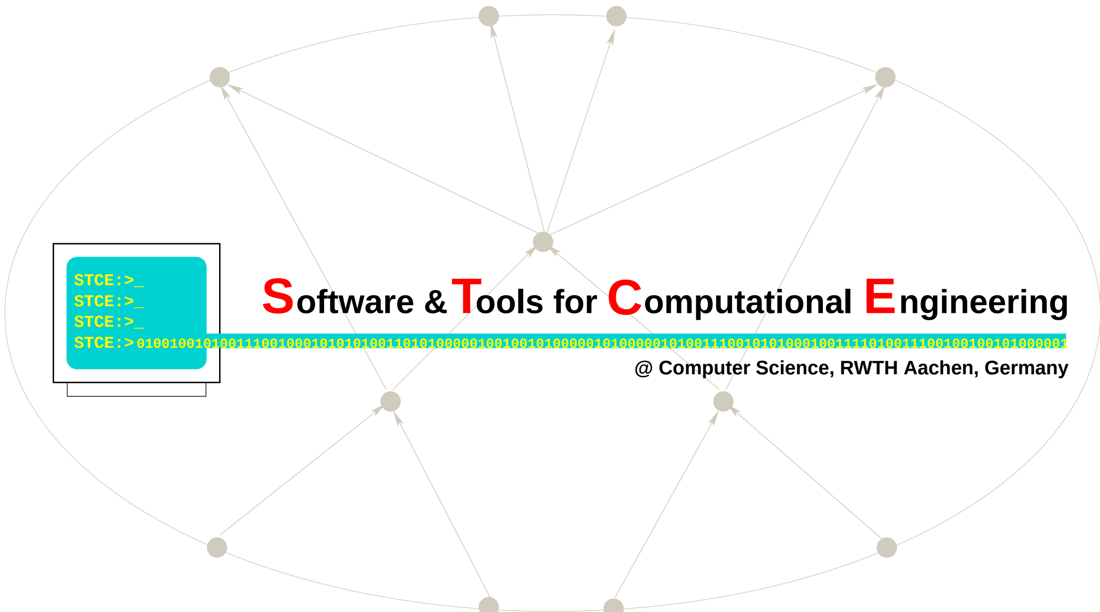
MinOps Jacobian Accumulation is NP-complete

Uwe Naumann



History – Proof – Discussion

History – Terminology

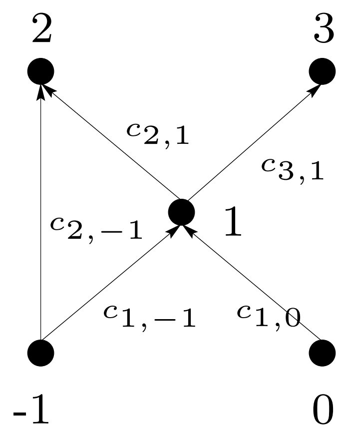
- numerical program + fixed flow of control
- single assignment code (code list) $v_j = \varphi_j(v_i)_{i \prec j}$
- computational graph $G(V, E)$
- linearized code list $c_{j,i}$
- linearized computational graph
- Jacobian entries as

