

Fundamentals of Data Structures

Projects2 : Autograd for Algebraic Expressions



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Chapter 1 : Introduction

Problem

Description

Nowadays the application of automatic differentiation technology has greatly facilitated people's implementation and training of deep learning algorithms. Our task is to create an automatic differentiation program for algebraic expressions.

Input

Input an infix expression composed of brackets, operators including power(^), multiplication(*), division(/), addition(+) and subtraction(-), variables(strings of lowercase English letters) and literal constant.

Output

For each variable in the expression, output an arithmetic expression that represents the derivative of the input expression with respect to the variable.

Arrange the output in the lexicographical order of the variables.

Sample Input

```
1 | a+b^c*d
```

Sample Output

```
1 | a: 1
2 | b: c*1/b*b^c*d
3 | c: 1*ln(b)*b^c*d
4 | d: b^c*1
```

Algorithm Analysis

The whole Algorithm can be divided into three main parts:

- Input the infix expression and create an expression tree.
- Store all the variable names in the expression and sort them in lexicographical order.
- Output the derivative of the input expression with respect to each variable.

Chapter 2 : Algorithm Specification

Step 1 : Create the expression tree

We create a **Struct** to store the information of the nodes in the expression tree. Every nodes in the expression tree has three components. One is a string indicating the value of the node (may be an operator, a variable name or a constant number) and the other two are two pointers respectively indicating leftchild and rightchild of the node.

We need the data structure **Stack** to assist building the expression tree. Nodestack stores the subtrees created from the expression while opstack stores all the operators. Pseudo-code is shown below:

```
1  for(every ch in the expression){
2      if(ch=='(')
3          push '(' into the opstack;
4      if(ch==')'){//build a subtree from the expression in the brackets
5          pop operator from opstack;
6          while(operator!='('){
7              pop a,b from nodestack;
8              create subtree (a,operator,b)
9              push the subtree into nodestack;
10             pop operator from opstack;
11         }
12         pop '(' from opstack;
13     }
14     if(ch is a letter or a number)
15         add ch to a variable name;//it must be a component of variable name/a number
16     if(ch is an operator){
17         pop a,b from nodestack;
18         create subtree (a,operator,b)
19         push the subtree into nodestack;
20     }
21 }
22 while(opstack is not empty){
23     pop operator from opstack;
24     pop a,b from nodestack;
25     create subtree (a,operator,b)
26     push the subtree into nodestack;
27 }
28 pop root from nodestack;//root is the root of expression tree;
```

Step 2 : Store all variable names and sort

We use a **String Array** to store all variable names. Pseudo-code is shown below:

```

1  for(every ch in the expression){
2      if(ch is a letter or a number)
3          add ch to a variable name;
4      else if (variable name is not in the array)
5          add the variable name to the String Array;
6  }
7  sort all variable names;

```

Step 3 : Output

We define a function `differentiate(root,var)` to build an expression tree of the answer. Pseudo-code is shown below:

```

1  if(root==NULL)
2      return NULL;
3  if(root->value is a constant number)//F(x)=c,F'(x)=0
4      return NULL;
5  if(root->value==var)//F(x)=x,F'(x)=1
6      return node("1");
7  if(root->value is an operator){
8      left=differentiate(root->left,var);//get the derivative of left expression
9      right=differentiate(root->right,var);//get the derivative of right expression
10     if(root->value=="+" )//F(x)=f(x)+g(x),F'(x)=f'(x)+g'(x)
11         return subtree (left,"+",right);
12     if(root->value=="-" )//F(x)=f(x)-g(x),F'(x)=f'(x)-g'(x)
13         return subtree (left,"-",right);
14     if(root->value=="*" ){//F(x)=f(x)*g(x),F'(x)=f'(x)*g(x)+f(x)*g'(x)
15         build subtree s1 (left,"*",root->right);
16         build subtree s2 (root->left,"*",right);
17         return subtree s3 (s1,"+",s2);
18     }
19     if(root->value=="/" ){//F(x)=f(x)/g(x),F'(x)=[f'(x)*g(x)-f(x)*g'(x)]/g(x)^2
20         build subtree s1 (left,"*",root->right);
21         build subtree s2 (root->left,"*",right);
22         build subtree s3 (s1,"-",s2);
23         build subtree s4 (root->right,"^","2");
24         return subtree s5 (s3,"/",s4);
25     }
26     if(root->value=="^" ){//F(x)=f(x)^[g(x)],F'(x)=
27         [g'(x)*lnf(x)+g(x)*f'(x)/f(x)]*f(x)^g(x)
28         build subtree s1 (right,"*",ln(root->left));
29         build subtree s2 (root->right,"*",left);
30         build subtree s3 (s2,"/",root->left);
31         build subtree s4 (s1,"+",s3);
32         build subtree s5 (root->left,"^",root->right);
33         return subtree s6 (s4,"*",s5);
34     }
35 }

