Optimal Derivative Accumulation on Series-Parallel Dags

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11/15/07

Outline

- Intro to Jacobians by AD
- The Optimal Jacobian Accumulation Problem
- Two-Terminal Series-Parallel Dags and Decomposition Trees
- Our Current View of OJA
- Single-Terminal Series-Parallel Dags and Vertex Elimination
- General Series-Parallel Dags
- Modular Decomposition: a Generalization

Jacobians by Automatic Differentiation (AD)

code for $F(\mathbf{x}_0) : \mathbb{R}^n \longrightarrow \mathbb{R}^m, \quad \mathbf{x} \mapsto \mathbf{y}$

$$\Big\downarrow \text{AD}$$

augmented code for $F(\mathbf{x}_0),\ F'(\mathbf{x}_0)$

$$\text{Jacobian } J \equiv F'(\mathbf{x}) = \left(\frac{\partial y_j}{\partial x_i}\right)_{i=1,\ldots,n}^{j=1,\ldots,m} \in \mathbb{R}^{m\times n}$$

Jacobians by Automatic Differentiation (AD)

$$\left[\; y_1 = x_1 * x_2 * \sin(x_1 * x_2), \quad y_2 = \cos(\sin(x_1 * x_2)) \;\right]^T$$

$(\mathtt{v}_{\text{-}1} = x_1,\ \mathtt{v}_0 = x_2)$

$\mathtt{v}_1 = v_{-1} * v_0$

$\mathtt{v}_2 = \sin(\mathtt{v}_1)$

$\mathtt{v}_3 = \mathtt{v}_1 * \mathtt{v}_2$

$\mathtt{v}_4 = \cos(\mathtt{v}_2)$

$(y_1 = \mathtt{v}_3,\ y_2 = \mathtt{v}_4)$

Generally

$$\mathtt{v}_j = \varphi_j(\mathtt{v}_i)_{i \prec j}$$

$$c_{ji} = \frac{\partial \varphi_j}{\partial \mathtt{v}_i} \in \mathbb{R}$$

Jacobians by Automatic Differentiation (AD)

$$\left[\ y_1 = x_1 * x_2 * \sin(x_1 * x_2), \quad y_2 = \cos(\sin(x_1 * x_2))\ \right]^T$$

$(\mathtt{v}_{-1} = x_1,\ \mathtt{v}_0 = x_2)$

$\mathtt{v}_1 = v_{-1} * v_0 \quad c_{1-1} = \mathtt{v}_0 \quad c_{10} = \mathtt{v}_{-1}$

$\mathtt{v}_2 = \sin(\mathtt{v}_1) \quad c_{21} = \cos(\mathtt{v}_2)$

$\mathtt{v}_3 = \mathtt{v}_1 * \mathtt{v}_2 \quad c_{31} = \mathtt{v}_2 \quad c_{32} = \mathtt{v}_1$

$\mathtt{v}_4 = \cos(\mathtt{v}_2) \quad c_{42} = -\sin(\mathtt{v}_2)$

$(y_1 = \mathtt{v}_3,\ y_2 = \mathtt{v}_4)$

Generally

$$\mathtt{v}_j = \varphi_j(\mathtt{v}_i)_{i \prec j}$$

$$c_{ji} = \frac{\partial \varphi_j}{\partial \mathtt{v}_i} \in \mathbb{R}$$

Linearized Computational Graph

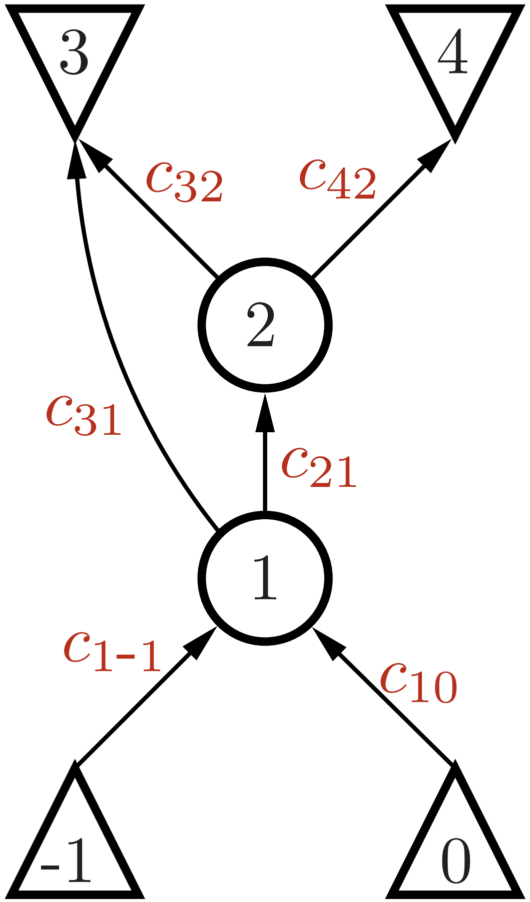
$$\mathtt{v_i} \prec \mathtt{v_j} \Leftrightarrow \mathtt{v_i} \text{ is an argument of } \varphi_j$$

