Lab 1

Trust-Region Methods

Lab Objective: *Explore Trust-Region methods for optimization.*

When it comes to optimizing high-dimensional functions, a common strategy is to break the problem up into a series of smaller, easier tasks, leading to a sequence of successive approximations to the optimizer. This is the approach taken by Line-Search algorithms such as Newton's method or conjugate gradient. The class of algorithms known as trust-region methods are also based on this strategy, although they differ from line-search methods in some important ways.

Overview of the Trust-Region Approach

Suppose we wish to minimize a function f. Given some particular point x_k in the domain of f, how do we select a new point x_{k+1} that better minimizes the function? A line-search algorithm solves this sub-problem by first choosing a search direction d_k (often related to the gradient of f), and then a step length α_k so as to minimize f along the direction d_k. The next point, then, is simply

$$x_{k+1} := x_k + \alpha_k d_k.$$

A trust-region algorithm, on the other hand, does away with a search direction and step length, and instead approximates the function f with some simpler function m_k (called the *model function*) in a neighborhood of x_k. The model m_k will likely not be a good approximation for f over the entire domain, and so we must restrict our attention to a ball of radius r_k centered at the point x_k, inside of which m_k is reasonably close to f. We then minimize m_k over this ball, and set x_{k+1} equal to this minimizer. That is, we compute x_{k+1} by solving the sub-problem

$$x_{k+1} := \underset{x \in B(x_k, r_k)}{\operatorname{argmin}} \; m_k(x).$$

The ball $B(x_k, r_k)$ is called the *trust region* because we trust that the model function m_k gives a reasonably accurate approximation of f on this region. Note that it is also possible to use other types of trust regions, such as ellipsoidal or box-like regions.

The Model Function

The model function is commonly taken to be a linear or quadratic approximation of f based on its Taylor Series expansion about the point x_k. In the linear case, our model function has the form

$$m_k(x) = f(x_k) + (x - x_k)^T \nabla f(x_k).$$

In the quadratic case, we simply add on a quadratic term to obtain

$$m_k(x) = f(x_k) + (x - x_k)^T \nabla f(x_k) + \frac{1}{2}(x - x_k)^T H_k (x - x_k),$$

where H_k is the Hessian matrix of f at x_k, or some approximation thereof. Given a trust region with radius r_k, note that our sub-problem can be written in the following way:

$$\begin{aligned} x_{k+1} &= \underset{x \in B(x_k, r_k)}{\operatorname{argmin}} \; m_k(x) \\ &= x_k + p_k, \end{aligned}$$

where

$$p_k = \underset{\|p\| < r_k}{\operatorname{argmin}} \{ f(x_k) + p^T \nabla f(x_k) + \frac{1}{2} p^T H_k p \}. \tag{1.1}$$

p_k is called a *step*. Also we define p to be

$$p = x - x_k \tag{1.2}$$

For the remainder of the lab, we define

$$m_k(p) = f(x_k) + p^T \nabla f(x_k) + \frac{1}{2} p^T H_k p,$$

and refer to *this* function as the model function.

The Trust-Region Radius

A crucial aspect of trust-region algorithms is the choice of radius r_k. If r_k is too small, then the algorithm will make slow progress toward the minimizer of f. If r_k is too large, the model function will be a poor fit for the objective function f, and the next iterate x_{k+1} may fail to decrease f. Of course, whether the radius is too small or large depends on the local behavior of f, which may change as the algorithm converges. A reasonably robust trust-region algorithm must therefore be able to adaptively choose the trust-region radius.

Our strategy for choosing an appropriate radius r_{k+1} for the $(k+1)$-th iterate involves evaluating the accuracy of the model function at the k-th iterate. If the model was accurate and a large step was taken, we can optimistically choose r_{k+1} to be larger than r_k in the hopes of achieving faster convergence. To prevent the radius from growing too large, we set an overall bound r_{max} on the trust-region radii. If the model was very inaccurate, we make r_{k+1} smaller than r_k, since the model function can't be trusted over such a large region. If the model was neither particularly accurate nor inaccurate, we simply choose $r_{k+1} = r_k$.

We measure the accuracy of the model by computing the following value:

$$\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}.$$

This value is the ratio of the *actual reduction* to the *predicted reduction* in the objective function. The closer ρ_k is to 1, the more accurate the model. Note that if ρ_k is negative or below a certain positive threshold η, then the point $x_k + p_k$ is a poor improvement over x_k (and perhaps is worse). In this case, we reject the new point and set $x_{k+1} = x_k$.

The Trust-Region Algorithm

We now combine the two steps of minimizing the model function and choosing the trust-region radius to build the algorithm. In practice, we halt the algorithm once $\|\nabla f(x_k)\|$ is less than some threshold value.