```

Chapter 3 : Testing Results

Test case 1

Test case 1 wants to test expression including "+,-,*,/"

Input

```
1 | a+b*c-d/e
```

Output

```
1 | a: 1
2 | b: 1*c
3 | c: b*1
4 | d: -1*e/e^2
5 | e: -(-d*1)/e^2
```

Test case 2

Test case 2 wants to test expression including "+,-,*,/,(,)"

Input

```
1 | (a+b)*c-(d-e)/f
```

Output

```
1 | a: 1*c
2 | b: 1*c
3 | c: (a+b)*1
4 | d: -1*f/f^2
5 | e: -(-1)*f/f^2
6 | f: -(-(d-e)*1)/f^2
```

Test case 3

Test case 3 wants to test expression including variables whose length is longer.

Input

```
1 | (aabbcc+ddffea)*ddfa-bb/ss*cc*(ddffs+ee)
```

Output

```
1 | aabbcc: 1*ddfa
2 | bb: -1*ss/ss^2*cc*(ddffs+ee)
3 | cc: -bb/ss*1*(ddffs+ee)
4 | ddfa: (aabbcc+ddffea)*1
5 | ddffea: 1*ddfa
6 | ddffs: -bb/ss*cc*1
7 | ee: -bb/ss*cc*1
8 | ss: -(-bb*1)/ss^2*cc*(ddffs+ee)
```

Test case 4

Test case 4 wants to test expression including forms of "^".

Input

```
1 | aa^2+2^aa+2^2+aa^aa
```

Output

```
1 | aa: 2*1/aa*aa^2+1*ln(2)*2^aa+(1*ln(aa)+aa*1/aa)*aa^aa
```

Test case 5

Test case 5 mix all the situations in Test case 1,2,3,4.

Input

```
1 | aa*10*bb+2^ab/ab+abb^abb/aab-(ba+bba)*baa^20
```

Output

```

1 aa: 1*10*bb
2 aab: (-abb^abb*1)/aab^2
3 ab: (1*ln(2)*2^ab*ab-2^ab*1)/ab^2
4 abb: (1*ln(abb)+abb*1/abb)*abb^abb*aab/aab^2
5 ba: -1*bba^20
6 baa: -(ba+bba)*20*1/baa*bba^20
7 bb: aa*10*1
8 bba: -1*bba^20

```

Chapter 4 : Analysis and Comments

Time Complexity

For step 1 : Creating the expression tree, we traverse all operators, variables and numbers in the expression, so the time complexity of step 1 is $O(n)$ (Assume the length of the expression is n).

