Second Order Derivatives with ADTAGEO

Algorithmic Differentiation Through Automatic Graph Elimination Ordering

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15th April 2005
Automatic Differentiation Workshop
Nice, France

Outline

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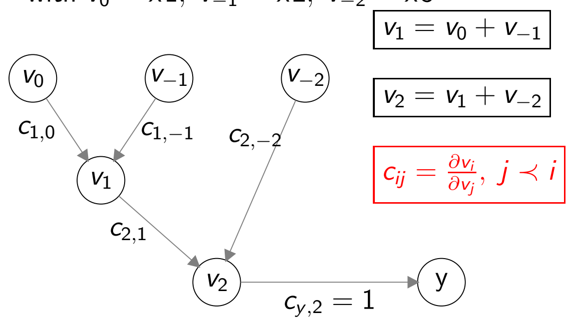
ADTAGEO Gradient-Mode – Example

Computational graph of statement:

`y = x1 + x2 + x3;`

with $v_0 = x1,\ v_{-1} = x2,\ v_{-2} = x3$

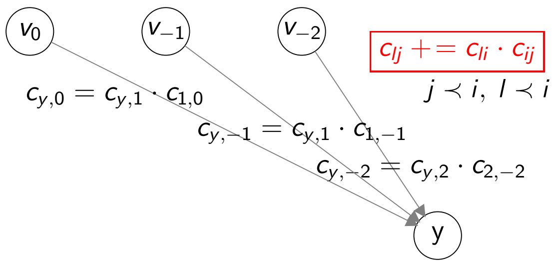


ADTAGEO Gradient-Mode – Elemination

After execution of the assignment:

Elimination of Intermediates:

```
y = x1 + x2 + x3;
```



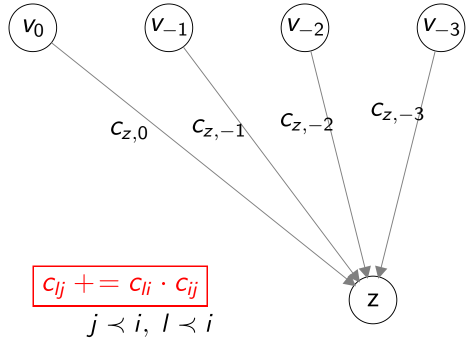
ADIFOR: Statement Level Reverse

AD-enabled NAGWare Fortran 95 compiler

ADTAGEO Gradient-Mode – Elemination

Program: y . . . local variable, leaving scope of y

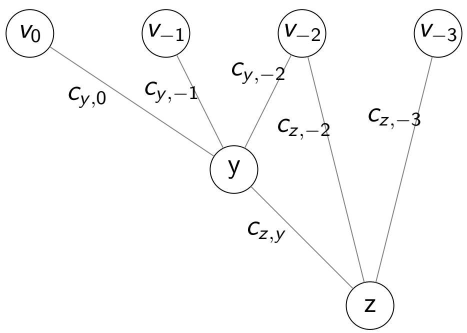
```
{ double y = x1 + x2 + x3;   z = x3 + x4 + y; }
```



ADTAGEO Gradient-Mode – Elemination

Program: y . . . local variable, inside scope of y

```
{ double y = x1 + x2 + x3;   z = x3 + x4 + y; }
```



ADTAGEO at a glance – The idea behind

- More talking about an **IDEA** than a another AD-*TOOL*
- A **new way** of doing Algorithmic Differentiation
- Do not build the computational graph of complete (sub)programs

  Instead:

Maintain a Life -DAG

- Eliminate as soon as possible as many vertexes as possible.
- Eliminate on the fly, Online elimination.
- DAG represents the active variables alive at any one time.

  → Small graph – Huge memory savings (gradients: factor 100)

ADTAGEO at a glance – Requirements

ADTAGEO performs vertex elimination whenever

(i) An active variable is deallocated/destroyed
(ii) An active variable is overwritten

Perfect fitting into OOP scenario

(i) is covered by Destructor (assuming it exists in language)
(ii) is covered by assignment operator

Implementation

- Proof of concept
  - optimized for understanding
  - not optimized for speed
- Implemented in C++
- Heavy use of class `map` from the *Standard Template Library* to store partials **locally** at every node (edges in graph)
- Rapid prototyping (First Order):
  - 140 lines of code for +-*/ and sin, cos, exp
  - One week (with basic testing)
- Any new operator / intrinsic requires 4 lines
  (2 lines for open and closing curly braces)
- Rapid prototyping – **Hessian**:
  - 100 additional lines of code for Hessian elimination
  - One additional day (plus two nights)

