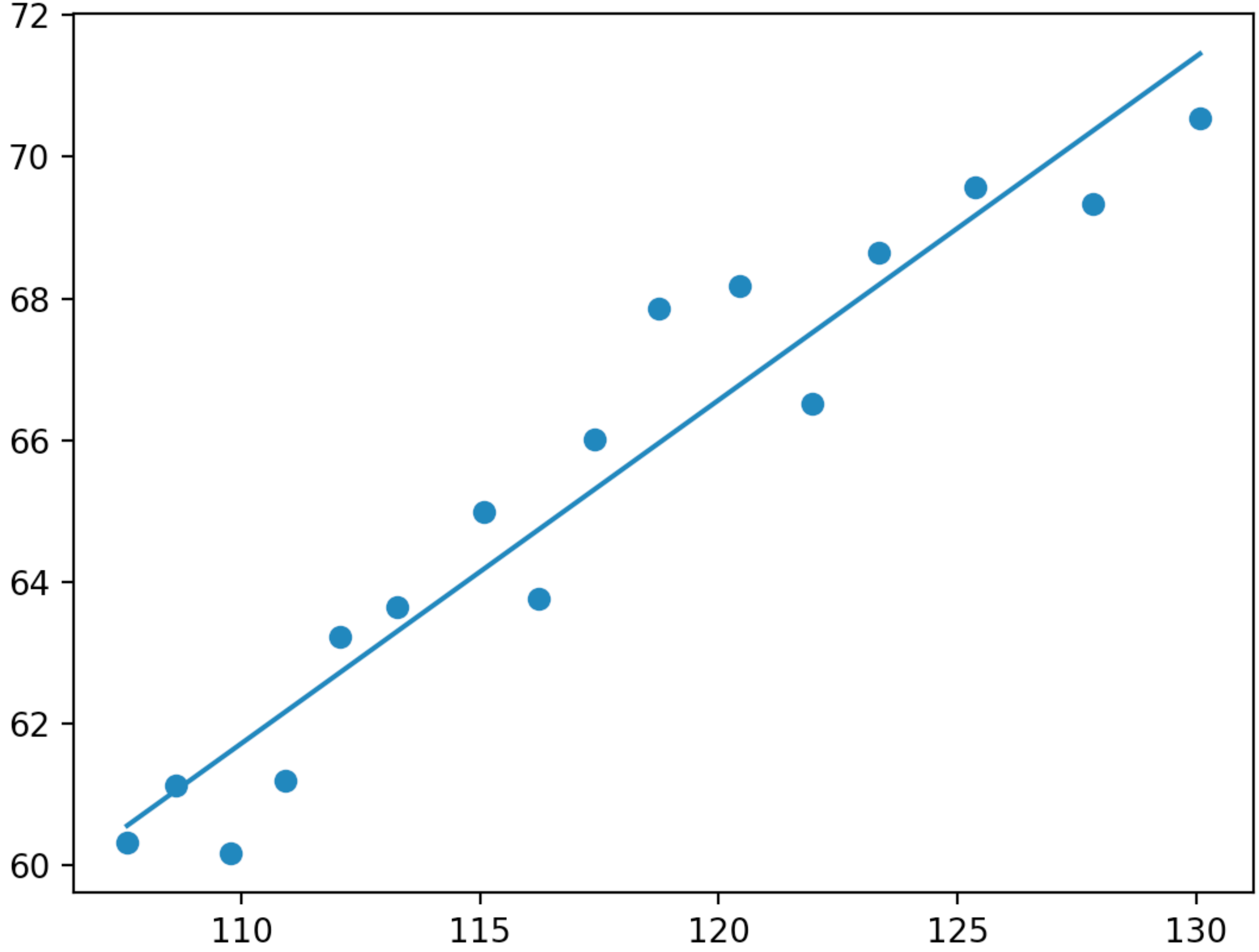
```
popt, pcov = opt.curve_fit(model, x, y)
print(popt)

a, b = popt

plt.scatter(x,y)
xrange = np.linspace(np.min(x), np.max(x), 3)
plt.plot(xrange, model(xrange, a, b))
plt.show()
```

```
[0.48487809 8.38067476]
```