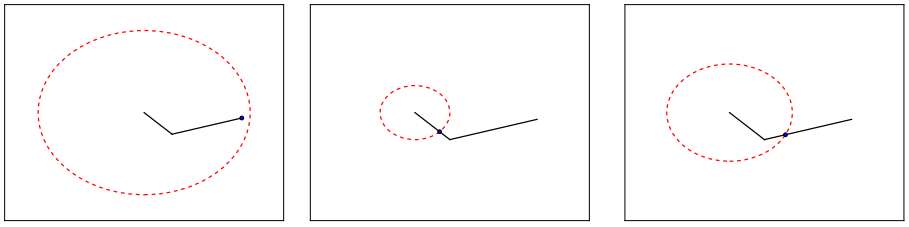
Algorithm 1.1 Trust-Region Algorithm

```
1:  procedure TRUST-REGION ALGORITHM
2:      Choose initial point x_0, initial radius r_0, and threshold η ∈ [0, 0.25).
3:      while ||∇f(x_k)|| > tol do
4:          Calculate p_k by solving the sub-problem in Equation 1.1.
5:          Compute ρ_k.
6:          if ρ_k < 0.25 then
7:              r_{k+1} = 0.25 r_k
8:          else
9:              if ρ_k > 0.75 and ||p_k|| = r_k then
10:                 r_{k+1} = min(2 r_k, r_max)
11:             else
12:                 r_{k+1} = r_k
13:         if ρ_k > η then
14:             x_{k+1} = x_k + p_k
15:         else
16:             x_{k+1} = x_k
```

Problem 1. Implement the trust-region algorithm (see the specifications file). At this stage, do not solve Equation (1.1) for p_k. Instead, assume the parameter `subprob` is a function that does that for you (see Problem 2) The function `subprob()` takes as parameters a gradient vector, hessian matrix, and radius.

Solving the Sub-problem: the Dogleg Method

Our trust-region algorithm is as yet incomplete, since we do not have a viable means solving the subproblem given by Equation 1.1. We may be tempted to search for



(a) Dogleg path completely within the trust region.

(b) Intersection in the first leg of the path.

(c) Intersection in the second leg of the path.

Figure 1.1: Relationships between the dogleg path (black solid line), the trust region boundary (red dashed circle), and the dogleg minimizer (blue dot).

the true minimizer of the model function over the trust region, but it turns out that we can get away with just an approximate minimizer. We will employ the "dogleg" method when selecting an approximate minimizer of the model function. This method works by minimizing the model function along a particular path extending from the origin out to the boundary of the trust region. This path is piecewise linear and has a shape vaguely reminiscent of a dog's leg, which explains the peculiar name of the method.

To calculate the dogleg minimizer of the model function, we first solve the unconstrained minimizer of the model function. We p^B as the unconstrained minimizer of the model function:

$$p^B = -H_k^{-1} \nabla f(x_k).$$

We then calculate the direction of steepest descent for the model function, given by

$$p^U = -\frac{\nabla f(x_k)^T \nabla f(x_k)}{\nabla f(x_k)^T H_k \nabla f(x_k)} \nabla f(x_k).$$

We define the dogleg path using these two points as follows:

$$\gamma(\tau) = \begin{cases} \tau p^U, & 0 \leq \tau \leq 1 \\ p^U + (\tau - 1)(p^B - p^U), & 1 \leq \tau \leq 2 \end{cases}$$

It can be shown that the model function decreases along this path. Thus, the dogleg minimizer is either the endpoint of the path if it lies completely within the trust region, or the point of intersection between the path and the boundary of the trust region. See Figure 1.1 for an illustration of the three salient cases. We consider each case in turn.

- When the path lies completely within the trust region, the dogleg minimizer is simply the endpoint, namely p^B. This is the case when $\|p^B\| \leq r_k$. See Figure 1.1a.

- When the path intersects the boundary of the trust region in the first line segment, the dogleg minimizer is $r_k p^U / \|p^U\|$. This is the case when $\|p^U\| \geq r_k$. See Figure 1.1b.

- When the path intersects the boundary of the trust region in the second line segment, the dogleg minimizer is given by $p^U + (\tau^* - 1)(p^B - p^U)$, where τ^* satisfies the quadratic equation

$$\|p^U + (\tau^* - 1)(p^B - p^U)\|^2 = r_k^2.$$

This quadratic equation can be simplified into

$$a(\tau^* - 1)^2 + b(\tau^* - 1) + c = 0$$

where the coefficients are defined to be

$$a = p_B^T p_B - 2p_B^T p_U + p_U^T p_U$$

$$b = 2p_B^T p_U - 2p_U^T p_U$$

$$c = p_U^T p_U - r_k^2.$$

See Figure 1.1c.

Problem 2. Implement the dogleg method. Remember to avoid calculating the inverse of a matrix.