ADTAGEO – And Sourcetransformation

- Requirements of ADTAGEO??
  (i) Recognise leaving of the scope of variables (deallocation)
  (ii) Recognise assignments (overwrites)
- Produce source code for graph manipulations
- therefore: one have access to the storage associated with pointers at runtime
  - no pointer aliasing problem
  - DEALLOCATE becomes your best friend: Eliminate all array elements at once opens possibility to optimise the elimination order
- Elements of arrays are handled as single entities
  - partial overwrites are no topic

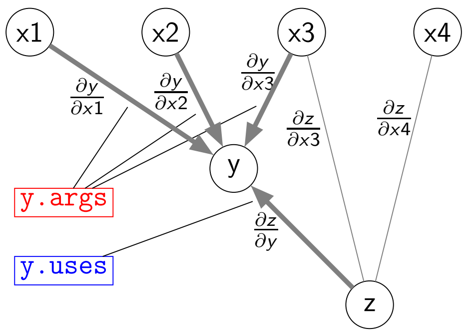
Implementation – DAGLAD

```
class daglad{
private:
 double val;                                            //function value
 map<daglad*, double> args;              //arguments = incoming edges
 map<daglad*, double> uses;                 //used by = outgoing edges
public:
 daglad() { ...};                                          //constructor
 void eliminate() {...};                        //eliminate current vertex
 ~daglad() { eliminate(); ...};                             //destructor
 void operator = (...)  { eliminate(); ...};     // asgnm.
 friend dagdoub operator + (...);       // arithmetic operators
 friend double operator % (...); ...               // retrieval op
}; /* class daglad */
```

Implementation – DAGLAD

Program:

```
y = x1 + x2 + x3;   z = x3 + x4 + y;
```



Implementation – Example

```
#include "daglad.hpp"
main(){
  daglad x1(0.5), x2(1.3), y;
  double xx1, xx2, yy, dy, dyy;

  y = exp(x1)*sin(x1+x2);                          // compute f(x)
  dyy = y%x1;                          // first element of gradient

  xx1 = x1.val(); xx2 = x2.val();                  //shortcuts
  dy = exp(xx1)*(sin(xx1+xx2)+cos(xx1+xx2));
  cout << " dF1 = " << dyy << " diff " << (dyy-dy) << endl;
  dyy = y%x2;                         // second element of gradient
  dy = exp(xx1)*cos(xx1+xx2);
  cout << " dF1 = " << dyy << " diff " << (dyy-dy) << endl;
  cout << " x1 = " << x1 << endl << " x2 = " << x2 << endl;
  cout << " y = " << y << endl;
}
```


Implementation – Usage (prototype)

- Easy mode:
  - Redeclare (required) variables to be of type `daglad`
  - Retrieve first order derivatives somewhere in the code using the % operator

$$\mathtt{y[j]\%x[i]} \equiv \frac{\partial y_j}{\partial x_i}$$

- Advanced mode:
  - Check/prepare/write code for better performance
    Right mixture of forward and reverse mode [see below]

Implementation – Example Output (reformatted)

```
dF1 = 1.23101 diff 2.22045e-16
dF2 = -0.374593 diff 0
x1 = |1,1:0,0.5,3, args={} , uses={[3,4,0,1.23101]}|
x2 = |2,1:0,1.3,2, args={} , uses={[3,4,0,-0.374593]}|
y = |3,1:4,1.6056,0,
    args={[2,0,2,-0.374593][1,0,3,1.23101]}
    uses={} |
```

Implementation – Highlights

- No specification of independents/dependents
- No call of forward / reverse sweeps
  mode is defined by variable allocation
- No tape, No top level routine
- Access to derivatives everywhere (Correctness of derivatives has to be ensured)
- Graph represents the sparsity structure
  - BUT: ADTAGEO is not only sparsity propagation
  - ADTAGEO computes derivatives in sparse mode, therefore no structural zeros are computed
  - Avoid propagation of a seed matrix / directions / ...
  - Avoid Jacobian compression

Implementation – Storing edges locally

Benefits of storing the edges locally

```
for (int i = 0; i < N; i++ )
    y = y*x1*x2*sin(x1)*x1+x2*sin(x1)*x2+x2;
```