Example



Example

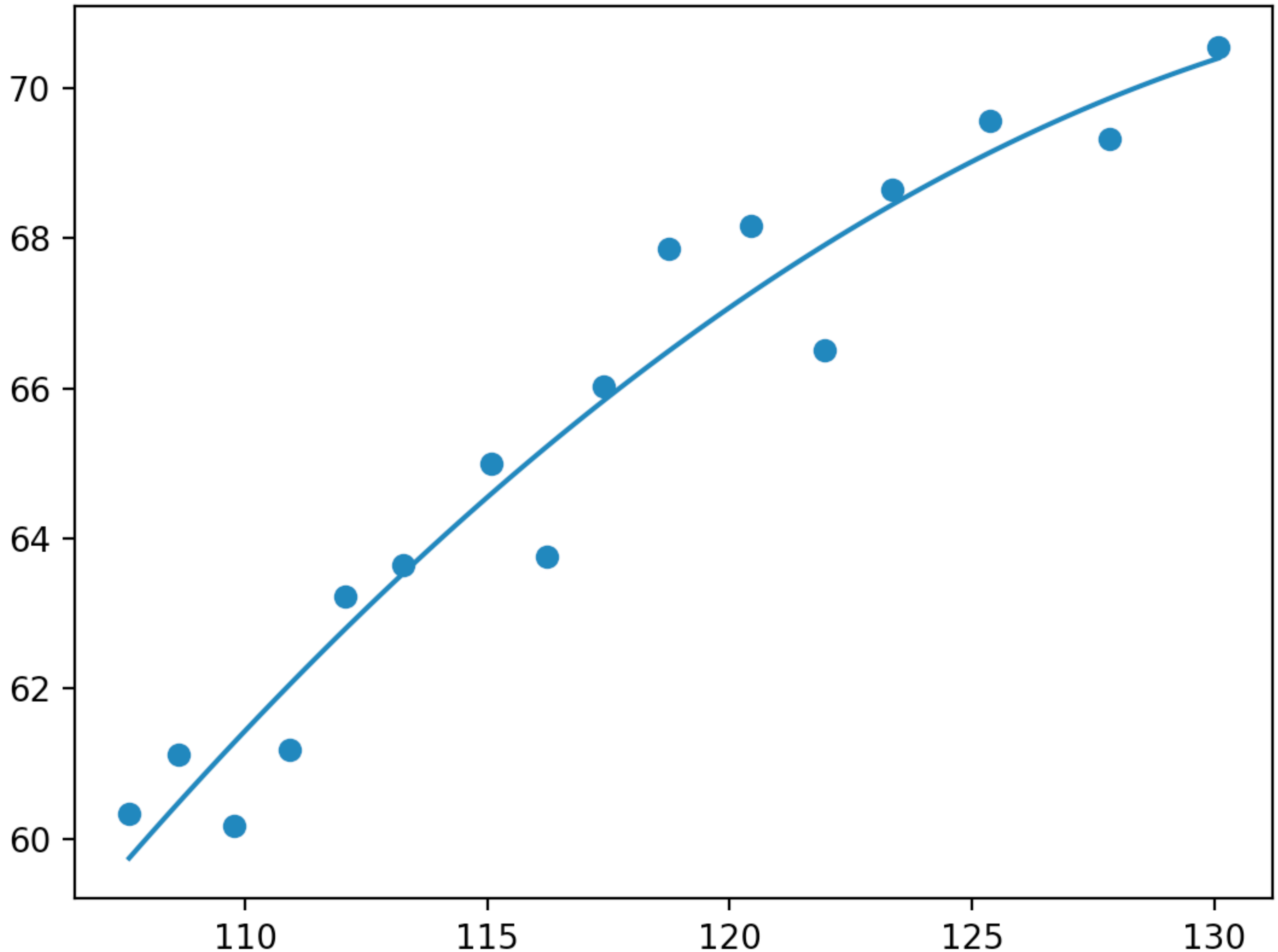
- Change the model by adding a quadratic component

```
def model(x, alpha, beta, gamma):
    return alpha*x**2+beta*x+gamma

popt, pcov = opt.curve_fit(model, x, y)
print(popt)
a, b, c = popt

plt.scatter(x,y)
xrange = np.linspace(np.min(x), np.max(x), 101)
plt.plot(xrange, model(xrange, a, b, c))
plt.show()
```

