

Problem Set # 3

Part A: Analytical (Due September 22, 2009)

1. The Armijo step size rule can be combined with a quadratic interpolation scheme as follows. Given s , s_{LB} (a lower bound on s), β , and σ such that $0 < s_{LB} < s$, $0 < \beta < 1$, $0 < \sigma < 1/2$, the current point \underline{x}_k and the direction \underline{d}_k , compute $f(\underline{x}_k + s\underline{d}_k)$. The procedure is:

a) Fit a parabola $h(\alpha) = a\alpha^2 + b\alpha + c$ such that $h(0) = f(\underline{x}_k)$, $h(s) = f(\underline{x}_k + s\underline{d}_k)$, and $h'(0) = \underline{g}_k^T \underline{d}_k$, where \underline{g}_k is the gradient of $f(\underline{x})$ at $\underline{x} = \underline{x}_k$. Determine a , b , and c . The minimum point is $\alpha_k^* = -b/2a$.

b) The initial step size for the Armijo rule is determined from:

$$s_k = \begin{cases} s & \text{if } f(\underline{x}_k + \alpha^* \underline{d}_k) \geq f(\underline{x}_k + s\underline{d}_k) \\ \alpha^* & \text{if } f(\underline{x}_k + \alpha^* \underline{d}_k) < f(\underline{x}_k + s\underline{d}_k) \\ s_{LB} & \text{otherwise} \end{cases}$$

c) Apply Armijo step size rule.

Devise an algorithm based on a), b) and c) above.

2. Use Golden Section Search to determine (within an interval of 0.6) the optimal solution to: $\min (e^x - x)$ subject to $-1 \leq x \leq 3$.

3. (How to Estimate the rate of convergence and number of iterations?)

Consider the problem

$$\text{minimize } f(x, y) = 5x^2 - xy + 5y^2 - 11x + 11y + 11$$

- Find a point satisfying the first-order necessary conditions for a solution.
- Show that the point is a global minimum.
- What would be the rate of convergence of steepest descent for this problem?
- Starting at $x=y=0$, how many steepest descent iterations would it take (at most) to reduce the function value to 10^{-11} ?

4. (How to effectively reduce the condition number or improve convergence rate?)

Let $\underline{\xi}_1, \underline{\xi}_2, \dots, \underline{\xi}_n$ denote the eigenvectors of the symmetric positive definite $n \times n$ matrix Q . For the quadratic problem considered in class, suppose \underline{x}_0 is chosen so that \underline{g}_0 belongs to a subspace M spanned by a subset of the $\{\underline{\xi}_j\}$. Show that for the method of steepest descent $\underline{g}_k \in M$ for all k . Find the rate of convergence in this case.

5. (Why Steepest Descent can tolerate inaccurate line searches?)

Suppose we use the method of steepest descent to minimize the quadratic function $f(\underline{x}) = \frac{1}{2}(\underline{x} - \underline{x}^*)^T Q(\underline{x} - \underline{x}^*)$ but we allow a tolerance of $\pm \delta \alpha_k, \delta \geq 0$ in the line search, that is,

$$\underline{x}_{k+1} = \underline{x}_k - \alpha_k \underline{g}_k,$$

where

$$(1 - \delta)\bar{\alpha}_k \leq \alpha_k \leq (1 + \delta)\bar{\alpha}_k$$

and $\bar{\alpha}_k$ minimizes $f(x_k - \alpha g_k)$ over α .

- a) Find the convergence rate of the algorithm in terms of λ_{\max} and λ_{\min} , the largest and the smallest eigenvalues of Q and the tolerance δ . (*Hint: Assume the extreme case $\alpha_k = (1 \pm \delta)\bar{\alpha}_k$*).
- b) What is the largest δ that guarantees convergence of the algorithm? Explain the result geometrically.
- c) Does the sign of δ make any difference?

6. (*Stopping Criterion and Aitken's acceleration process*)

A question that arises in using an algorithm such as the steepest descent to minimize an objective function f is when to stop the iterative process. In other words, how can one tell when the current point is close to a solution? If, as with the steepest descent, it is known that convergence is linear, this knowledge can be used to develop a stopping criterion. Let $\{f_k\}_{k=0}^{\infty}$ be the sequence of values obtained by the algorithm. We assume that $f_k \rightarrow f^*$ linearly, but both f^* and the convergence ratio β are unknown. However, we know that, at least approximately,

$$f_{k+1} - f^* = \beta(f_k - f^*)$$

and

$$f_k - f^* = \beta(f_{k-1} - f^*)$$

These two equations can be solved for β and f^* .