$$f'_{k,l} = \sum_{[l \to k]} \prod_{(i,j) \in [l \to k]} c_{j,i}$$

$t = x_1 * x_2$

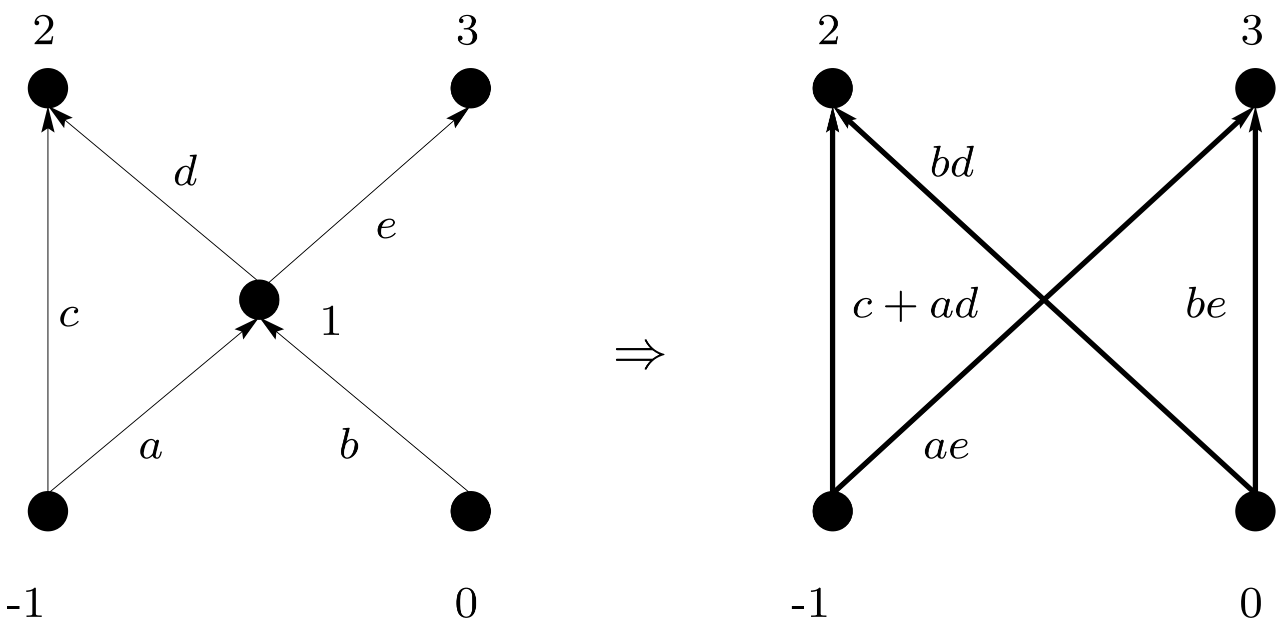
$y_1 = x_1 - t$

$y_2 = \sin(t)$



▶ W. Baur and V. Strassen. The complexity of partial derivatives. 1983

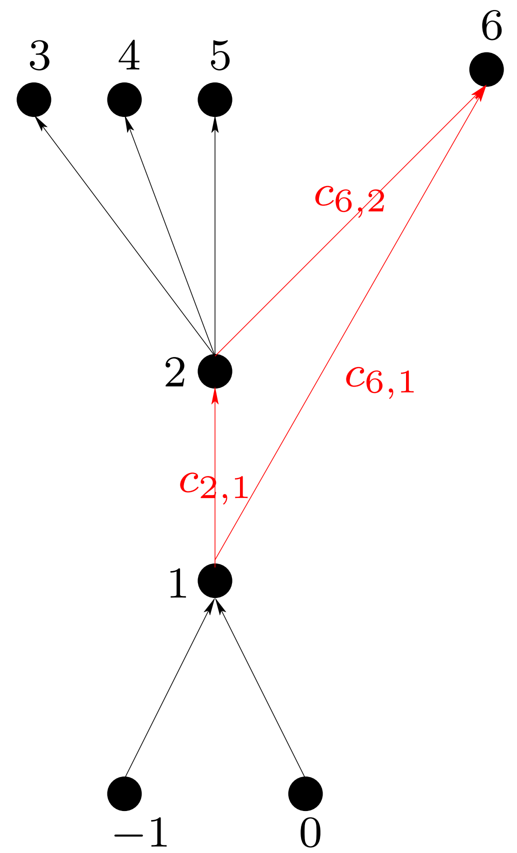
History – Vertex Elimination



Markovitz Degree $m_j = |\{i : i \prec j\}||\{k : j \prec k\}|$

- A. Griewank and S. Reese. On the calculation of Jacobian Matrices by the Markovitz rule. AD1991, 1991
- K. Herley. On minimal fill-in Jacobian accumulation. ANL, 1992