N	100.000			250.000		
	CPU	SYS	ELP	CPU	SYS	ELP
map	7.19	0.63	7.85	19.22	2.40	72.00
hash-map	5.53	0.60	6.17	12.87	1.40	14.50
local	2.30	0.00	2.35	5.77	0.00	5.89

Implementation – Memory consumption

```
y[1] = 0;
for( i = 0; i < 100000; i++ ) {
     y[0] = y[1] + x[0] + x[1];
     y[1] = y[0] + x[0] + x[1];
     y[0] = x[0] + x[1];
}
```

complete DAG 82 Megabyte
ADTAGEO 880 Kilobyte

It is a tiny, but perfect example for ADTAGEO

- It is in fact a small **gather-scatter-loop** !!
- Eliminate instead of storing or recompute!

Implementation – Cache behavior (n=250.000)

```
for (int i = 0; i < N; i++ )
    y = y*x1*x2*sin(x1)*x1+x2*sin(x1)*x2+x2;
```

	major	minor
	page faults	
map	6.817	188.676
hash-map	–	≈ 70.000
local	–	≈ 300

Implementation – Mixing Forward and Reverse

Talking about the loop in Speelpennings example

```
void speelforw( int dim, daglad* x, daglad& y ) {
   y = 1;                                        // initialise
   for ( int i = 0; i < dim; i++ )         // loop over elements
      y = y * x[i];                          // compute product
}                                              // end of speelforw
```

Hybrid mode

- Split loop into chunks of C elements
  $\Longrightarrow$ spent small amount of additional memory (compared with forward)
- Loop over chunks
- Deallocate / Eliminate inside of loop over chunks

Runtime Forward / Reverse / R-Split / F-Split

Size of chunks: C = 100

N	1.000	2.500	5.000	10.000	25.000	50.000	100.000
Forward	1.9	14.8	62.5	–	–	–	–
Reverse	0.0	0.0	0.1	0.2	0.5	0.9	1.9
R-Split	0.0	0.1	0.7	2.8	17.3	70.0	280.1
F-Split	0.0	0.3	1.1	3.6	19.3	73.9	286.9

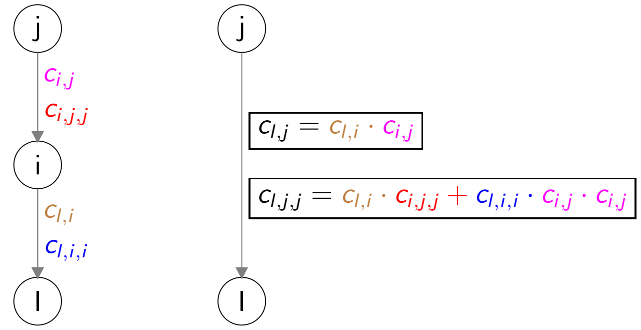
Notes:

- Surprising runtime behavior of Forward Split mode
- Memory used: Reverse 32MB R-Split 11MB F-Split 19MB

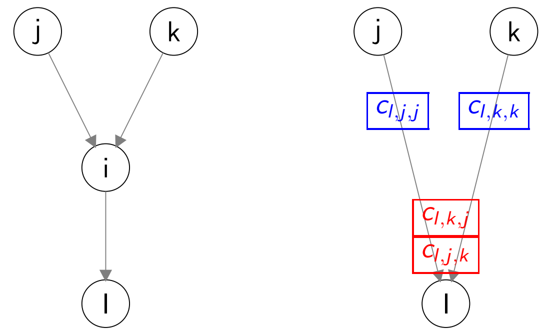
Hessian Elimination – Simplest Case

Looking at a graph snippet, only dealing with

$$c_{i,j} = \frac{\partial v_i}{\partial v_j} \qquad c_{i,j,k} = \frac{\partial^2 v_i}{\partial v_j \partial v_k}$$



