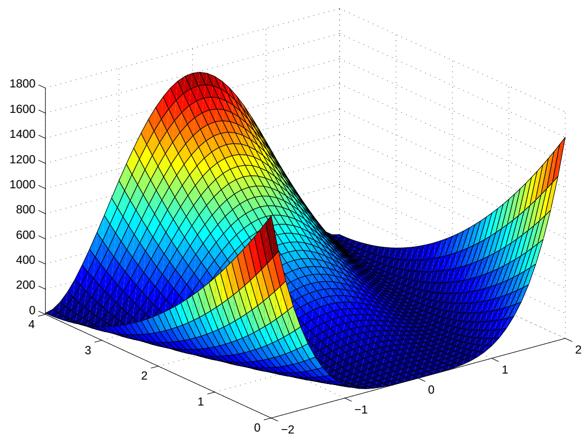
CS5321 Numerical Optimization Homework 3

Due April 8

1. (50%) The Rosenbrock function $f(x, y) = (1-x)^2 + 100(y-x^2)^2$ is shown below, whose minimizer is at $(1, 1)$.[1]



   (a) Derive the gradient and the Hessian of $f(x, y)$.

   (b) Read the Matlab code `polyline.m` and `polymod.m` in

   `http://www4.ncsu.edu/~ctk/matlab_darts.html`

   and explain which line search algorithm they are implemented.

   (c) Use $(x_0, y_0) = (-1.2, 1.0)$ to test the steepest descent method with the line search algorithm, implemented in `steep.m` (in the same repository as (b)), and plot its trace $\{(x_k, y_k)\}$. When calling `steep`, the code is like `[x, ...]=steep(x0,@rosenbrock, ...)`. You may modify the code to recode the $\{(x_k, y_k)\}$ and use the plotting code from homework 2.

   (d) Implement Newton's method with line search algorithm, and test it with $(x_0, y_0) = (-1.2, 1.0)$. Plot its trace and compare the results, such as the number of iterations, to (c).

[1] You can find reference of this function in MO and Wikipedia.

2. (25%) We had shown in class that when the line-search algorithm satisfies the Wolfe conditions, $\cos^2\theta_k\|\nabla f_k\|^2 \to 0$, where $\cos\theta_k = \frac{-\vec{p}_k^T\nabla f_k}{\|\nabla f_k\|\|\vec{p}_k\|}$. (Assume $\|\vec{p}_k\| \neq 0$ and $\|\nabla f_k\| \neq 0$.) Therefore, if the search direction of a method satisfies $|\cos\theta_k| > \delta$ for all k, then we can prove that $\nabla f_k \to \vec{0}$.

(a) Assume the matrix norm used satisfies the submultiplicative property, i.e. $\|AB\| \leq \|A\|\|B\|$. Prove that $1/\|\vec{x}\| \geq 1/(\|B\vec{x}\|\|B^{-1}\|)$ for any nonsingular matrix B.

$$\|\vec{x}\| = \|B^{-1}B\vec{x}\| \leq \|B^{-1}\|\|B\vec{x}\|$$

Therefore, $1/\|\vec{x}\| \geq 1/(\|B\vec{x}\|\|B^{-1}\|)$.

(b) In the Newton-like methods, we replace the Hessian matrix with a symmetric positive definite matrix B_k, and use $\vec{p}_k = -B_k^{-1}\nabla f_k$ as the search direction. Use (a) to prove that if B_k is well conditioned, i.e. $\|B_k\|\|B_k^{-1}\| \leq M$ for some constant M, then

$$|\cos\theta_k| \geq \frac{1}{M}.$$

(Hint: you may use the following property directly: For any symmetric positive definite matrix B, $\vec{u}^TB\vec{u} \geq 1/\|B^{-1}\|$, where $\vec{u}$ is a unit vector, $\|\vec{u}\| = 1$.)

$$\begin{aligned}
|\cos\theta_k| &= \frac{|\vec{p}_k^T\nabla f_k|}{\|\nabla f_k\|\|\vec{p}_k\|} && \text{(by the definition of } \cos\theta_k.) \\
&= \frac{|\vec{p}_k^T B_k p_k|}{\|\nabla f_k\|\|\vec{p}_k\|} && \text{(by the relation } \vec{p}_k = -B_k^{-1}\nabla f_k.) \\
&\geq \frac{\|\vec{p}_k\|^2}{\|\nabla f_k\|\|\vec{p}_k\|\|B_k^{-1}\|} && \text{(by the property } \vec{u}^TB\vec{u} \geq 1/\|B^{-1}\|.) \\
&= \frac{\|\vec{p}_k\|}{\|\nabla f_k\|\|B_k^{-1}\|} && \text{(cancel out one } \|\vec{p}_k\|) \\
&\geq \frac{\|\vec{p}_k\|}{\|B_k^{-1}\nabla f_k\|\|B_k\|\|B_k^{-1}\|} && \text{(by (a))} \\
&= \frac{\|\vec{p}_k\|}{\|\vec{p}_k\|\|B_k\|\|B_k^{-1}\|} && \text{(by the relation } \vec{p}_k = -B_k^{-1}\nabla f_k.) \\
&= 1/\|B_k\|\|B_k^{-1}\| \geq 1/M && \text{(cancel out } \|\vec{p}_k\| \text{ and use the assumption.)}
\end{aligned}$$

3. (25%) Prove the formula of SR1.