For step 2 : Store all variable names and sort, we traverse the expression again and sort all variable names. The time complexity of Quick_sort Algorithm is $O(m \log m)$, so the time complexity of step 2 is $O(n) + O(m \log m) = O(n + m \log m)$ (Assume there are m variable names in the expression)

For step 3 : Output, firstly we differentiate all m variables and use the function m times. The function differentiate traverse all operators, variables and numbers in the expression tree and extend constant number of nodes, so the time complexity of step 3 is $O(mp)$ (Assume there are p nodes in the expression tree)

To sum up, the total time complexity of the program is $O(n + m \log m + mp)$ (n indicates the length of the expression, m indicates the number of the variables, p indicates the number of nodes in the expression tree)

Space Complexity

The whole program construct $c_1 * p$ nodes (c_1 is a constant), c_2 strings (c_2 is a constant) to store the expression and a string array (but the total length is the length of the expression). So the total space complexity is $O(p + n)$ (n indicates the length of the expression, p indicates the number of nodes in the expression tree)

Comments

The function of this program is still limited, for it can't support mathematic functions such as $\sin x$, $\cos x$, $\tan x$, $\ln x$, $\log(x, y)$, $\exp(x)$... Also it can't simplify both the input expression or the output expression. It still needs to be improved.

Appendix : Source Code

```
1  #include<iostream>
2  #include<string>
3  #include<algorithm>
4  using namespace std;
5
6  struct TreeNode{
7      string value;
8      TreeNode *left;
9      TreeNode *right;
10 };
11
12 struct Stack{//define a stack to build the expression tree from inorder expression
13     TreeNode *data[100];
14     int top;
15
16     void push(TreeNode *node){//pushing the node into the stack
17         data[++top]=node;
18     }
19
20     TreeNode *pop()//pop and acquire the top element in the stack
21     {
22         return data[top--];
23     }
24
25     TreeNode *visit()//acquire the top element in the stack
26     {
27         return data[top];
28     }
29
30     bool empty()//judge whether the stack is empty
31     {
32         return top==--1;
33     }
34 };
35
36 int precedence(char op){//get the precedence of the operator
37     switch(op){
38         case '^':return 3;break;
39         case '*':return 2;break;
40         case '/':return 2;break;
41         case '+':return 1;break;
42         case '-':return 1;break;
43         default:return -1;//define the precedence of a number or a variable is the
lowest
44     }
45 }
46
47 bool cmp(string s1,string s2){//the assisting function for quick_sort algorithm
48     return s1<s2;
49 }
50
51 bool isnumber(string s){//determine whether s is a number
52     for(int i=0;i<(int)s.length();i++)
53         if((s[i]<'0')||(s[i]>'9'))
```

```

51         return false;
52     return true;
53 }
54
55 bool isoperator(string s){//determine whether s is an operator
56     return (s[0]=='+' || (s[0]=='-') || (s[0]=='*') || (s[0]=='/') || (s[0]=='^'));
57 }
58
59 TreeNode* createnode(string s){//function for creating a new treenode
60     TreeNode *temp=new TreeNode;
61     temp->value=s;
62     temp->left=NULL;temp->right=NULL;
63     return temp;
64 }
65
66 TreeNode* buildtree(string expression){//function for building a tree
67     Stack nodestack,opstack;//nodestack stores variables,numbers;opstack stores
operators
68     nodestack.top=opstack.top=-1;//set the two tops
69     string var;//collect the variable name/number
70     for(int i=0;i<(int)expression.length();i++){
71         if(expression[i]=='(')//if we encounter left bracket,push it into opstack
for encountering right bracket
72             opstack.push(createnode(string(1,expression[i])));
73         else if(isalnum(expression[i]))//if expression[i] is a letter or
number,collect it into var
74             var+=expression[i];
75         else if(expression[i]==')'){//if we encounter right bracket,then create
expression tree in the brackets
76             if(!var.empty())//push the new variable into the stack
77             {
78                 nodestack.push(createnode(var));
79                 var.clear();//clear the string and start over
80             }
81             while((!opstack.empty())&&(opstack.visit()->value!="(")){//create until
we encounter left bracket
82                 TreeNode *op=opstack.pop();//get the operator
83                 TreeNode *rightnode=nodestack.pop();//get the numbers
84                 TreeNode *leftnode=nodestack.pop();
85                 op->left=leftnode;op->right=rightnode;//create the tree
86                 nodestack.push(op);//push the new tree back into the stack
87             }
88             opstack.pop();//pop the left bracket
89         }
90         else{//if expression[i] is an operator,then get two numbers from nodestack
and create the tree
91             if(!var.empty()){
92                 nodestack.push(createnode(var));
93                 var.clear();
94             }
95             while((!opstack.empty())&&(precedence(opstack.visit()-
>value[0])>precedence(expression[i]))){//if the precedence of previous operator is
greater,handle the operator first
96                 TreeNode *op=opstack.pop();
97                 TreeNode *rightnode=nodestack.pop();