Hessian Elimination – Becoming more general



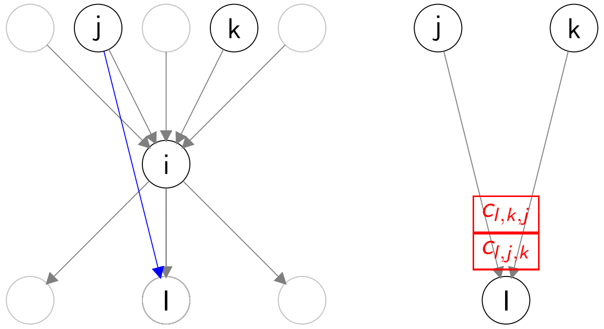
$$c_{l,j,j} = c_{l,i} \cdot c_{i,j,j} + c_{l,i,i} \cdot c_{i,j} \cdot c_{i,j}$$

$$c_{l,j,k} = c_{l,i} \cdot c_{i,j,k} + c_{l,i,i} \cdot c_{i,j} \cdot c_{i,k}$$

Hessian Elimination – Even more general

$$\boxed{c_{l,j,k} \mathrel{+}= c_{l,i} \cdot c_{i,j,k} + c_{l,i,i} \cdot c_{i,j} \cdot c_{i,k}}$$

$j \prec i,\ k \prec i,\ i \prec l$



Hessian Elimination – Summary

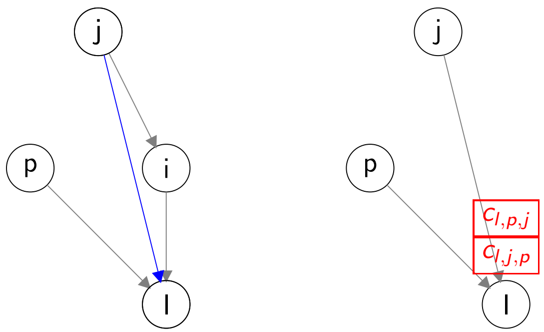
$j \prec i,\ k \prec i,\ i \prec l$:

$$\boxed{c_{l,j,k} \mathrel{+}= c_{l,i} \cdot c_{i,j,k} + c_{l,i,i} \cdot c_{i,j} \cdot c_{i,k}}$$

$j \prec i,\ i \prec l,\ p \prec l,\ p \neq i$:

$$\boxed{\begin{array}{l} c_{l,p,j} \mathrel{+}= c_{l,p,i} \cdot c_{i,j} \\ c_{l,j,p} \mathrel{+}= c_{l,i,p} \cdot c_{i,j} \end{array}}$$

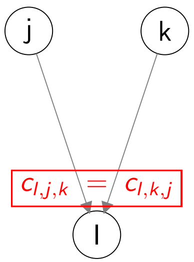
Hessian Elimination – Even more general



$$\boxed{c_{l,p,j} \mathrel{+}= c_{l,p,i} \cdot c_{i,j}}$$

$j \prec i,\ i \prec l,\ p \prec l,\ p \neq i$

Hessian Elimination – What's about Hessian Symmetry?



Can be exploited with canonicalised keys:

$$\boxed{(j,k) \equiv c_{l,j,k} \quad \textit{always fulfills} \quad j \geq k}$$

Hessian Elimination – Symmetric Elimination

$j \prec i,\ k \prec i,\ \boxed{j \geq k},\ i \prec l$:

$$\boxed{c_{l,j,k} \mathrel{+}= c_{l,i} \cdot c_{i,j,k} + c_{l,i,i} \cdot c_{i,j} \cdot c_{i,k}}$$

$j \prec i,\ i \prec l,\ p \prec l,\ p \neq i$:

if($\boxed{p \neq j}$)

$$\boxed{c_{l,p,j} \mathrel{+}= c_{l,p,i} \cdot c_{i,j}}$$

else

$$\boxed{c_{l,p,p} \mathrel{+}= 2 \cdot c_{l,p,i} \cdot c_{i,p}}$$

Hessian Elimination – Hessian Example Output (reformatted)

```
dF1 = 1.23101 difference 2.22045e-16
dF1 = -0.374593 difference 0
x1 = |1,1:0,0.5,3, args={} , uses={[3,4,0,1.23101]} |
x2 = |2,1:0,1.3,2, args={} , uses={[3,4,0,-0.374593]} |
y = |3,1:4,1.6056,0,
    args={[2,0,2,-0.374593][1,0,3,1.23101]} ,
    uses={} ,
    hessian={[(5,6),1],           // BUG has to be removed
            [(2,2),-1.6056],
            [(1,4),-0.374593],    // BUG has to be removed
            [(1,5),1.64872],      // BUG has to be removed
            [(1,2),-1.9802],
            [(1,1),-0.749186], }|
```