(a) Verify the Sherman-Morrison-Woodbury formula.
For $\hat{A} = A + \vec{a}\vec{b}^T$,

$$\hat{A}^{-1} = A^{-1} - \frac{A^{-1}\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}}.$$

(Hint: prove $\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = I$.)

$$\begin{aligned}
\hat{A}\hat{A}^{-1} &= (A + \vec{a}\vec{b}^T)\left(A^{-1} - \frac{A^{-1}\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}}\right) \\
&= AA^{-1} - \frac{AA^{-1}\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}} + \vec{a}\vec{b}^T A^{-1} - \frac{\vec{a}\vec{b}^T A^{-1}\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}} \\
&= I + \vec{a}\vec{b}^T A^{-1} - \frac{\vec{a}\vec{b}^T A^{-1} + (\vec{b}^T A^{-1}\vec{a})\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}} \\
&= I + \vec{a}\vec{b}^T A^{-1} - \vec{a}\vec{b}^T A^{-1}\frac{1 + \vec{b}^T A^{-1}\vec{a}}{1 + \vec{b}^T A^{-1}\vec{a}} = I \\
\hat{A}^{-1}\hat{A} &= \left(A^{-1} - \frac{A^{-1}\vec{a}\vec{b}^T A^{-1}}{1 + \vec{b}^T A^{-1}\vec{a}}\right)(A + \vec{a}\vec{b}^T) \\
&= A^{-1}A - \frac{A^{-1}\vec{a}\vec{b}^T A^{-1}A}{1 + \vec{b}^T A^{-1}\vec{a}} + A^{-1}\vec{a}\vec{b}^T - \frac{A^{-1}\vec{a}\vec{b}^T A^{-1}\vec{a}\vec{b}^T}{1 + \vec{b}^T A^{-1}\vec{a}} \\
&= I + A^{-1}\vec{a}\vec{b}^T - \frac{A^{-1}\vec{a}\vec{b}^T + (\vec{b}^T A^{-1}\vec{a})A^{-1}\vec{a}\vec{b}^T}{1 + \vec{b}^T A^{-1}\vec{a}} \\
&= I + A^{-1}\vec{a}\vec{b}^T - A^{-1}\vec{a}\vec{b}^T\frac{1 + \vec{b}^T A^{-1}\vec{a}}{1 + \vec{b}^T A^{-1}\vec{a}} = I
\end{aligned}$$

(b) Use (a) and the fact that B_k is symmetric to prove that if $B_k = B_{k-1} + \frac{(\vec{y}_k - B_{k-1}\vec{p}_k)(\vec{y}_k - B_{k-1}\vec{p}_k)^T}{(\vec{y}_k - B_{k-1}\vec{p}_k)^T\vec{p}_k}$, then

$$B_k^{-1} = B_{k-1}^{-1} + \frac{(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)^T}{\vec{y}_k^T(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)}.$$

Let $\vec{a} = \vec{y}_k - B_{k-1}\vec{p}_k$, $\vec{b} = \vec{a}/\rho$, where $\rho = \vec{a}^T\vec{p}_k = (\vec{y}_k - B_{k-1}\vec{p}_k)^T\vec{p}_k = \vec{y}_k^T\vec{p}_k - \vec{p}_k^T B_{k-1}\vec{p}_k$. Then we can rewrite $B_k = B_{k-1} + \vec{a}\vec{b}^T$. Compute the following terms

$$\begin{aligned}
B_{k-1}^{-1}\vec{a} &= B_{k-1}^{-1}(\vec{y}_k - B_{k-1}\vec{p}_k) = B_{k-1}^{-1}\vec{y}_k - \vec{p}_k && (1)\\
\vec{b}^T B_{k-1}^{-1} &= \frac{1}{\rho}(\vec{y}_k - B_{k-1}\vec{p}_k)^T B_{k-1}^{-1} = \frac{1}{\rho}(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)^T && (2)\\
\vec{b}^T B_{k-1}^{-1}\vec{a} &= \frac{1}{\rho}(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)^T(\vec{y}_k - B_{k-1}\vec{p}_k)\\
&= \frac{1}{\rho}(\vec{y}_k^T B_{k-1}^{-1} - \vec{p}_k^T)(\vec{y}_k - B_{k-1}\vec{p}_k)\\
&= \frac{1}{\rho}(\vec{y}_k^T B_{k-1}^{-1}\vec{y}_k - \vec{y}_k^T\vec{p}_k - \vec{p}_k^T\vec{y}_k + \vec{p}_k^T B_{k-1}\vec{p}_k)\\
&= \frac{1}{\rho}(\vec{y}_k^T B_{k-1}^{-1}\vec{y}_k - \vec{y}_k^T\vec{p}_k - \rho) && (3)
\end{aligned}$$

By the Sherman-Morrison-Woodbury formula,

$$\begin{aligned}
B_k^{-1} &= B_{k-1}^{-1} - \frac{B_{k-1}^{-1}\vec{a}\vec{b}^T B_{k-1}^{-1}}{1 + \vec{b}^T B_{k-1}^{-1}\vec{a}}\\
&= B_{k-1}^{-1} - \frac{(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)^T/\rho}{1 + (\vec{y}_k^T B_{k-1}^{-1}\vec{y}_k - \vec{y}_k^T\vec{p}_k - \rho)/\rho} \text{(using(1)(2)(3))}\\
&= B_{k-1}^{-1} - \frac{(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)(B_{k-1}^{-1}\vec{y}_k - \vec{p}_k)^T}{\rho + (\vec{y}_k^T B_{k-1}^{-1}\vec{y}_k - \vec{y}_k^T\vec{p}_k - \rho)} \text{(scaling by } \rho\text{)}\\
&= B_{k-1}^{-1} + \frac{(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)^T}{\vec{y}_k^T(\vec{p}_k - B_{k-1}^{-1}\vec{y}_k)} \text{(flipping the sign.)}
\end{aligned}$$