```

```

98         TreeNode *leftnode=nodestack.pop();
99         op->left=leftnode;op->right=rightnode;
100         nodestack.push(op);
101     }
102     opstack.push(createnode(string(1,expression[i])));//push the new
operator into opstack
103     }
104 }
105 /*there is still a variable in var,a operator in opstack,a variable in
nodestack,create the tree*/
106 if(!var.empty()){
107     nodestack.push(createnode(var));
108     var.clear();
109 }
110 while(!opstack.empty()){
111     TreeNode *op=opstack.pop();
112     TreeNode *rightnode=nodestack.pop();
113     TreeNode *leftnode=nodestack.pop();
114     op->left=leftnode;op->right=rightnode;
115     nodestack.push(op);
116 }
117 return nodestack.pop();//return the headnode
118 }
119
120 TreeNode* addnodes(TreeNode *left,TreeNode *right){//merge leftnode,rightnode and
operator "+"
121 if(left==NULL)//if left is NULL then there is no need to print "+"(in case
"a")
122     return right;
123 if(right==NULL)//if right is NULL then there is no need to print "+"(in case
"a")
124     return left;
125     TreeNode *temp=createnode("+");
126     temp->left=left;temp->right=right;
127     return temp;
128 }
129
130 TreeNode* subnodes(TreeNode *left,TreeNode *right){//merge leftnode,rightnode and
operator "-"
131 if(right==NULL)//if right is NULL then there is no need to print "-"(in case
"a-")
132     return left;
133     TreeNode *temp=createnode("-");
134     temp->left=left;temp->right=right;
135     return temp;
136 }
137
138 TreeNode* mulnodes(TreeNode *left,TreeNode *right){//merge leftnode,rightnode and
operator "*"
139 if((left==NULL)|| (right==NULL))//if right or left is NULL then the whole result
is 0
140     return NULL;
141     TreeNode *temp=createnode("*");
142     temp->left=left;temp->right=right;
143     return temp;

```

```

144 }
145
146 TreeNode* divnodes(TreeNode *left,TreeNode *right){//merge leftnode,rightnode and
operator "/"
147     if((left==NULL)||(right==NULL))//if right or left is NULL then the whole result
is 0
148         return NULL;
149     TreeNode *temp=createnode("/");
150     temp->left=left;temp->right=right;
151     return temp;
152 }
153
154 TreeNode* powernodes(TreeNode *left,TreeNode *right){//merge leftnode,rightnode and
operator "^"
155     TreeNode *temp=createnode("^");
156     temp->left=left;temp->right=right;
157     return temp;
158 }
159
160 TreeNode* differentiate(TreeNode *root,string var){
161     if(root==NULL)
162         return NULL;
163     if(isnumber(root->value))//the derivative of constant number is 0
164         return NULL;
165     else if(root->value==var)//the derivative of the var is 1
166         return createnode("1");
167     else{//root->value is an operator
168         TreeNode *leftchild=differentiate(root->left,var);//get the derivative of
leftchild
169         TreeNode *rightchild=differentiate(root->right,var);//get the derivative of
rightchild
170
171         if(root->value=="+"//F(x)=f(x)+g(x),F'(x)=f'(x)+g'(x)
172             return addnodes(leftchild,rightchild);
173         if(root->value=="-"//F(x)=f(x)-g(x),F'(x)=f'(x)-g'(x)
174             return subnodes(leftchild,rightchild);
175         if(root->value=="*"//F(x)=f(x)*g(x),F'(x)=f'(x)*g(x)+f(x)*g'(x)
176             return addnodes(mulnodes(leftchild,root->right),mulnodes(root->
left,rightchild));
177         if(root->value=="/"//F(x)=f(x)/g(x),F'(x)=[f'(x)*g(x)-f(x)*g'(x)]/g(x)^2
178             TreeNode *term1=mulnodes(leftchild,root->right);
179             TreeNode *term2=mulnodes(root->left,rightchild);
180             TreeNode *term3=powernodes(root->right,createnode("2"));
181             return divnodes(subnodes(term1,term2),term3);
182         }
183         if(root->value=="^"//F(x)=f(x)^[g(x)],F'(x)=
[g'(x)*lnf(x)+g(x)*f'(x)/f(x)]*f(x)^g(x)
184             TreeNode *term1=mulnodes(rightchild,createnode("ln("+root->left-
>value+"")));
185             TreeNode *term2=divnodes(mulnodes(root->right,leftchild),root->left);
186             TreeNode *term3=powernodes(root->left,root->right);
187             return mulnodes(addnodes(term1,term2),term3);
188         }
189     }
190 }