Test your implementation of the trust-region algorithm on the Rosenbrock function contained the `scipy.optimize` module. Compare your answer with that obtained by SciPy's trust-region implementation. The code to accomplish this, together with the correct results, is given below.

```
>>> from scipy import optimize as op
>>> x = np.array([10.,10])
>>> rmax=2.
>>> r=.25
>>> eta=1./16
>>> tol=1e-5
>>> opts = {'initial_trust_radius':r, 'max_trust_radius':rmax, 'eta':eta, 'gtol':↩
    tol}
>>> sol1 = op.minimize(op.rosen, x, method='dogleg', jac=op.rosen_der, hess=op.↩
    rosen_hess, options=opts)
>>> sol2 = trustRegion(op.rosen, op.rosen_der, op.rosen_hess, dogleg, x, r, rmax,↩
     eta, gtol=tol)
>>> print np.allclose(sol1.x, sol2)
True
```

Problem 3. Test your `trustRegion()` and `dogleg()` methods on the Rosenbrock function. Use the `rosen()`, `rosen_der()`, and `rosen_hess()` methods from `scipy.optimize`. Return the solution `x*` from the `trustRegion()` method.

Solving Systems of Nonlinear Equations

Trust-region methods can be used to find solutions of systems of nonlinear equations, which arise in applications across science and engineering. Suppose we have a vector function $r : \mathbb{R}^n \to \mathbb{R}^n$, written as

$$r(x) = \begin{bmatrix} r_1(x) \\ r_2(x) \\ \vdots \\ r_n(x) \end{bmatrix},$$

where each r_i is a nonlinear smooth function mapping from $\mathbb{R}^n$ into $\mathbb{R}$. Our goal is to find $x \in \mathbb{R}^n$ that satisfies $r(x) = 0$; such an x is called a solution or root of the nonlinear system. In general, there may be several roots (even infinitely many), or there may be none at all. Solving the equations by hand can range from arduous to impossible, so we turn to trust-region methods for help.

In order to use our trust-region method to find the roots of a system of equations, we need to come up with an objective function whose minima correspond to roots of the system. As such, we consider the *merit function*

$$f(x) = \frac{1}{2}\|r(x)\|_2^2 = \frac{1}{2}\sum_{i=1}^{n} r_i(x)^2,$$

which, roughly speaking, measures how close a point x is to being a root of r. Note that $f(x) = 0$ if and only if $r(x) = 0$. Thus, if we can successfully find a global minimum of f, we will have found a root to the nonlinear system.

Now that we have an objective function, we need to create a quadratic model function. If we let J_k be the Jacobian matrix of r at the point x_k, i.e.

$$J_k = \begin{bmatrix} \nabla r_1(x_k)^T \\ \nabla r_2(x_k)^T \\ \vdots \\ \nabla r_n(x_k)^T \end{bmatrix},$$

then we can write the gradient $\nabla f(x_k) = J_k^T r(x_k)$ and the Hessian $H_k = J_k^T J_k$. We can now use the same model function described earlier.

Let's work through an example. Consider the system

$$r(x, y) = \begin{bmatrix} -\sin x \cos y - 2\cos x \sin y \\ -\sin y \cos x - 2\cos y \sin x \end{bmatrix}.$$

Observe that the Jacobian takes the form

$$J(x) = \begin{bmatrix} -\cos x \cos y + 2\sin x \sin y & \sin x \sin y - 2\cos x \cos y \\ \sin y \sin x - 2\cos y \cos x & -\cos y \cos x + 2\sin y \sin x \end{bmatrix}.$$

In Python, we initialize all of the requisite functions and then find a root as follows:

```
>>> # define the system of equations
>>> def r(x):
```

```
>>>     return np.array([-sin(x[0])*cos(x[1]) - 2*cos(x[0])*sin(x[1]),
>>>                      -sin(x[1])*cos(x[0]) - 2*cos(x[1])*sin(x[0])])
>>>
>>> # define the merit function
>>> def f(x):
>>>     return .5*(r(x)**2).sum()
>>>
>>> # define the jacobian function
>>> def J(x):
>>>     return np.array([[-cos(x[0])*cos(x[1]) + 2*sin(x[0])*sin(x[1]),
>>>                       sin(x[0])*sin(x[1]) - 2*cos(x[0])*cos(x[1])],
>>>                      [sin(x[1])*sin(x[0]) - 2*cos(x[1])*cos(x[0]),
>>>                       -cos(x[1])*cos(x[0]) + 2*sin(x[1])*sin(x[0])]])
>>>
>>> # define the gradient function
>>> def g(x):
>>>     return J(x).dot(r(x))
>>>
>>> # define the Hessian function
>>> def H(x):
>>>     return J(x).T.dot(J(x))
>>>
>>> # set trust-region parameters
>>> rmax=2.
>>> rr=.25
>>> eta=1./16
>>> tol=1e-5
>>> # set initial point
>>> x = np.array([3.5, -2.5])
>>> # find a minimizer of f
>>> xstar = trustRegion(f,g,H,dogleg,x,rr,rmax,eta=eta,gtol=tol)
>>> print xstar
[ 3.14159265 -3.14159265]
>>> # verify that it is a root of r
>>> print r(xstar)
[ -7.75116117e-09   7.75147025e-09]
```

Of course, we are not guaranteed to always find a root, as convergence depends on the choice of initial point. However, by running the algorithms with several randomly selected starting points, we are more likely to be successful.

Problem 4. Solve the following nonlinear system.

$$r(x,y) = \begin{bmatrix} \sin x \cos y - 4\cos x \sin y \\ \sin y \cos x - 4 \cos y \sin x \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$