$$\mathtt{v}_1 = \varphi_1(\mathtt{v}_{-1}, \mathtt{v}_0)$$

$$\mathtt{v}_2 = \varphi_2(\mathtt{v}_1)$$

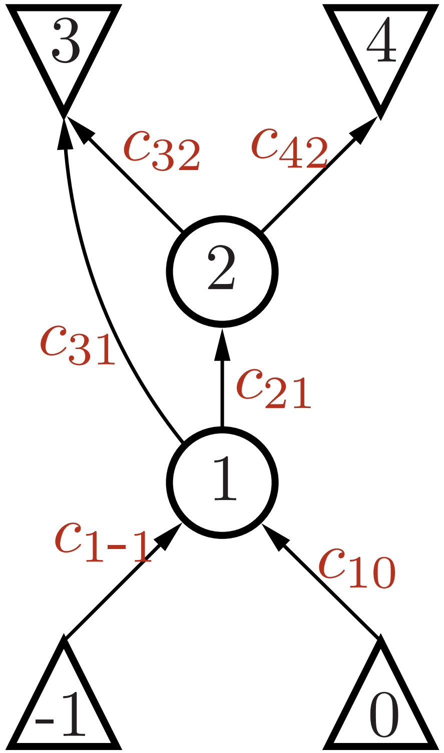
$$\mathtt{v}_3 = \varphi_3(\mathtt{v}_1, \mathtt{v}_2)$$

$$\mathtt{v}_4 = \varphi_4(\mathtt{v}_2)$$



Baur's Formula (Baur, Strassen 1983)

$$J_{y_\ell,x_k} = \frac{\partial y_\ell}{\partial x_k} = \sum_{[x_k \to y_\ell] \in \mathbf{G}} \ \prod_{c_{ji} \in [x_k \to y_\ell]} c_{ji}$$



$$J = \begin{pmatrix} c_{1\text{-}1}c_{31} + c_{1\text{-}1}c_{21}c_{32} & c_{10}c_{31} + c_{10}c_{21}c_{32} \\ c_{1\text{-}1}c_{21}c_{42} & c_{10}c_{21}c_{42} \end{pmatrix}$$

The Optimal Jacobian Accumulation Problem

Given an LCG G for the evaluation procedure for some 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 $c_{i,j}$ for some $(j, i) \in E$ or $u_{k'}$ for some $k' < k$ such that $\omega \leq \Omega$ and for every Jacobian entry there is some identical $u_k, k \leq \omega$?

or

Evaluate F' with as few operations ($*$ or $+$) as possible.

The Optimal Jacobian Accumulation Problem

Evaluate F' with as few operations ($*$ or $+$) as possible.

We restrict ourselves to "pure chain rule methods":

- OJA is NP-complete (Naumann 2005). We assume all edge labels algebraically independent (the "structural" problem)
- Don't consider rerouting (Griewank, Vogel 2004)

Accumulation Dags

computational graphs for Jacobians

- Every non-minimal vertex is an operation ($+$ or $*$) and has exactly two predecessors (the operands).
- Minimal vertices are the edge labels in E (the local partials)
- Maximal vertices are Jacobian entries

Each vertex is an operation $\Rightarrow$ We want to find an accumulation dag with a minimum number of vertices