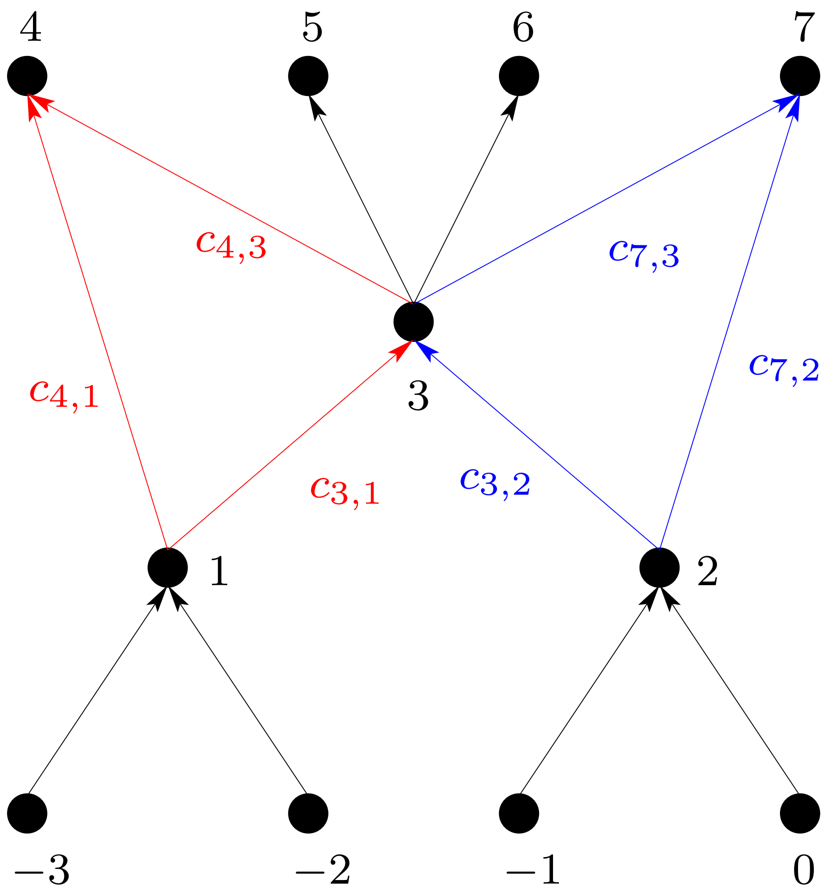
History – Edge Elimination



Lion graph

- U. Naumann. Elimination techniques for cheap Jacobians. AD2000, 2001
- U. Naumann. The no-free-refill conjecture. AD Fest, 2003

