4. Implicit Loop and Vecorization

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Lab Note for MAT325 Numerical Analysis

Contents

1 Introduction

This lab note introduces how to reduce loops through vectorization. For any vectorized language, there are different extensions such as user-defined functions and routines to carry vectorized operation instead of element-wise operation. Most R functions are vectorized. We will use some examples to illustrate how a loop can be avoided if vectorization is available.

2 Implicit in R Primitive Functions

R was written in C. It has a long list of primitive functions written in C. Most of these functions are vectorized. Calling an internal vectorized function is the same as performing an implicit loop.

Example 1: Consider the sum of two matrices with the same dimension. Define

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 7 & 9 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 5 & 2 & 7 \\ 4 & 1 & 6 \end{pmatrix}$$

We find the sum of A and B

$$A + B = \begin{pmatrix} 6 & 4 & 10 \\ 7 & 8 & 15 \end{pmatrix}$$

Method 1: Using explicit loops. Since the sum of compatible matrices is an element-wise operation, in order to access individual elements, we need to use two indexes - one for the row and one for the column. We use the double loops to calculate the sum of two matrices in the following code.

```
loopSum = function(A,B){
    sumAB = matrix(0, nrow = dim(A)[1], ncol = dim(A)[2])
        for(i in 1:dim(A)[1]) {
            for (j in 1:dim(A)[2]){
                sumAB[i,j] = A[i,j] + B[i,j]
             }
         }
    sumAB
 }
```

We can also use R primitive function + to perform the matrix summation.

```
vectorSum = function(A,B) {A + B}
```

```
A = matrix(c(1,2,3,3,7,9), ncol = 3, byrow = TRUE)
B = matrix(c(5,2,7,4,1,6), ncol = 3, byrow = TRUE)
```

```
start <- Sys.time()
loopSum(A,B)
```

```
##      [,1] [,2] [,3]
## [1,]    6    4   10
## [2,]    7    8   15
```

```
print( Sys.time() - start )
```

```
## Time difference of 0.01308799 secs
```

```
start <- Sys.time()
vectorSum(A,B)
```

```
##      [,1] [,2] [,3]
## [1,]    6    4   10
## [2,]    7    8   15
```

```
print( Sys.time() - start )
```

```
## Time difference of 0.001881123 secs
```

Example 2: Summation of large matrices.

```
A0 = matrix(runif(10000000), ncol = 5000)
B0 = matrix(runif(10000000), ncol = 5000)
```

```
start <- Sys.time()
AplusB.lp = loopSum(A0,B0)
print( Sys.time() - start )
```

```
## Time difference of 1.402006 secs
```

```
start <- Sys.time()
AplusB.vec = vectorSum(A0,B0)
print( Sys.time() - start )
```

```
## Time difference of 0.06303811 secs
```

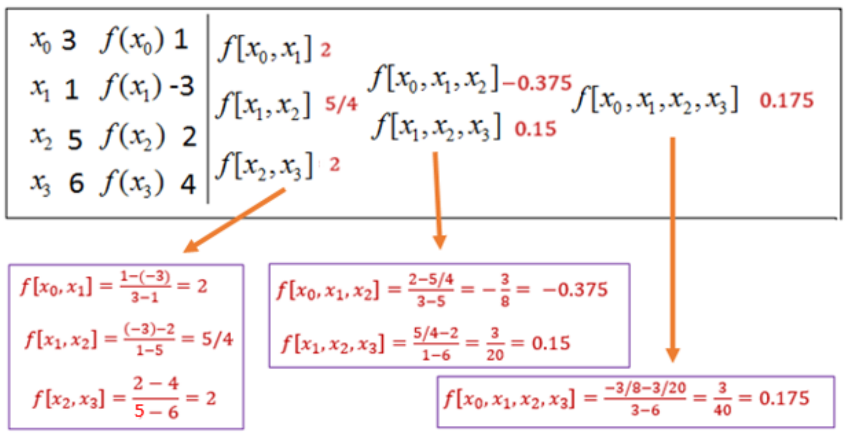
The obvious benefits of using an implicit vectorized primitive function to perform matrix operation:

1. The code is simple.
2. It is faster.

3 Some Vectorized Primitive Functions

Since the numerator and denominator are defined as the difference between adjacent terms. We can vectorize these differences using the R function **diff()** that computes the difference between pairs of consecutive elements of a numeric vector.