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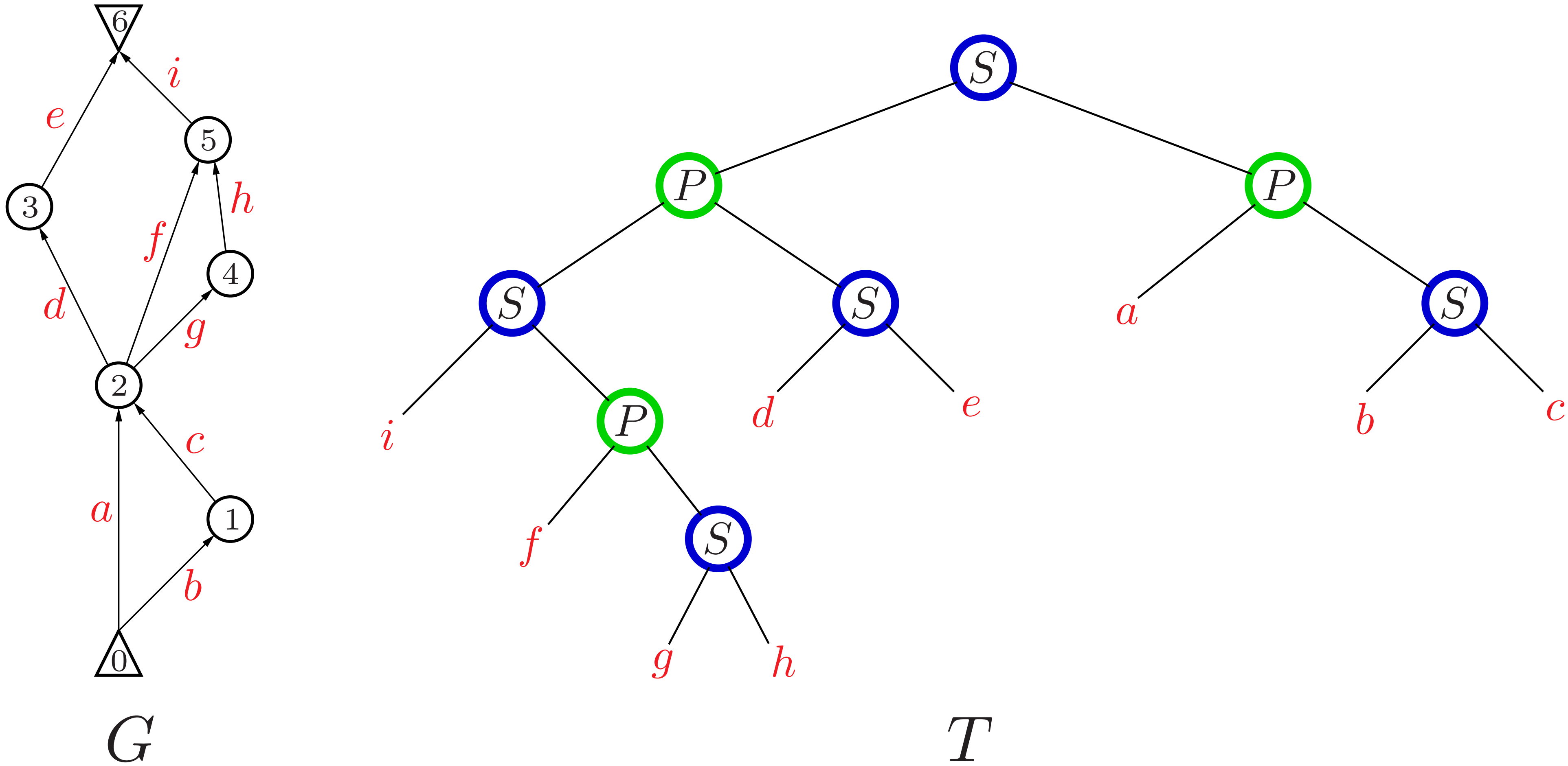
Two-Terminal Series-Parallel dags

Recursive definition:

- An isolated edge is TTSP
- If two graphs G_1, G_2 are TTSP, then so is...
  - *Series composition:* Identifying source of G_1 with sink of G_2
  - *Parallel composition:* Identifying sources, sinks of G_1, G_2