History – Face Elimination

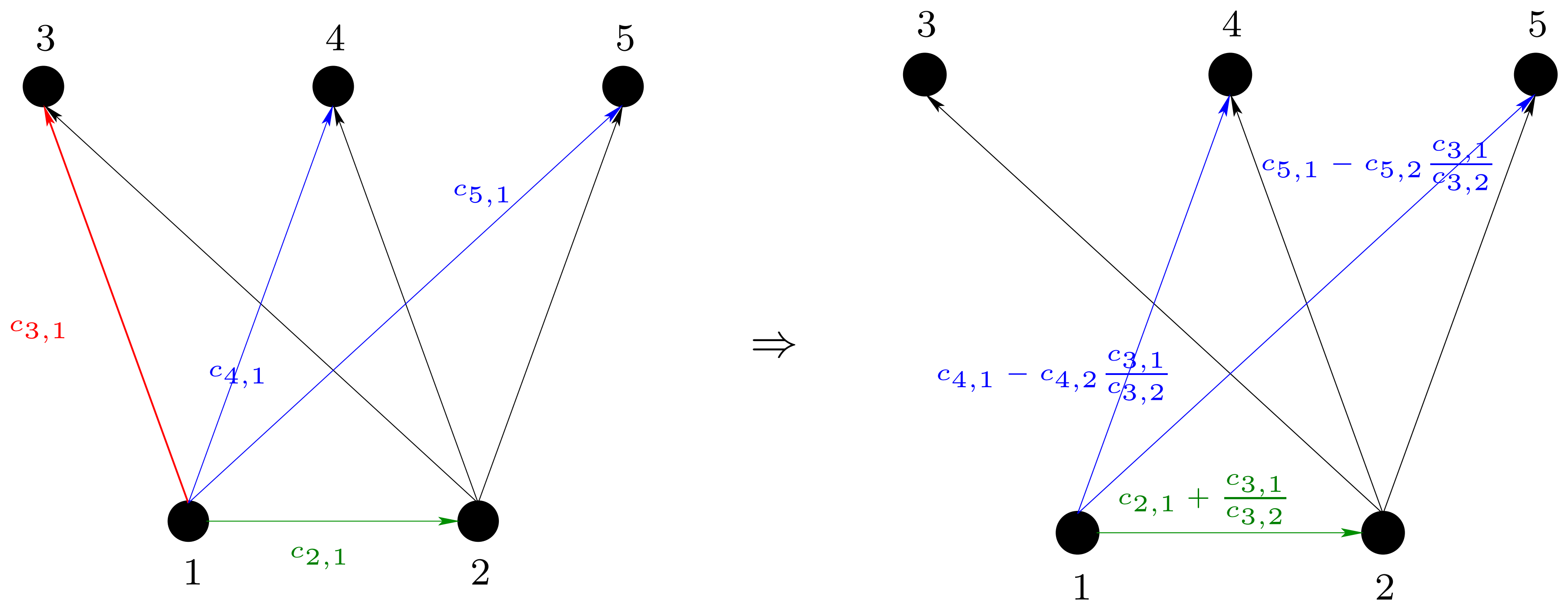


Bat graph

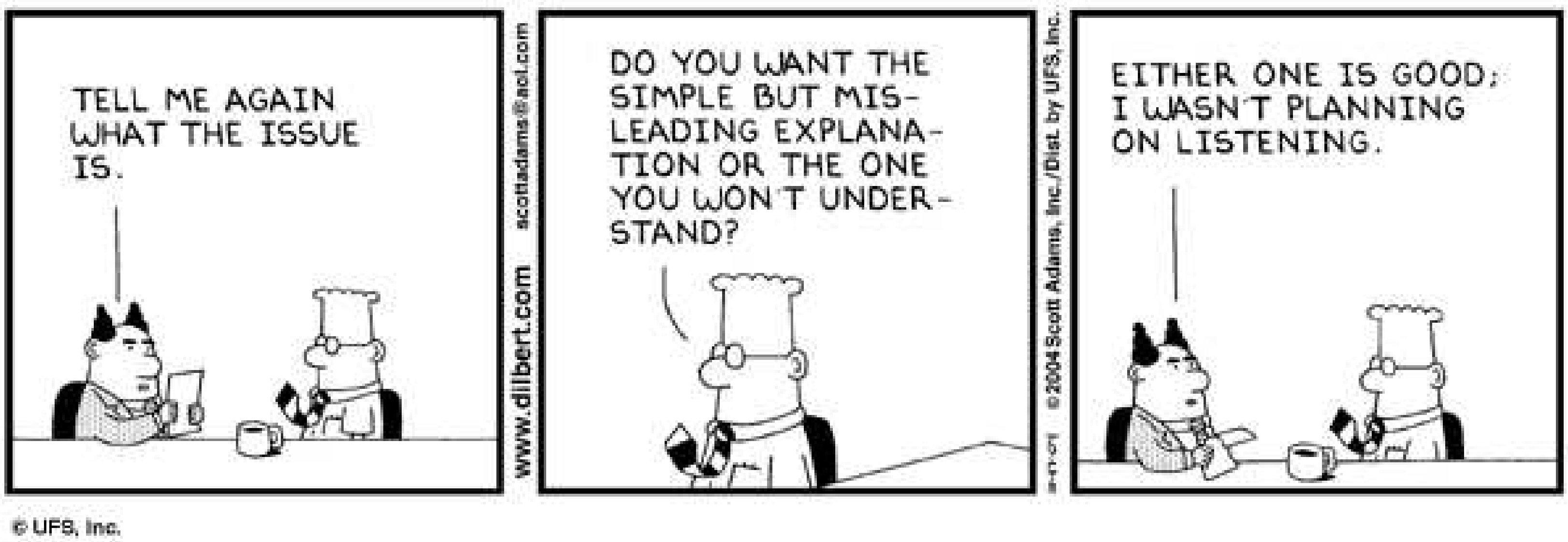
▶ U. Naumann. Optimal Accumulation of Jacobian matrices by elimination methods on the dual computational graph. Math. Prog. 2004