Example 2: Consider `vec.x = (1, 1.3, 1.6, 1.9, 2.2)` and `vec.y = (0.7651977, 0.6200860, 0.4554022, 0.2818186, 0.1103623)`. We use the **diff()** to calculate the divided differences in the following table step by step.



The following are manual steps for calculating the divided differences in the above table.

- *Step 1*: zero-th order divided differences (i = 1)

```
vec.x = c(3,1,5,6)
vec.y = c(1,-3,2,4)
n = length(vec.x)
```

- *Step 2*: The first order divided differences (i = 2)

```
i=2
## divided difference
i2.y = diff(vec.y)
i2.x = vec.x[-(1:(i-1))] - vec.x[-((n+2-i):n)]
i2.divDif = i2.y/i2.x
cbind(i2.y = i2.y, i2.x = i2.x, i2.divDif = i2.divDif)
```

```
##      i2.y i2.x i2.divDif
## [1,]   -4   -2      2.00
## [2,]    5    4      1.25
## [3,]    2    1      2.00
```

- *Step 3*: The first order divided differences (i = 3)

```
i = 3
i3.y = diff(i2.divDif)    # Caution
i3.x = vec.x[-(1:(i-1))] - vec.x[-((n+2-i):n)]
i3.divDif = i3.y/i3.x
cbind(i3.y = i3.y, i3.x = i3.x, i3.divDif = i3.divDif)
```

```
##       i3.y i3.x i3.divDif
## [1,] -0.75    2    -0.375
## [2,]  0.75    5     0.150
```

- *Step 4*: The first order divided differences (i = 4)

```
i = 4
i4.y = diff(i3.divDif)
i4.x = vec.x[-(1:(i-1))] - vec.x[-((n+2-4):n)]
i4.divDif = i4.y/i4.x
cbind(i4.y = i4.y, i4.x = i4.x, i4.divDif = i4.divDif)
```

```
##       i4.y i4.x i4.divDif
## [1,] 0.525    3     0.175
```

4 Divided Difference Variants

Recall the definitions of the divided difference in the Newton form interpolation.

$$N_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \cdots + f[x_0, \cdots, x_n](x - x_0)\cdots(x - x_{n-1})$$

x	$f(x)$	First divided differences	Second divided differences	Third divided differences
x_0	$f[x_0]$			
		$f[x_0,x_1] = \dfrac{f[x_1]-f[x_0]}{x_1-x_0}$		
x_1	$f[x_1]$		$f[x_0,x_1,x_2] = \dfrac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$	
		$f[x_1,x_2] = \dfrac{f[x_2]-f[x_1]}{x_2-x_1}$		$f[x_0,x_1,x_2,x_3] = \dfrac{f[x_1,x_2,x_3]-f[x_0,x_1,x_2]}{x_3-x_0}$
x_2	$f[x_2]$		$f[x_1,x_2,x_3] = \dfrac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$	
		$f[x_2,x_3] = \dfrac{f[x_3]-f[x_2]}{x_3-x_2}$		$f[x_1,x_2,x_3,x_4] = \dfrac{f[x_2,x_3,x_4]-f[x_1,x_2,x_3]}{x_4-x_1}$
x_3	$f[x_3]$		$f[x_2,x_3,x_4] = \dfrac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$	
		$f[x_3,x_4] = \dfrac{f[x_4]-f[x_3]}{x_4-x_3}$		$f[x_2,x_3,x_4,x_5] = \dfrac{f[x_3,x_4,x_5]-f[x_2,x_3,x_4]}{x_5-x_2}$
x_4	$f[x_4]$		$f[x_3,x_4,x_5] = \dfrac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}$	
		$f[x_4,x_5] = \dfrac{f[x_5]-f[x_4]}{x_5-x_4}$		
x_5	$f[x_5]$			

```
NewtonInterp = function(xvec,
                        yvec = NULL,
                        fn = NULL,
                        pred.x
                        ){
 if(length(yvec)==0) yvec = fn(xvec)
 n=length(xvec)
 DivDiff = rep(0,n)          # zero vector to store divided differences
 NewtonBasis = rep(0,1)      # zero vector to store Newton form basis polynomial
 DivDiff[1]=yvec[1]          # 1st order divided difference loaded to the first
 NewtonBasis[1]=1            # zero-degree basis polynomial
 old.NewtonBasis = 1         # initialize Newton basis polynomial for updating newer basis
 ##
 for (i in 2:n){
```

```
    NewtonBasis[i] = old.NewtonBasis*(pred.x-xvec[i-1])  # updating Basis polynomial
    dfx = xvec[-(1:(i-1))] - xvec[-((n-(i-2)):n)]         # denominator in the divided difference
    dy = diff(yvec)              # difference of lower order divided difference for the numerator
    ##
    DivForm = dy/dfx                    # new vector of divided differences
    DivDiff[i]=DivForm[1]               # pick the top one store in the vector of DivDiff
    yvec = DivForm                      # updating for operation in the next row
    old.NewtonBasis = NewtonBasis[i]    # updating Newton basis polynomial
   }
 Nx=sum(DivDiff*NewtonBasis)            # predicted y value of the given pred.x
 list(Pred.y = Nx, DividedDifference = DivDiff, NewtonBasis = NewtonBasis)
}
```