```

```

191
192 void printtree(TreeNode *root){//print the expression tree back to inorder
expression
193     if(root==NULL)
194         return;
195     if(root->left!=NULL){
196         if(isoperator(root->value)&&isoperator(root->left->value)){
197             bool flag=precedence(root->value[0])>precedence(root->left->value[0]);
198             if(flag)//if root's operator is higher than root's leftchild's
operator,then expression in leftchild need brackets
199                 cout<<"(";
200                 printtree(root->left);
201                 if(flag)
202                     cout<<")";
203             }
204             else
205                 printtree(root->left);
206         }
207         cout<<root->value;
208         if(root->right!=NULL){
209             if(isoperator(root->value)&&isoperator(root->right->value)){
210                 bool flag=precedence(root->value[0])>precedence(root->right->value[0]);
211                 if(flag)//if root's operator is higher than root's rightchild's
operator,then expression in rightchild need brackets
212                     cout<<"(";
213                     printtree(root->right);
214                     if(flag)
215                         cout<<")";
216                 }
217                 else
218                     printtree(root->right);
219             }
220         }
221     }
222
223 int main(){
224     string expression;
225     cin>>expression;
226
227     /*build the expression tree*/
228     TreeNode* root=buildtree(expression);
229
230     /*count all the variable names*/
231     string variables[100];
232     string var;
233     int total=0;
234     for(int i=0;i<(int)expression.size();i++){
235         if(isalnum(expression[i]))
236             var+=expression[i];
237         else{
238             if(!var.empty()){
239                 bool flag=true;//flag=true means the new variable name is not in
the old set of variable names
240                 for(int i=1;i<=total;i++){
241                     if(var==variables[i]){
242                         flag=false;
243                     }
244                 }
245                 if(flag){
246                     variables[total]=var;
247                     total++;
248                 }
249                 var="";
250             }
251         }
252     }
253
254     cout<<endl;
255     cout<<total<<endl;
256     cout<<endl;
257     printtree(root);
258     cout<<endl;
259 }

```

```

242         break;
243     }
244     if(flag)//add the new variable name
245         variables[++total]=var;
246     var.clear();
247 }
248 }
249 }
250 if(!var.empty()){
251     bool flag=true;
252     for(int i=1;i<=total;i++)
253         if(var==variables[i]){
254             flag=false;
255             break;
256         }
257     if(flag)
258         variables[++total]=var;
259     var.clear();
260 }
261 /*sort all the variable name in lexicographical order*/
262 sort(variables+1,variables+total+1,cmp);
263
264 for(int i=1;i<=total;i++)
265     if(!isnumber(variables[i])){
266         cout<<variables[i]<<": ";
267         TreeNode *ans=differentiate(root,variables[i]);//differentiate all
variables
268         printtree(ans);
269         cout<<endl;
270     }
271     return 0;
272 }

```

Declaration

I hereby declare that all the work done in this project titled “Autograd for Algebraic Expressions” is of my independent effort.