牛顿法解RosenBrock函数最小值问题

quandy2020@126.com

1 Rosenbrock函数

- Rosenbrock function

$$f(x,y)=(a-x)^2+b(y-x^2)^2$$

其中全局最小值$(x,y)=(a,a^2)$, 当$a=1,b=100$

$$f(x,y)=(1-x)^2+100(y-x^2)^2$$

优化问题：

$$argminf(x)$$

- **Gradient**

$$\nabla f=\begin{bmatrix}-400xy+400x^3+2x-2\\ 200y-200x^2\end{bmatrix}$$

- **Hessian**

$$H=\begin{bmatrix}-400y+1200x^2+2 & -400x\\ -400x & 200\end{bmatrix}$$

2 Newton's method

梯度下降（或称最陡下降）是一种用于寻找函数最小值的一阶迭代优化算法。为了通过梯度下降找到函数的局部最小值，沿着当前点处函数梯度（或近似梯度）的负方向迈出一步。如果沿着梯度的正方向迈出一步，那么就是在逼近该函数的局部最大值；这个过程则被称为梯度上升。

这一方法基于这样的观察：如果一个多变量函数在某点的邻域内被定义并且可微，那么该函数在负梯度方向下降最快。由此可得，如果：

$$x_{n+1}=x_n-\alpha\nabla F(x)$$

- 梯度处处垂直于等高线。
- 在每次线搜索后，新的梯度始终与先前的步进方向正交（对于任何线搜索都成立）。
- 因此，迭代往往以非常低效的方式在山谷中蜿蜒前行。

Algorithm 1 Newton's Method

```
Initialize at $x^0$, and set $k \leftarrow 0$ .
At iteration $k$ :
1. $d^k := -H(x^k)^{-1}\nabla f(x^k)$. If $d^k = 0$, then stop.
2. Choose step-size $\alpha^k = 1$ .
3. Set $x^{k+1} \leftarrow x^k + \alpha^k d^k$, $k \leftarrow k+1$ .
```

3 Python code

- Rosenbrock function

```python
def Rosenbrock(x,y):
    return (1 + x)**2 + 100*(y - x**2)**2
```

- Rosenbrock gradient

```python
def Grad_Rosenbrock(x,y):
    g1 = -400*x*y + 400*x**3 + 2*x -2
    g2 = 200*y -200*x**2
    return np.array([g1,g2])
```

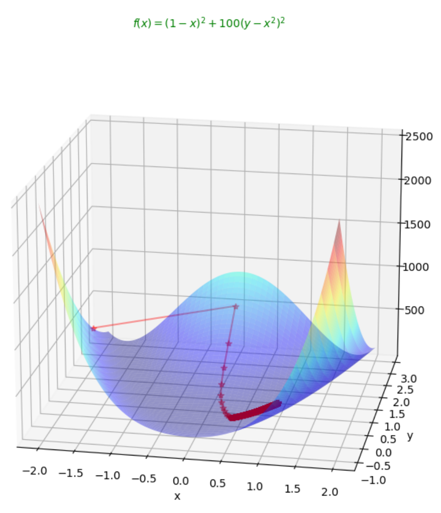
- Rosenbrock Hessian

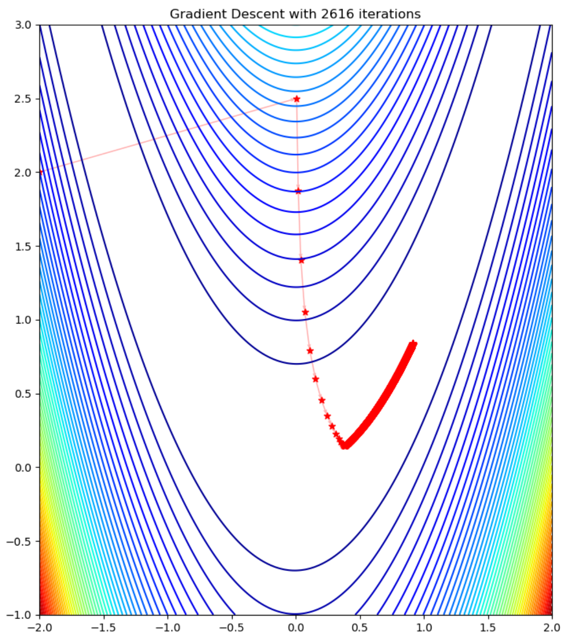
```python
def Hessian_Rosenbrock(x,y):
    h11 = -400*y + 1200*x**2 + 2
    h12 = -400 * x
    h21 = -400 * x
    h22 = 200
    return np.array([[h11,h12],[h21,h22]])
```