History – Rerouting

Example: Prerouting $(1,3)$ with pivot $(2,3)$



▶ A. Griewank and O. Vogel. Analysis and explotation of Jacobian scarcity. HPSC, 2003


TELL ME AGAIN WHAT THE ISSUE IS.
DO YOU WANT THE SIMPLE BUT MIS-LEADING EXPLANA-TION OR THE ONE YOU WON'T UNDER-STAND?
EITHER ONE IS GOOD; I WASN'T PLANNING ON LISTENING.
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www.dilbert.com
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Complexity Proofs – Prior Attempts

Approach

1. pick known NP-complete problem (NPP)
2. derive polynomially instance of your problem for each instance of NPP
3. verify given solution in polynomial time

Prior Attempts

- Max Clique
  ($C(K_n) = \binom{n-1}{2}$ by forward/reverse)
- Longest Common Subsequence
  (*abc* and *aec* not representable in DAG, but there is hope...)

Ensemble Computation Problem (EC)

Given a collection $C = \{C_\nu \subseteq A : \nu = 1, \ldots, |C|\}$ (Jacobian) of subsets $C_\nu = \{c_i^\nu : i = 1, \ldots, |C_\nu|\}$ (Jacobian entries) of a finite set A (elemental partial derivatives) and a positive integer Ω (max. nr. of scalar multiplications) is there a sequence $u_i = s_i \cup t_i$ (scalar multiplications) for $i = 1, \ldots, \omega$ of $\omega \leq \Omega$ union operations, where each s_i and t_i is either $\{a\}$ (elemental partial derivative) for some $a \in A$ or u_j (previously accumulated partial derivative) for some $j < i$, such that s_i and t_i are disjoint for $i = 1, \ldots, \omega$ and such that for every subset $C_\nu \in C$, $\nu = 1, \ldots, |C|$, there is some u_i, $1 \leq i \leq \omega$, that is identical to C_ν (all Jacobian entries are computed).

Theorem 1 *EC is NP-complete.*

M. Garey and D. Johnson. Computers and Intractability. 1979

EC Example

Let an instance of EC be given by

$$A = \{a_1, a_2, a_3, a_4\}$$

$$C = \{\{a_1, a_2\}, \{a_2, a_3, a_4\}, \{a_1, a_3, a_4\}\}$$

and $\Omega = 4$. The answer to the decision problem is positive with a corresponding instance given by

$$\begin{aligned} C_1 = u_1 &= \{a_1\} \cup \{a_2\} \\ u_2 &= \{a_3\} \cup \{a_4\} \\ C_2 = u_3 &= \{a_2\} \cup u_2 \\ C_3 = u_4 &= \{a_1\} \cup u_2 \quad . \end{aligned}$$

Optimal Jacobian Accumulation Problem

Given a linearized computational graph G of a vector function F and a positive integer Ω is there a sequence of scalar assignments $u_k = s_k \circ t_k,\ \circ \in \{+, *\},\ k = 1, \ldots, \omega,$ where each s_k and t_k is either $c_{j,i}$ for some $(i,j) \in E$ or $u_{k'}$ for some $k' < k$ such that $\omega \leq \Omega$ and for every Jacobian entry there is some identical u_k, $k \leq \omega$?

Example: *Lion*

$c_{6,1} := c_{6,1} + c_{6,2}c_{2,1};\ c_{2,-1} = c_{2,1}c_{1,-1};\ c_{2,0} = c_{2,1}c_{1,0}$

$c_{6,-1} = c_{6,1}c_{1,-1};\ c_{6,0} = c_{6,1}c_{1,0};\ c_{3,-1} = c_{3,2}c_{2,-1};\ c_{3,0} = c_{3,2}c_{2,0}$

$c_{4,-1} = c_{4,2}c_{2,-1};\ c_{4,0} = c_{4,2}c_{2,0};\ c_{5,-1} = c_{5,2}c_{2,-1};\ c_{5,0} = c_{5,2}c_{2,0}$