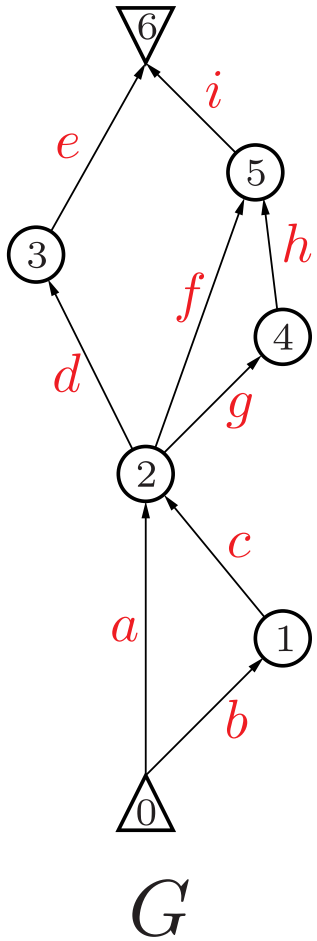
Note: in LCGs, cannot combine two isolated edges in parallel

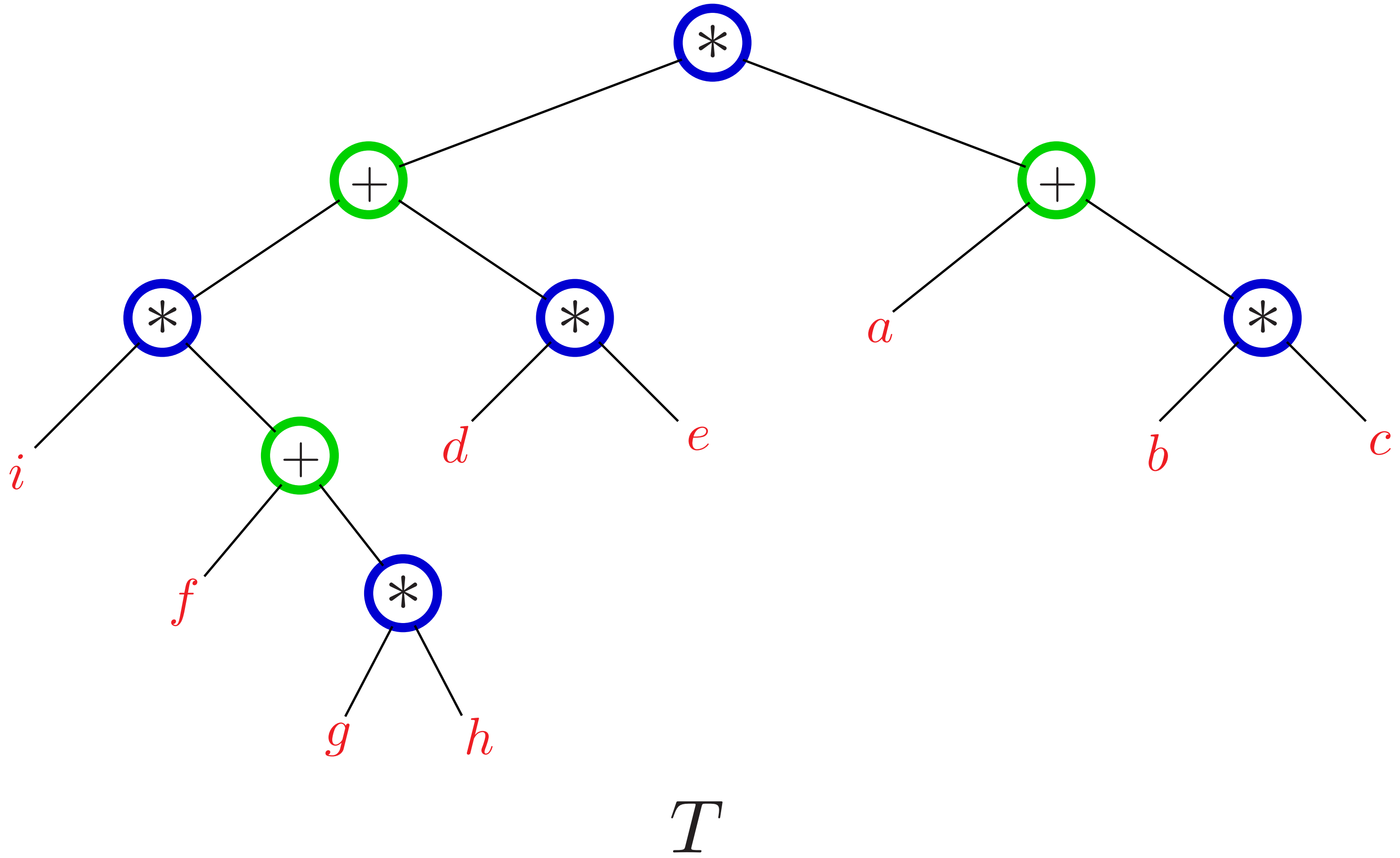
Decomposition Trees



Binary/canonical versions

Decomposition Trees $\longrightarrow$ Accumulation dags





SP Decomposition Solves OJA

Claims:

- The SP decomposition tree computes J
- The SP decomposition tree solves OJA

SP Decomposition Solves OJA

<u>Any</u> (full) binary tree contains $|E| - 1$ non-minimal nodes (operations)

TTSP dags are recognizable in linear time, and the decomposition tree (binary or canonical) can be built in linear time (Valdes, Tarjan, Lawler 1982)

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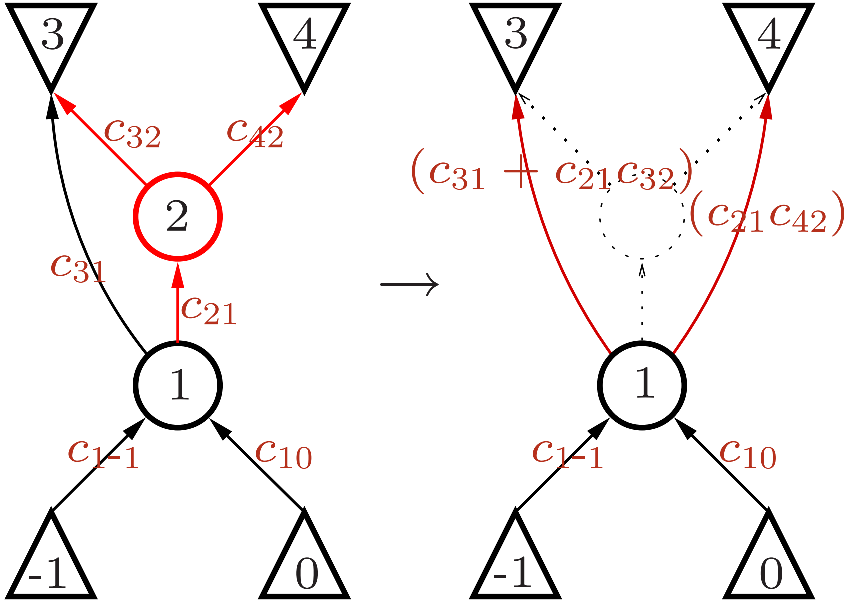
Vertex Elimination (Griewank, Reese 1991)