Example



Optimization

- Global optimizers:
  - Grid search: Start out at a large number of starting positions
  - Try out several methods
    - If possible, calculate the gradient and the Hessian yourself
    - Can use scipy.optimize.check_grad( ) to see whether you calculated correctly

Curve Fitting

- Need to have a good model:
  - Avoids under- and over-fitting
  - Find a way to measure success
    - E.g. time series: You want to remove trends and have white noise left over

Constraints

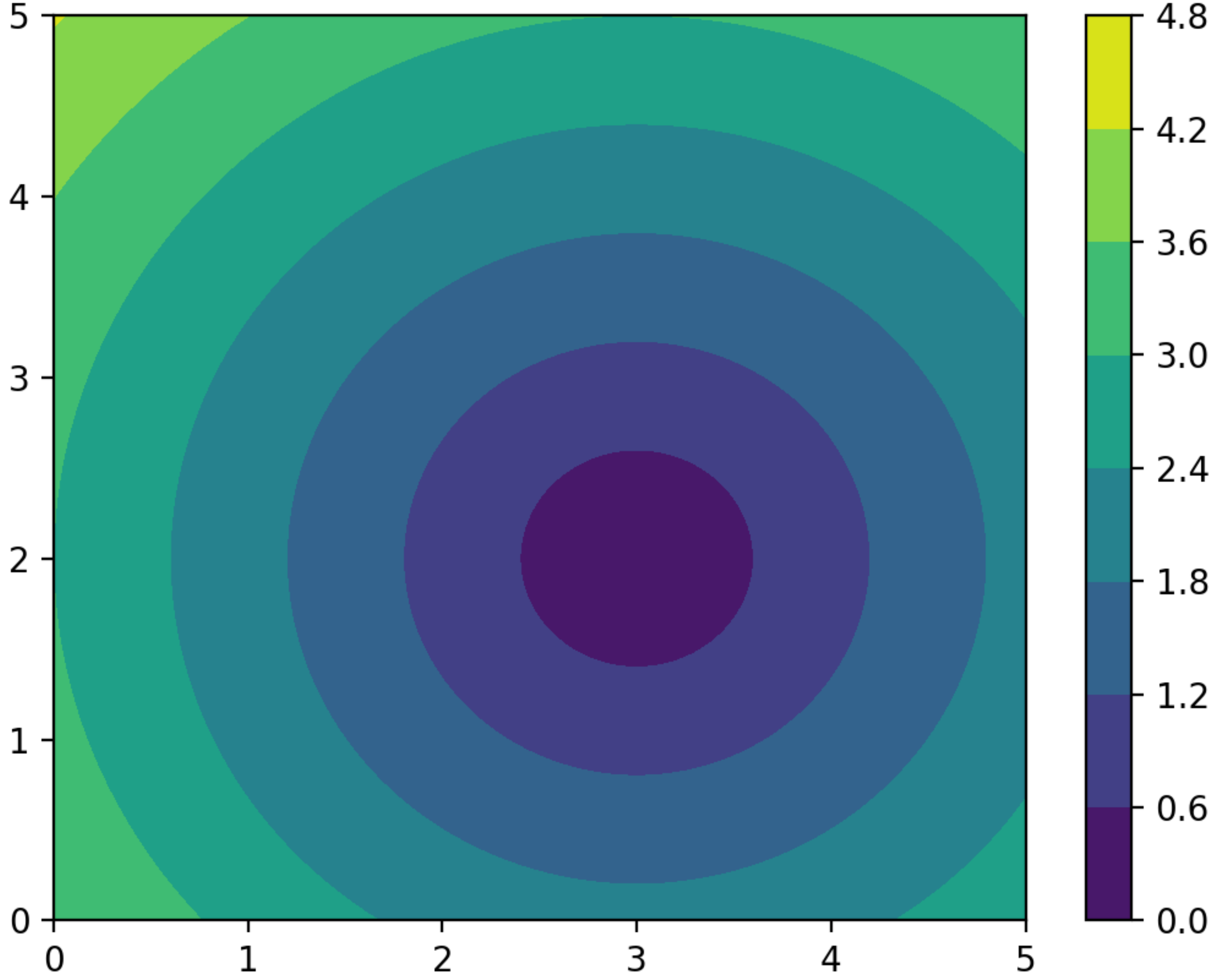
- Often need to optimize under constraints
  - Easiest constraints are for box bounds:
    - Variables need to be within a certain range