- a) Show that

$$f^* = \frac{f_k^2 - f_{k-1}f_{k+1}}{2f_k - f_{k-1} - f_{k+1}}$$

$$\beta = \frac{f_{k+1} - f_k}{f_k - f_{k-1}}$$

- b) Motivated by the above, we form the sequence $\{f_k^*\}$ defined by

$$f_k^* = \frac{f_k^2 - f_{k-1}f_{k+1}}{2f_k - f_{k-1} - f_{k+1}}$$

as the original sequence is generated. This procedure of generating $\{f_k^*\}$ from $\{f_k\}$ is called the Aitken δ^2 -process. If $|f_k - f^*| = \beta^k + O(\beta^k)$, show that $|f_k^* - f^*| = O(\beta^k)$, which means that $\{f_k^*\}$ converges to f^* faster than $\{f_k\}$ does. The iterative search for the minimum can then be terminated when $(f_k - f_k^*)$ is smaller than some prescribed tolerance.

7. Problem 1.2.6 of Bertsekas, Page 55.

Part B: Computational (Due October 6, 2009)

Extensively test the computer subroutines LSEARCH (Golden section + quadratic interpolation) and LSEARCH2 (Armijo + quadratic interpolation) for minimizing a scalar function $(0,\infty)$. The program LSEARCH operates in three steps:

1. Finds three point pattern;
2. Use golden section search until the uncertain interval is cut sufficiently short;
3. Use quadratic fit to obtain the final result.

Sample MATLAB code is in huskyct for LSEARCH and LSEARCH2, as well as some old Fortran code for LSEARCH only below. My recommendation is that you use the attached code as a guideline for writing your own code. The inputs of LSEARCH (for the Fortran version below) include: FNCL (function value at $x=0$), EST (a priori estimate of the optimal), DELTA (step length to obtain a three point pattern), and HOF (value of the function for a given x). The outputs include: ALPHA (the optimal step size), FNCL (optimal function value), and NFCNS (number of function evaluations). You should write a routine that computes EST and DELTA. The choice of a rich set of test functions that demonstrate your effort and ideas will be critical. Test functions should include at least 10 scalar functions of your choice. These functions should span polynomials, ratio of polynomials, trigonometric and logarithmic functions. Furthermore, you should consider functions that are piecewise polynomial and discontinuous. Note that all functions must have derivatives less than zero at zero.

1. Examine 2 or more techniques for picking the initial parameters EST and DELTA. For this part, assume the following values for two parameters: $PG=30$ and $PQ = 10$. Discuss your results in detail. Tell which technique you recommend on the basis of numerical testing using your set of test functions.
2. Determine the "best" value of PG if PQ is fixed at 10, 100, 1000, and 10000 (Note that $PG > PQ$). For this work, assume EST is as you found in part 1, but take $DELTA = EST$.

Note that you will need to write specific code for each function to be minimized. Also, you may need a function that returns $df(x)/dx$, especially if you plan to get EST from $df(x)/dx|_{x=0}$. **Do this and all future computer assignments in Teams of two.**

All future programs will be graded as follows:

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| a. Working program | 25% |
| b. Program and Algorithm Documentation | 25% |
| c. Extensive Testing | 25% |
| d. Discussion of Results | 25% |

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c
c  Subroutines for line search algorithms
c
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  subroutine lsearch(fxk,gradf,xk,dk,alpha,nfcnev)
  include 'param.dim'
  real xk(nn),dk(nn),gradf(nn),fxk,alpha,eta,est,
    $      gfder,delta,s,sigma,scale
  integer nfcnev,flag1,lines,nfcnf
  common/line/lines,eta,flag1,s,sigma,scale
  common/gradn/n,h,idiff
  if (lines.eq.1) then
c  **  Check function and derivative
    if (fxk.eq.0.) fxk=fxk+eta
102   gfder=dot(n,gradf,dk)
    if (gfder.le.0) then
      if (gfder.eq.0) gfder=gfder-eta
      if (flag1.eq.1) call init1(n,fxk,gfder,est,delta)
      if (flag1.eq.2) then
        call init2(n,xk,dk,fxk,gfder,nfcnf,est,delta)
        nfcnev=nfcnev+nfcnf
      endif
    else
      do 120 i=1,n
        dk(i)=-gradf(i)
120   continue
      print *,''
c      print *,'***** ERROR :Gradient TOO BIG *****'
c      STOP
    endif
    call lserch(n,xk,dk,alpha,fxk,nfcns,est,delta,pq,pg,tol)
    nfcnev=nfcnev+nfcns
  else