Reduction EC → OJA

Consider $\boldsymbol{y} = F(\boldsymbol{x}, \boldsymbol{a})$ where $\boldsymbol{x} \in \mathbb{R}^{|C|}$, $\boldsymbol{a} \in \mathbb{R}^{|A|}$ is a vector containing all elements of A, and $F : \mathbb{R}^{|C|+|A|} \to \mathbb{R}^{|C|}$ defined as

$$y_\nu = x_\nu * \prod_{j=1}^{|C_\nu|} c_j^\nu$$

for $\nu = 1, \ldots, |C|$ and where c_j^ν is equal to some $a \in A$ for all ν and j. This transformation is linear with respect to the original instance of Ensemble Computation in both space and time. The Jacobian $F'(\boldsymbol{x}, \boldsymbol{a})$ is a diagonal matrix with nonzero entries

$$f_{\nu,\nu} = \prod_{j=1}^{|C_\nu|} c_j^\nu$$

for $\nu = 1, \ldots, |C|$.

Example

$A = \{a_1, a_2, a_3, a_4\}$

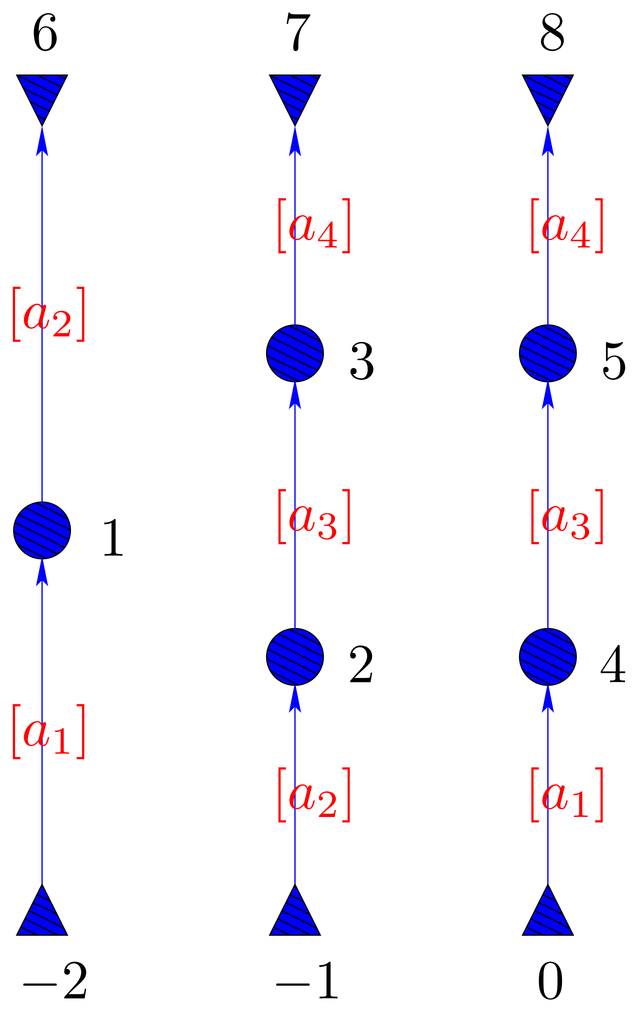
$C = \{\{a_1, a_2\}, \{a_2, a_3, a_4\}, \{a_1, a_3, a_4\}\}$

$f'_{1,1} = c_{6,-2} = a_1 * a_2$

$u_2 = c_{7,2} = c_{8,4} = a_3 * a_4$

$f'_{2,2} = c_{7,-1} = a_2 * u_2$

$f'_{3,3} = c_{8,0} = a_1 * u_2$



EC $\Leftrightarrow$ OJA

$\Leftarrow$: Simply subsitute $*$ for $\cup$.

$\Rightarrow$: 1. No additions; simply subsitute $*$ for $\cup$.

2. Suppose that there is some $i \leq \omega$ such that $s_i \cap t_i = \{b\}$. Hence the computation of u_i in the Jacobian accumulation code involves a factor $b * b$. Note that such a factor is not part of any Jacobian entry which implies that the computation of u_i is obsolete and therefore cannot be part of an optimal Jacobian accumulation code.