- Gradient Descent implementation

```python
def GradientDescent(Grad,x,y, gamma = 0.00125, epsilon=0.0001, nMax = 10000 ):
    #Initialization
    i = 0
    iter_x, iter_y, iter_count = np.empty(0),np.empty(0), np.empty(0)
    error = 10
    X = np.array([x,y])

    #Looping as long as error is greater than epsilon
    while np.linalg.norm(error) > epsilon and i < nMax:
        i +=1
        iter_x = np.append(iter_x,x)
        iter_y = np.append(iter_y,y)
        iter_count = np.append(iter_count ,i)
        #print(X)

        X_prev = X
        X = X - gamma * Grad(x,y)
        error = X - X_prev
        x,y = X[0], X[1]

    print(X)
    return X, iter_x,iter_y, iter_count
```

最优解：[0.91654302 0.83970004]





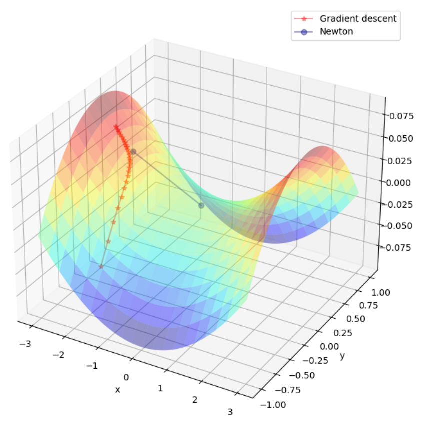
- Python完整代码

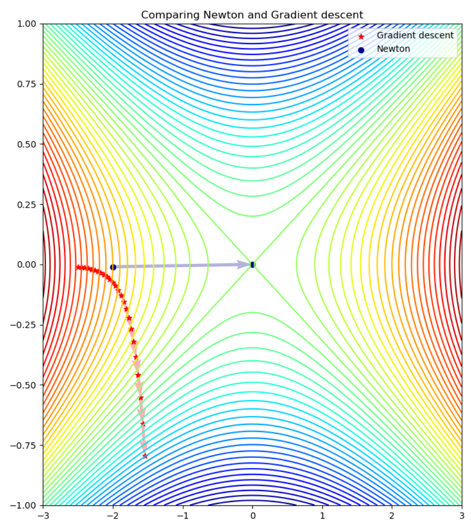
```python
import matplotlib.pyplot as plt
import numpy as np
from mpl_toolkits import mplot3d

# https://xavierbourretsicotte.github.io/Intro_optimization.html

def Rosenbrock(x,y):
    return (1 + x)**2 + 100*(y - x**2)**2

def GradRosenbrock(x,y):
    g1 = -400*x*y + 400*x**3 + 2*x -2
    g2 = 200*y -200*x**2
    return np.array([g1,g2])

def HessianRosenbrock(x,y):
    h11 = -400*y + 1200*x**2 + 2
    h12 = -400 * x
    h21 = -400 * x
    h22 = 200
    return np.array([[h11,h12],[h21,h22]])

def GradientDescent(Grad,x,y, gamma = 0.00125, epsilon=0.0001, nMax =
10000 ):
    #Initialization
    i = 0
    iter_x, iter_y, iter_count = np.empty(0),np.empty(0), np.empty(0)
    error = 10
    X = np.array([x,y])
    #Looping as long as error is greater than epsilon
    while np.linalg.norm(error) > epsilon and i < nMax:
        i +=1
        iter_x = np.append(iter_x,x)
        iter_y = np.append(iter_y,y)
        iter_count = np.append(iter_count ,i)

        X_prev = X
        X = X - gamma * Grad(x,y)
        error = X - X_prev
        x,y = X[0], X[1]
    print(X)
    return X, iter_x,iter_y, iter_count

def NewtonMethod():
    ## 1 Newton's Method
    root,iter_x,iter_y, iter_count = GradientDescent(GradRosenbrock,-2,2)
    x = np.linspace(-2,2,250)
    y = np.linspace(-1,3,250)
    X, Y = np.meshgrid(x, y)
    Z = Rosenbrock(X, Y)

    #Angles needed for quiver plot
    anglesx = iter_x[1:] - iter_x[:-1]
    anglesy = iter_y[1:] - iter_y[:-1]

    ## 2 Surface plot
    fig = plt.figure(figsize = (16,8))
    ax = fig.add_subplot(1, 2, 1, projection='3d')
    ax.plot_surface(X,Y,Z,rstride = 5, cstride = 5, cmap = 'jet', alpha = .4, edgecolor = 'none' )
    ax.plot(iter_x,iter_y, Rosenbrock(iter_x,iter_y),color = 'r', marker = '*', alpha = .4)

    ax.view_init(45, 280)
    ax.set_xlabel('x')
    ax.set_ylabel('y')

    ax.set_title(r"$f(x) = (1 - x)^2 + 100(y - x^2)^2$", c='g', horizontalalignment='center', fontsize=10)

    #Contour plot
    ax = fig.add_subplot(1, 2, 2)
    ax.contour(X,Y,Z, 50, cmap = 'jet')
    #Plotting the iterations and intermediate values
    ax.scatter(iter_x,iter_y,color = 'r', marker = '*')
    ax.quiver(iter_x[:-1], iter_y[:-1], anglesx, anglesy, scale_units = 'xy', angles = 'xy', scale = 1, color = 'r', alpha = .3)
    ax.set_title('Gradient Descent with {} iterations'.format(len(iter_count)))
    plt.show()

def main():
    NewtonMethod()

if __name__ == '__main__':
    main()
```