Example 3: Reproduce the result in the above illustrative table.

```
vec.x = c(3,1,5,6)
vec.y = c(1,-3,2,4)
example1 = NewtonInterp(yvec = vec.y, xvec = vec.x, pred.x = 5)
example1
```

```
## $Pred.y
## [1] 2
##
## $DividedDifference
## [1]  1.000  2.000 -0.375  0.175
##
## $NewtonBasis
## [1] 1 2 8 0
```

```
sum(example1$DividedDifferenc* example1$NewtonBasis)
```

```
## [1] 2
```

Example 5: Reproduce *Example 1* of Burden and Faires' textbook, 9th edition, page 127) Complete the divided difference table for the following data.

x	y
1.0	0.7651977
1.3	0.6200860
1.6	0.4554022
1.9	0.2818186
2.2	0.1103623

```
vec.x = c(1, 1.3, 1.6, 1.9, 2.2)
vec.y = c(0.7651977, 0.6200860, 0.4554022, 0.2818186, 0.1103623)
example2 = NewtonInterp(yvec = vec.y, xvec = vec.x, pred.x = 1)
example2
```

```
## $Pred.y
## [1] 0.7651977
##
## $DividedDifference
## [1]  0.765197700 -0.483705667 -0.108733889  0.065878395  0.001825103
##
## $NewtonBasis
```

```
## [1] 1 0 0 0 0
```

```
sum(example2$DividedDifferenc* example2$NewtonBasis)
```

```
## [1] 0.7651977
```

5 Vectorizing NewtonInterp()

Next, we vectorize the above R function for Newton interpolation polynomial so that it can take a vector input. We will also compare this new function with the two R functions created in the lecture note.

```
Vectorizing.Newton = function(xvec,
                                yvec = NULL,
                                fn = NULL,
                                pred.x     # numerical vector or scalar input
                        ){
 if(length(yvec) == 0) yvec = fn(xvec)
 n = length(xvec)
 m = length(pred.x)            # dimension of the input vector for prediction
 NewtonPolynomial = rep(0, m)  # predicted value of the Newton interpolation polynomial
 for (k in 1:m){
    yvec0 = yvec     # CAUTION: Must be REINSTATED! diff(yvec) will change its original values!!
    DivDiff = rep(0,n)         # zero vector to store divided differences
    NewtonBasis = rep(0,1)     # zero vector to store Newton form basis polynomial
    DivDiff[1] = yvec[1]       # 1st order divided difference loaded to the first
    NewtonBasis[1] = 1         # zero-degree basis polynomial
    old.NewtonBasis = 1        # initialize Newton basis polynomial for updating the newer basis
    ##
    for (i in 2:n){
       NewtonBasis[i] = old.NewtonBasis*(pred.x[k]-xvec[i-1])  # updating basis polynomial
       dfx = xvec[-(1:(i-1))] - xvec[-((n-(i-2)):n)]     # denominator in the divided difference
       dy = diff(yvec0)         # difference of lower order divided difference for the numerator
       DivForm = dy/dfx         # new vector of divided differences
       #cat("\n\n Inner loop:",i,". dfx =",dfx, ". dy =", dy, ". ")
       DivDiff[i] = DivForm[1]  # pick 1st component to store in vector DivDiff
       yvec0 = DivForm          # updating for operation in the next row
       old.NewtonBasis = NewtonBasis[i]
      }
      NewtonPolynomial[k] = sum(DivDiff*NewtonBasis)
      #cat("\n\n",k,"-th Pred.y:",NewtonPolynomial,", Diff:", DivDiff, ", Basis:", NewtonBasis,".")
     }
 NewtonPolynomial
}
```

```
vec.x = c(1, 1.3, 1.6, 1.9, 2.2)
vec.y = c(0.7651977, 0.6200860, 0.4554022, 0.2818186, 0.1103623)
Vectorizing.Newton(yvec = vec.y, xvec = vec.x, pred.x = c(1, 2))
```

```
## [1] 0.7651977 0.2238754
```