Consequences

1. "Rows and columns" of F' are NP-complete.

$$y=\sum_{\nu=1}^{|C|} y_\nu = \sum_{\nu=1}^{|C|}\left(x_\nu * \prod_{j=1}^{|C_\nu|} c_j^\nu\right) \quad .$$

2. "Tangents and adjoints" are NP-complete.

$$y_\nu = x * \dot{x}_\nu * \prod_{j=2}^{|C_\nu|} c_j^\nu \quad .$$

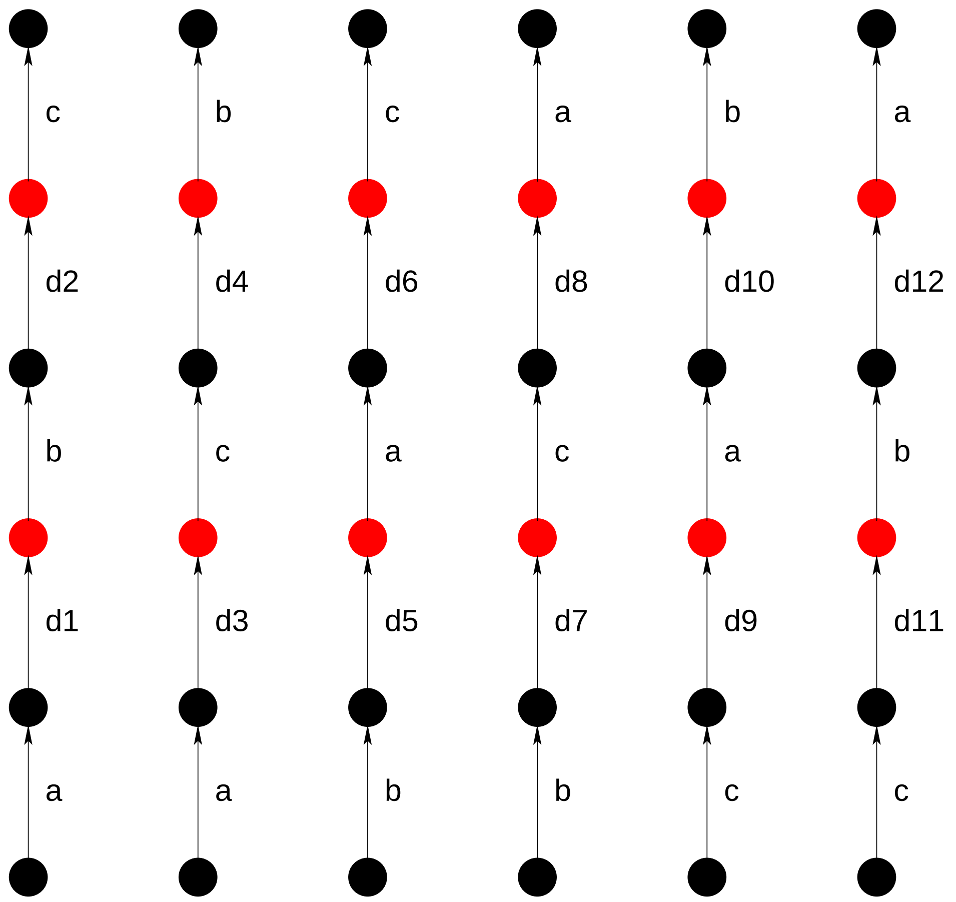
3. "Scalar partial derivatives" are NP-complete.

$$y=\sum_{\nu=1}^{|C|}\left(x * \prod_{j=1}^{|C_\nu|} c_j^\nu\right) \quad .$$

4. "Partial derivatives of arbitrary order" are NP-complete.

$$y_\nu = \frac{x_\nu^q}{q!} \prod_{j=1}^{|C_\nu|} c_j^\nu \quad .$$

Discussion



$$OPS(F) = 6 * 5 = 30$$
$$OPS(F') = 2 + 6 * 2 = 14$$

Conclusion

- *1.5 decades of work on heuristics not for the bin...*
- Combine previous and new wisdom.
- How cheap can Jacobians be?

We need more insight into the theory and new algorithms :-)))