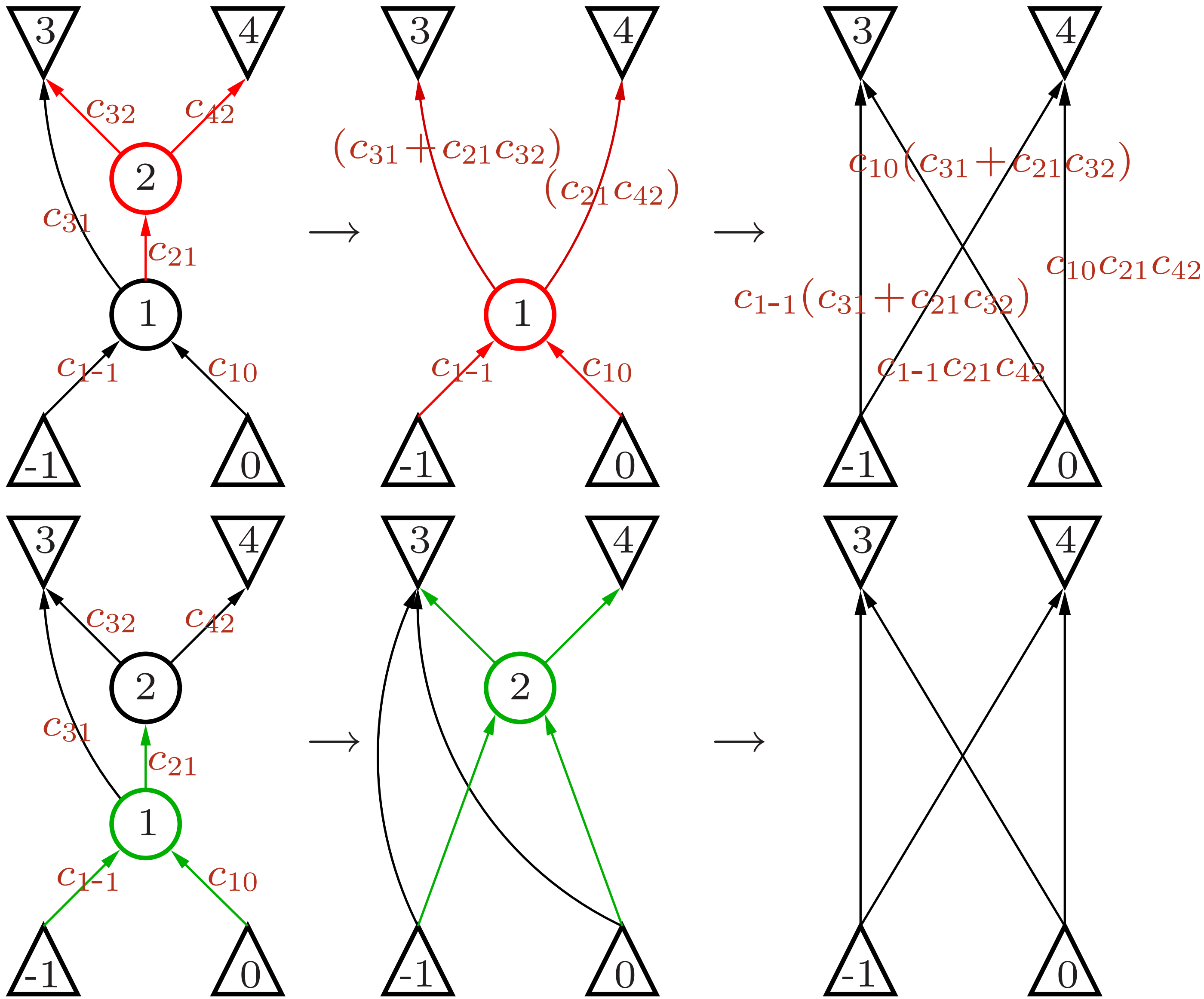
$$\mathtt{dv}_1 = c_{31} + c_{32} * c_{21}$$
$$\mathtt{dv}_2 = c_{21} * c_{42}$$

$$\begin{pmatrix} c_{1\text{-}1}c_{31} + c_{1\text{-}1}c_{21}c_{32} & c_{10}c_{31} + c_{10}c_{21}c_{32} \\ c_{1\text{-}1}c_{21}c_{42} & c_{10}c_{21}c_{42} \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} c_{1\text{-}1}(c_{31} + c_{21}c_{32}) & c_{10}(c_{31} + c_{21}c_{32}) \\ c_{1\text{-}1}(c_{21}c_{42}) & c_{10}(c_{21}c_{42}) \end{pmatrix}$$

Vertex Elimination (Griewank, Reese 1991)