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        call lserc2(n,gradf,dk,nfcnf,s,sigma,scale,alpha,fxk,xk)
        nfcnev=nfcnev+nfcnf
    endif
return
end

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c
c  SUBROUTINE line search : uses GOLDEN SECTION rule and
c                          QUADRATIC INTERPOLATION
c
c  SUBROUTINE LSEARCH(n,xk,dk,alpha,fxk,nfcns,est,delta,pq,pg,tol)
include 'param.dim'
integer n
real xk(nn),dk(nn)
real *8 dble,x0,y0,s1,s2
common/a3/nfcnev,ndrv,iter,ipr,ifg
alpmax = 10000
alpmin = 1e-05
nalpha = 0
alpha = 0.0
tau = 1.61803
rtau = 0.61803
nfcns=0
z0 = 0.0
hz0 = fxk

c
c  Three point pattern set up
c      if delta = est use h(0,0) point
c      if delta .ne. est use h(est-delta) point
c
c  if(abs(delta-est).le.tol*est) goto 400
z1 = est
hz1 = hof(n,xk,z1,dk)
nfcns=nfcns+1
if(hz1 .ge. hz0) goto 100

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380 z0 = z1 - delta
    if(z0.gt.alpmin)      goto 390
    z0=alpmin
    hz0=hof(n,xk,z0,dk)
    nfcns=nfcns+1
    goto 500
390    hz0 = hof(n,xk,z0,dk)
    nfcns=nfcns+1
    if(hz0.gt.hz1)  goto 156
    z2=z1
    z1 = z0
    hz2=hz1
    hz1 = hz0
    goto 380
400    z0 = 0.0
    hz0 = fxx
155    z1 = delta + z0
    hz1 = hof(n,xk,z1,dk)
    nfcns=nfcns+1
    if(hz1.ge.hz0)  goto 100
156 r = 1.0
    l = 1
300    l = l + 1
    r = r*tau
    z2 = z1 + r*delta
c
c    Check if z2 is still within allowable range
c
    if(z2.le.alpmax)  goto 302
c
c    Have hit the boundary in an attempt to set up a 3 point pattern
c    set alpha to alpmax and see if hof(alpmax) < hof(z1)
c
    z2 = alpmax
    hz2 = hof(n,xk,z2,dk)

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nfcns=nfcns+1
if(hz2.gt.hz1) goto 500
c
c hz2>hz1 ==>3 point pattern found( not in GS): goto Quadratic fit,
c hz2<hz1 ==>alpmax is best alpha in this direction
c
goto 305
302 hz2 = hof(n,xk,z2,dk)
nfcns=nfcns+1
if(hz2.ge.hz1) goto 200
z0 = z1
hz0 = hz1
z1 = z2
hz1 = hz2
if(l.lt.15) goto 300
print *,'could not bracket minimum in 15 steps'
305 alpha = z2
hz1 = hz2
306 print *,' Could not set up 3-pt pattern; returning best alpha'
goto 900
100 z2 = z1
hz2 = hz1
z1 = z0 + rtau*rtau*(z2-z0)
hz1 = hof(n,xk,z1,dk)
nfcns=nfcns+1
if(hz1.lt.hz0) goto 200
if(abs(z1).ge.alpmin) goto 100
747 continue
alpha = 0.0
hz1 = hz0
goto 900
c
c Start the GOLDEN SECTION search to PG accuracy
c
200 continue