For comparison, we copy the two functions in the lecture note.

```
Divided.Dif = function(
        vec.x,          # input nodes:
        vec.y = NULL,   # one of vec.y and fn must be given
        fn = NULL,
```

```
        pred.x          # scalar x for predicting pn(pred.x)
         ){
   n = length(vec.x)
   if (length(vec.y) == 0) vec.y = fn(vec.x) #
   node.x = vec.x
   A = matrix(c(rep(0,n^2)), nrow = n, ncol = n, byrow = TRUE)
   A[1,] = vec.y     # fill the first row with vec.y
   #
   for(i in 2:(n)){
     for(j in 1:(n-i+1)){
      denominator = vec.x[j] - vec.x[j+1+(i-2)]
      numerator = A[i-1,j]- A[i-1,j+1]
      A[i,j] = numerator/denominator
      }
    }
  A
 }
```

```
##################################################################################
##  Newton Interpolated Polynomial Approximation: vector-enabled input
##################################################################################

Looping.Newton = function( vec.x,            # input interpolation nodes
                                vec.y = NULL,
                                fn = NULL,        # either vec.y or fn must be provided
                                pred.x            # VECTOR INPUT!!!
                              ){
   if(length(vec.y) ==0) vec.y = fn(vec.x)
   DivDif = Divided.Dif(vec.x, vec.y)[,1]       # the values in the first column of the div dif matrix
   n = length(vec.x)
   ############
   m = length(pred.x)
   NV = rep(0, m)                  # values of Nn(pred.x)
   for(k in 1:m) {
   ################
   Nn = vec.y[1]                   # f[xo]
   for (i in 1:(n-1)){             # Must be n - 1 according to the last term in the polynomial
     cumProd = 1                   # initial value to calculate the cumulative product
     for(j in 1:i){                # forward difference formula
       cumProd = cumProd*(pred.x[k]-vec.x[j])   # updating the cumulative product in the inner loop
     }
      Nn = Nn + DivDif[i+1]*cumProd    # adding high order terms alliteratively to the Nn(x)
    }
    NV[k] = Nn                                 # return the value the Newton polynomial
   }
 NV
}
```

5.1

```
start <- Sys.time()
pred.x = c(1.6, 1.1, 2.0)   # pred.x is the argument is a local variable!
pred.NIPO = Vectorizing.Newton(xvec = c(1, 1.3, 1.6, 1.9, 2.2),
```

```
                    yvec = c(0.7651977, 0.6200860, 0.4554022, 0.2818186, 0.1103623),
                    pred.x = c(1.6, 1.1, 2.0))
pander(cbind(pred.x = pred.x, pred.NIP=pred.NIP0))
```

pred.x	pred.NIP
1.6	0.4554
1.1	0.7196
2	0.2239

```
print( Sys.time() - start )
```

```
## Time difference of 0.01124501 secs
```

```
start <- Sys.time()
pred.x = c(1.6, 1.1, 2.0)    # pred.x is the argument is a local variable!
pred.NIP = Looping.Newton(vec.x = c(1, 1.3, 1.6, 1.9, 2.2),
                    vec.y = c(0.7651977, 0.6200860, 0.4554022, 0.2818186, 0.1103623),
                    pred.x = c(1.6, 1.1, 2.0))
pander(cbind(pred.x = pred.x, pred.NIP=pred.NIP))
```

pred.x	pred.NIP
1.6	0.4554
1.1	0.7196
2	0.2239

```
print( Sys.time() - start )
```

```
## Time difference of 0.03061414 secs
```