Constraints

- Function:

```
def f(x):
    return np.sqrt((x[0]-3)**2 + (x[1]-2)**2)
```

Constraints



Constraints

- Optimization:
  - `result = optimize.minimize(f, np.array([0, 0]), bounds=((-1.5, 1.5), (-1.5, 1.5)))`

Constraints

- Result:

```
>>> result
      fun: 1.5811388300841898
 hess_inv: <2x2 LbfgsInvHessProduct with dtype=float64>
      jac: array([-0.94868331, -0.31622778])
  message: b'CONVERGENCE:
NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
     nfev: 9
      nit: 2
   status: 0
  success: True
        x: array([1.5, 1.5])
```

Constraints

- We can use minimize with a tuple of constraints
  - Assume we want to optimize a sum of Gaussian functions

```
def f(x):
    return -(np.exp(-(x[0]+1)**2/(2.1**2))+
             np.exp(-(x[1]-0.3)**2/(0.8**2))+
             np.exp(-(x[2]-2.1)**2/(1.7**2)))
```

  - By looking at the function, we know that the optimum of -3 is reached at x[0]=1, x[1]=0.3, x[2]=2.1

Constraints

```
result = opt.minimize(f,
                      x0=np.array([0,0,0]),
                      method='SLSQP',
                      #constraints = my_constraints,
                      options={'maxiter':1000})

print(result)
```

Constraints

- With result

```
     fun: -2.9999996182639146
     jac: array([-8.09729099e-05, -2.40176916e-04,
7.11053610e-04])
 message: 'Optimization terminated successfully'
    nfev: 34
     nit: 8
    njev: 8
  status: 0
 success: True
       x: array([-1.00017856,  0.29992313,  2.10102744])
```

Constraints

- SLSQP allows constraints
  - Define constraints as functions

```
def constraint(x):
    return 1-(x[0]**2+2*x[1]**2+3*x[2]**2)
```

  - Put them into a dictionary, and make a tuple of them

```
my_constraints = ({'type': 'ineq','fun': constraint})
```

  - Read: $x_0^2 + 2 \cdot x_1^2 + 3 \cdot x_2^2 < 1$

Constraints

```
def constraint(x):
    return 1-(x[0]**2+2*x[1]**2+3*x[2]**2)

my_constraints = ({'type': 'ineq','fun': constraint})

result = opt.minimize(f,
                      x0=np.array([0,0,0]),
                      method='SLSQP',
                      constraints = my_constraints,
                      options={'maxiter':1000})

print(result)
```

Constraints

- Result:

```
     fun: -2.3352953005679837
     jac: array([ 0.19044936, -0.16718537, -0.44114104])
 message: 'Optimization terminated successfully'
    nfev: 33
     nit: 8
    njev: 8
  status: 0
 success: True
       x: array([-0.56132919,  0.2462587 ,  0.43344502])
```

HELP!!!!

- Get Scipy Lecture notes (for free)
    - www.scipy-lectures.org