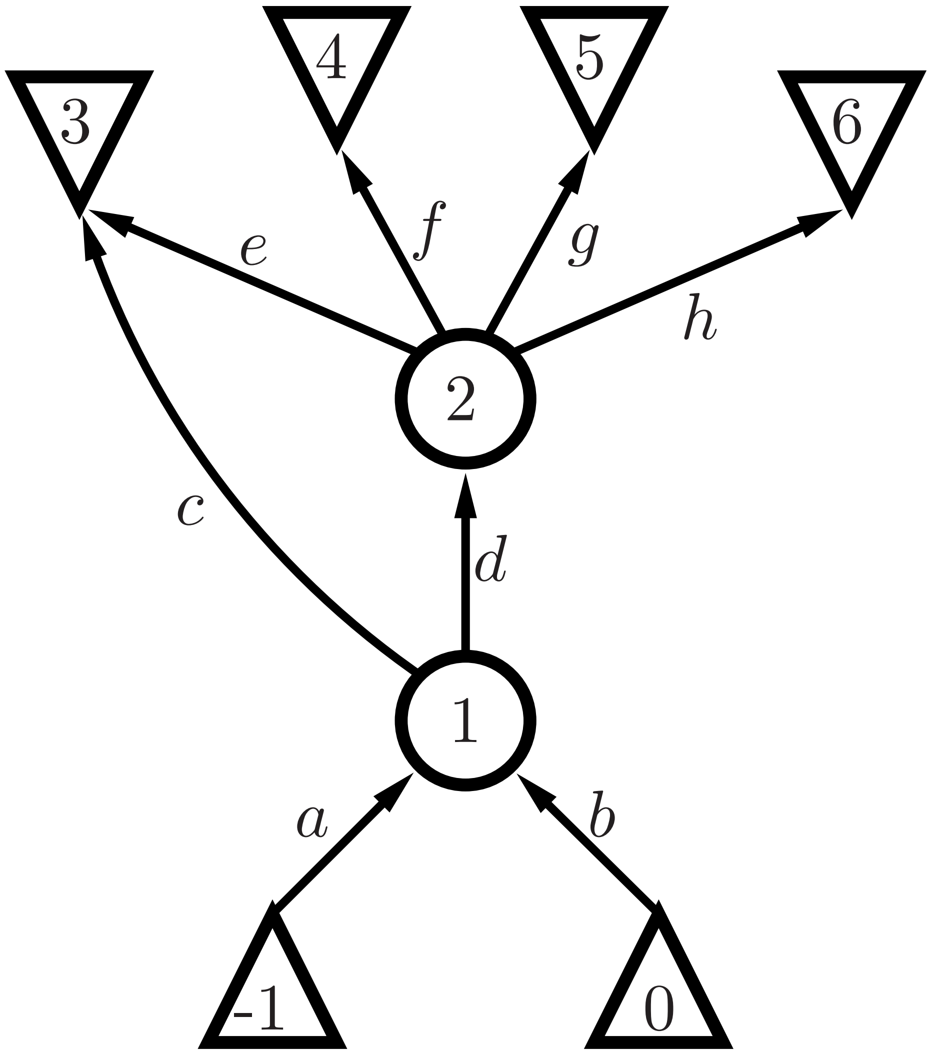


Vertex Elimination (Griewank, Reese 1991)

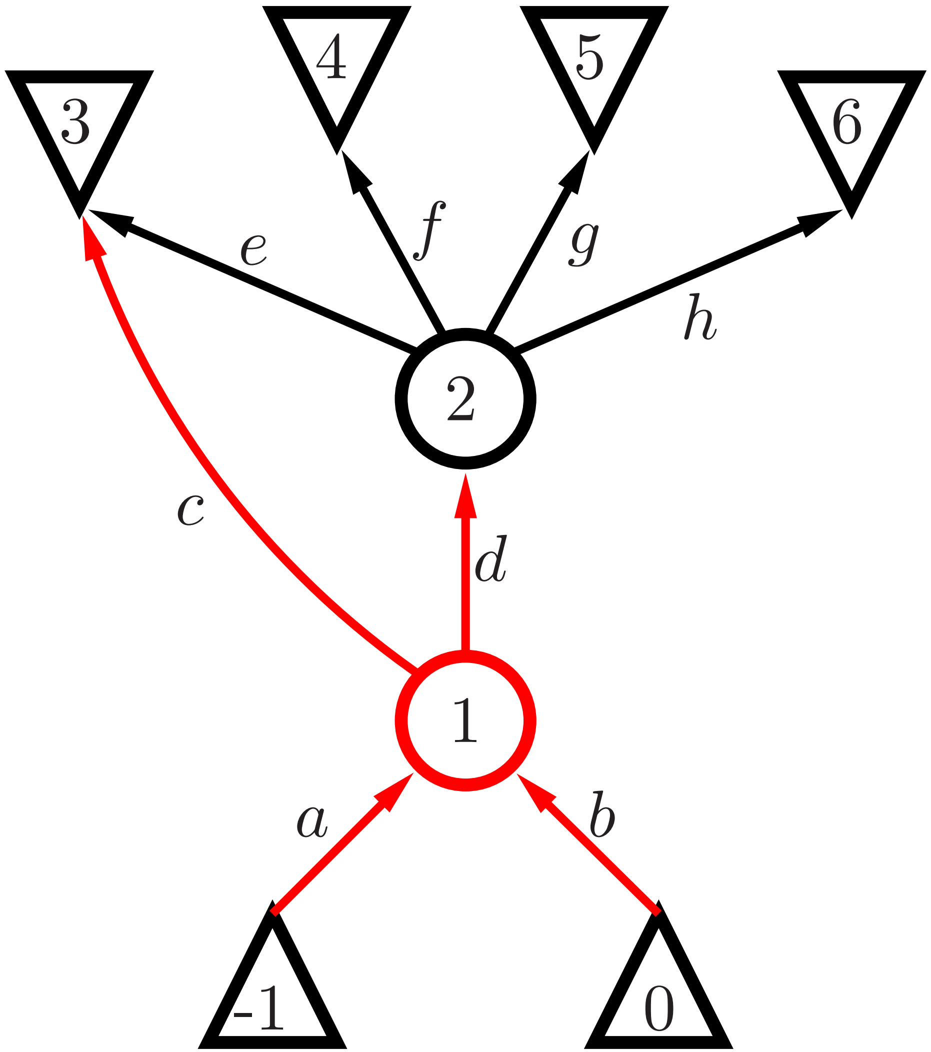
Cost of eliminating a vertex: $|P_v| * |S_v|$ multiplications