4 鞍点函数测试

- a single saddle point function

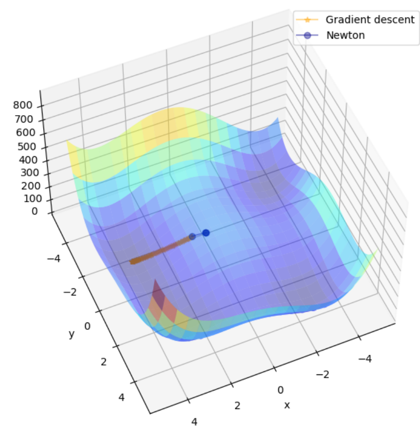
$$f(x,y) = 0.01x^2 - 0.1y^2$$

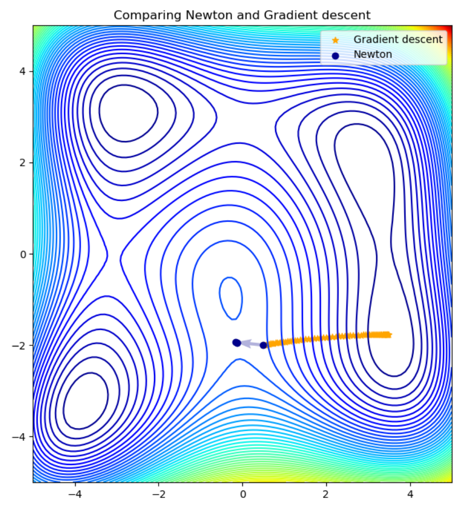




- multiple saddle points function

$$f(x,y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$





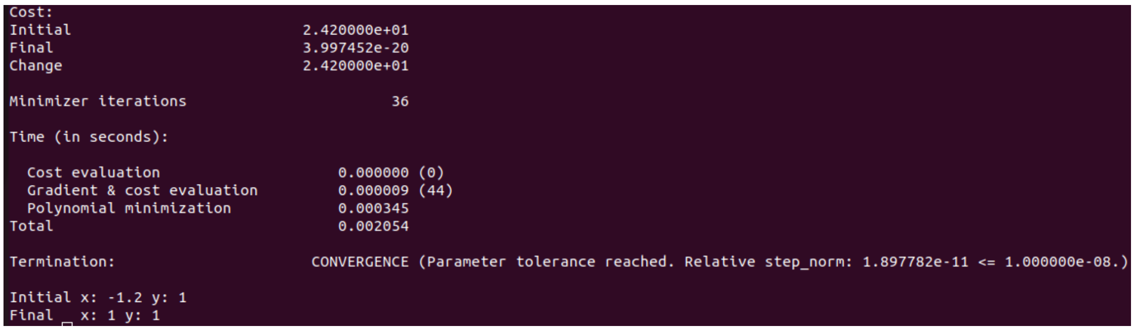
5 Ceres code

- Ceres Solver求解Rosenbrock函数极值

```
// f(x,y) = (1-x)^2 + 100(y - x^2)^2;
struct Rosenbrock {
  bool operator()(const double* parameters, double* cost) const {
    const double x = parameters[0];
    const double y = parameters[1];
    cost[0] = (1.0 - x) * (1.0 - x) + 100.0 * (y - x * x) * (y - x * x);
    return true;
  }

  static ceres::FirstOrderFunction* Create() {
    constexpr int kNumParameters = 2;
    return new ceres::NumericDiffFirstOrderFunction<Rosenbrock,
                                                    ceres::CENTRAL,
                                                    kNumParameters>(
        new Rosenbrock);
  }
};
```

- C++完整代码

```cpp
#include "ceres/ceres.h"
#include "glog/logging.h"

// f(x,y) = (1-x)^2 + 100(y - x^2)^2;
struct Rosenbrock {
  bool operator()(const double* parameters, double* cost) const {
    const double x = parameters[0];
    const double y = parameters[1];
    cost[0] = (1.0 - x) * (1.0 - x) + 100.0 * (y - x * x) * (y - x * x);
    return true;
  }

  static ceres::FirstOrderFunction* Create() {
    constexpr int kNumParameters = 2;
    return new ceres::NumericDiffFirstOrderFunction<Rosenbrock,
                                                    ceres::CENTRAL,
                                                    kNumParameters>(
        new Rosenbrock);
  }
};

int main(int argc, char** argv) {
  google::InitGoogleLogging(argv[0]);

  double parameters[2] = {-1.2, 1.0};

  ceres::GradientProblemSolver::Options options;
  options.minimizer_progress_to_stdout = true;

  ceres::GradientProblemSolver::Summary summary;
  ceres::GradientProblem problem(Rosenbrock::Create());
  ceres::Solve(options, problem, parameters, &summary);

  std::cout << summary.FullReport() << "\n";
  std::cout << "Initial x: " << -1.2 << " y: " << 1.0 << "\n";
  std::cout << "Final   x: " << parameters[0] << " y: " << parameters[1]
            << "\n";
  return 0;
}
```



```
Cost:
Initial                           2.420000e+01
Final                             3.997452e-20
Change                            2.420000e+01

Minimizer iterations                        36

Time (in seconds):

  Cost evaluation                     0.000000 (0)
  Gradient & cost evaluation          0.000009 (44)
  Polynomial minimization             0.000345
Total                                 0.002054

Termination:                       CONVERGENCE (Parameter tolerance reached. Relative step_norm: 1.897782e-11 <= 1.000000e-08.)

Initial x: -1.2 y: 1
Final   x: 1 y: 1
```