Hessian Elimination – Hessian Example

```
#include "daglad.hpp"
main(){
  daglad x1(0.5), x2(1.3), y;
  double xx1, xx2, yy, dy, dyy;

  y = exp(x1)*sin(x1+x2);                    // compute f(x)
  dyy = y%x1;                       // first element of gradient

  xx1 = x1.val(); xx2 = x2.val();              //shortcuts
  dy = exp(xx1)*(sin(xx1+xx2)+cos(xx1+xx2));
  cout << " dF1 = " << dyy << " diff " << (dyy-dy) << endl;
  dyy = y%x2;                      // second element of gradient
  dy = exp(xx1)*cos(xx1+xx2);
  cout << " dF1 = " << dyy << " diff " << (dyy-dy) << endl;
  cout << " x1 = " << x1 << endl << " x2 = " << x2 << endl;
  cout << " y = " << y << endl;
}
```


Hessian implementation – Easy part

- `map<pair<daglad*,daglad*>,double> hessian;`
  to store existing Hessian elements at node / active variable
- add additional parameters for Hessian elements to constructors (2 places)
- extend operators and intrinsics

```
daglad sin (const daglad &a)
{                              // has hessian: -sin(a) = -t
  double t = sin(a.val);
  return daglad( t, a, cos(a.val),
    true, -t
  );
};
```

Hessian implementation – Easy part

- extend operators and intrinsics (cont'd)

```
// daglad * daglad
daglad operator * (const daglad &a,
                   const daglad &b)
{                                //has hessian: [ 0 1; 1 0]
  return daglad( a.val * b.val, a, b.val, b, a.val,
                 true, 0, 1, 0
               );
};
```


Hessian implementation – Not so easy part

- extend `eliminate()` to deal with hessians based on the elimination rules seen

Overall changes on prototype to got Hessians

- roughly 100 lines of code added
- 80% in `eliminate()`

Outlook – Todo

Hessian retrieval – User interface

- Complete Hessians
- Hessian - Vector - Products

Bugfix

- Delete all Hessian elements storing derivatives with respect to eliminated nodes
  - Problems arises from the += if the corresponding variable is overwritten

Outlook – Future research

- Detect and exploit partial separability
- Propagate residuals

$$R \to 0 \quad \Longleftrightarrow \quad (A * R)' = \underbrace{A'R}_{\to 0} + AR' = AR'$$

- Performance Analysis

Outlook – ADTAGEO $\longrightarrow$ ALLEGRO

Making prototype faster:

- Instant elimination: reduce number of vertexes
  - Easy for unary operators
  - Open question: How to avoid copy/delete in DAG?
- Replace `maps` by `hashmap`, attemp to avoid use of `STL`
- Elimination of LHS intermediates in assignments already
  - Never more than 2 edges for intermediate vertexes
    $\longrightarrow$ Specialised class for intermediate vertexes
  - Statement Level Reverse Mode ala `ADIFOR`

Conclusions

We have seen (Pros)

- A new view to AD, strongly based **Life-DAG**
- Easy to implement
- Convenient to use (at least C++ implementation)
- Throws away/changes/mix up some of the good old AD-terms:
  - Independent / Dependent
  - Forward and Reverse mode
  - Seeding, Compression of Jacobians
- Elimination rules for Hessians keeping symmetry

We have also seen (Cons)

- Dynamic sparsity handling (Overhead)
- STL `map`: Handling dynamic data structures all the time (Overhead)

We have not seen (so far)

- Performance tests/Comparisons

Outlook – ADTAGEO $\longrightarrow$ ALLEGRO

- Classes for vectors of `daglad`'s
  - Destructor: access to a whole bunch of vertexes
  - Optimize elimination sequence: heuristics, `ANGEL`
  - Test: Speelpenning, randomised element ordering

N	FM	elim	RM	elim	OM	elim
500000	30s	92%	25s	92%	12s	75%

- Extend user interface
  - Develop Hessian retrieval machanism
  - Return compressed rows / columns of Jacobian / Hessian too
  - Sparse Jacobian/Hessian-Vector products
  - Enforce accumulation / elimination
  - Self verifying mode: Derivatives completely accumulated ?

Thank you!

Additionally:

Many thanks to Till Tantau, author of **BEAMER** and **PGF** (Portable Graphics Format, used to draw the graphs):

`http://sourceforge.net/projects/latex-beamer/`