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iflg = 1
alpha = z1
450   ppg = ((z2-z0)/(2.0*z1))*100.0
451   nalpha = nalpha + 1
      if(nalpha.lt.11)      goto 505
      alpha = z1
      goto 900
505   if(ppg.le.pg) goto 500
      if(abs(z1).lt.alpmin) goto 747
      if(iflg.eq.1) goto 250
      z = z1
      hz = hz1
      z1 = z0 + rtau*(z-z0)
      hz1 = hof(n,xk,z1,dk)
      nfcns=nfcns+1
      goto 800
250   z = z0 + rtau*(z2-z0)
      hz = hof(n,xk,z,dk)
      nfcns=nfcns+1
800   if(hz.gt.hz1) goto 600
      z0 = z1
      hz0 = hz1
      z1 = z
      hz1 = hz
      iflg = 1
      goto 450
600   z2 = z
      hz2 = hz
      iflg = 0
      goto 450
c
c   Start QUADRATIC fit to PQ accuracy
c
500   continue
510   alpha = z1

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      ppq = ((z2-z0)/(2.0*z1))*100.0
455 if(nalpha.gt.20)      goto 900
      if(ppq.le.PQ) goto 900
      if(abs(z1).lt.alpmin) goto 747
      nalpha = nalpha + 1
      A32 = z2 - z1
      A21 = z1 - z0
      s1 = dble(hz0 - hz1)/dble(A21)
      s2 = dble(hz2 - hz1)/dble(A32)
      if(s1.lt.0.0000000001.And.s2.lt.0.0000000001) goto 900
456      x0= dble(A32)*s1 - dble(A21)*s2
      y0= s1 + s2
      x0= (x0/y0) * 0.5D0
      amin = dble(z1) + x0
      if(amin.lt.alpmax) goto 512
      alpha = z1
      goto 900
512 if(abs(amin-z1).le.tol*z1) goto 900
      hmin = hof(n,xk,amin,dk)
      nfcns=nfcns+1
      if(amin.gt.z1) goto 540
      if(hmin.ge.hz1) goto 530
      z2 = z1
      hz2 = hz1
525 z1 = amin
      hz1 = hmin
      goto 510
530      z0 = amin
      hz0 = hmin
      goto 510
540      if(hmin.ge.hz1) goto 550
      z0 = z1
      hz0 = hz1
      goto 525
550      z2 = amin

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        hz2 = hmin
        goto 510
900 fvk=hz1
        do 50 i=1,n
            xk(i)=xk(i)+alpha*dk(i)
50 continue
        return
        end
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c
c  SUBROUTINE line search : uses ARMIJO STEP SIZE rule and
c                           QUADRATIC INTERPOLATION
c
c  SUBROUTINE LSERC2(n,gradf,dk,nfcnf,s,sigma,scale,alpha,fxk,
    $                      xk)
c  include 'param.dim'
c  integer n,nfcnf
c  real hof,gradf(nn),dk(nn),s,sigma,scale,alpha,lambdak,xk(nn),
    $      temp,galpha,glambda,fxk,l
c  l=.1
c  alpmax=1000
c  alpmin=1e-07
c  nfcnf=0
c  alpha=s
c  temp=dot(n,gradf,dk)
100 galpha=hof(n,xk,alpha,dk)
    nfcnf=nfcnf+1
    if (nfcnf.ge.100) then
        print *, '# of fn evaluations exceeded; nfcnf =',nfcnf
        goto 200
    endif
c  execute this while condition on alpha holds; else exit
    if (galpha.gt.(fxk+sigma*alpha*temp)) then
        lambdak=-0.5*(alpha*alpha*temp)/(galpha-alpha*temp-fxk)
        glambda=hof(n,xk,lambdak,dk)

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        nfcnf=nfcnf+1
c   update alpha
        if (glambda.lt.galpha) then
            if (lambdak.ge.l*alpha) then
                alpha=lambdak
            else
                alpha=l*alpha
            endif
        else
            alpha=alpha/scale
        endif
c   check if we have hit the boundary; then exit
        if (alpha.gt.alpmax) then
            alpha=alpmax
            galpha=hof(n,xk,alpha,dk)
            nfcnf=nfcnf+1
            goto 200
        endif
        if (alpha.lt.alpmin) then
            alpha=alpmin
            galpha=hof(n,xk,alpha,dk)
            nfcnf=nfcnf+1
            goto 200
        endif
        goto 100
    else
200   fvk=galpha
        do 50 i=1,n
            xk(i)=xk(i)+alpha*dk(i)
50   continue
        endif
    return
end

```