Lower bound for vertex elimination: $|\underline{P_v}| * |\underline{S_v}|$ for each v

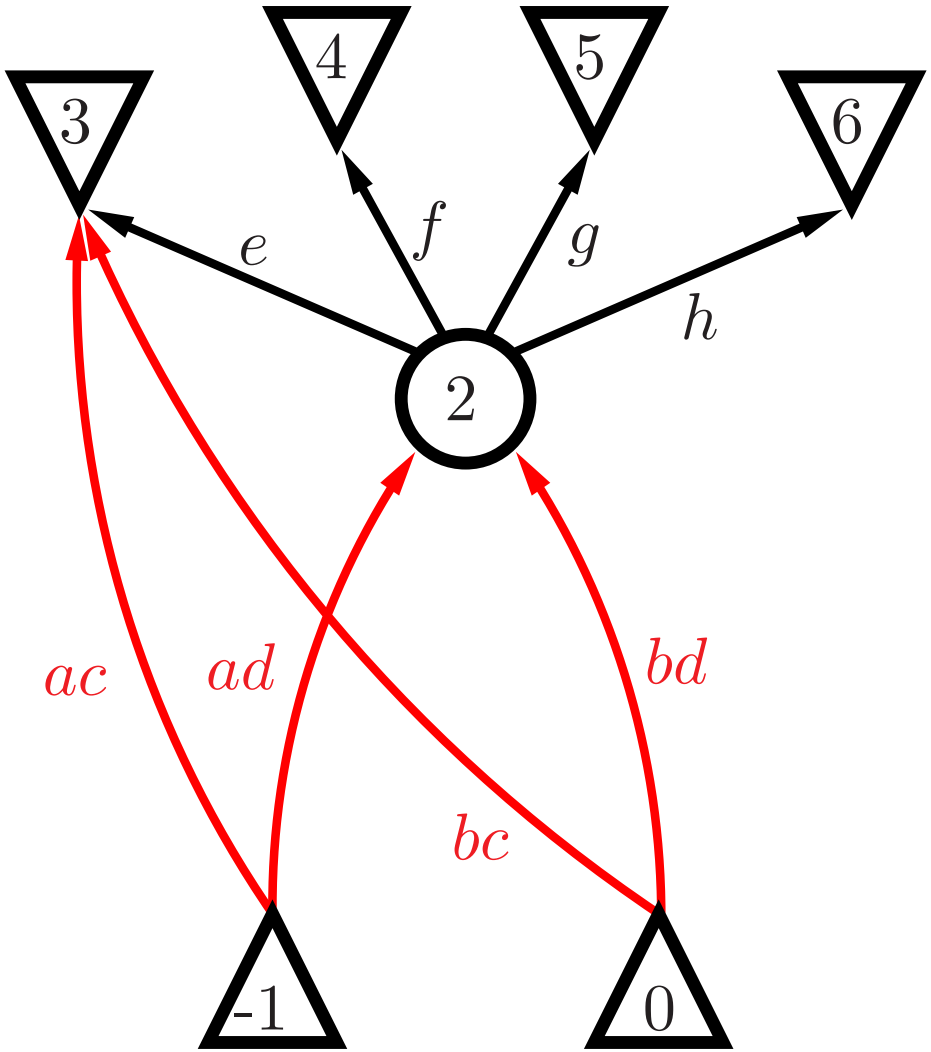
Vertex Elimination



Vertex Elimination

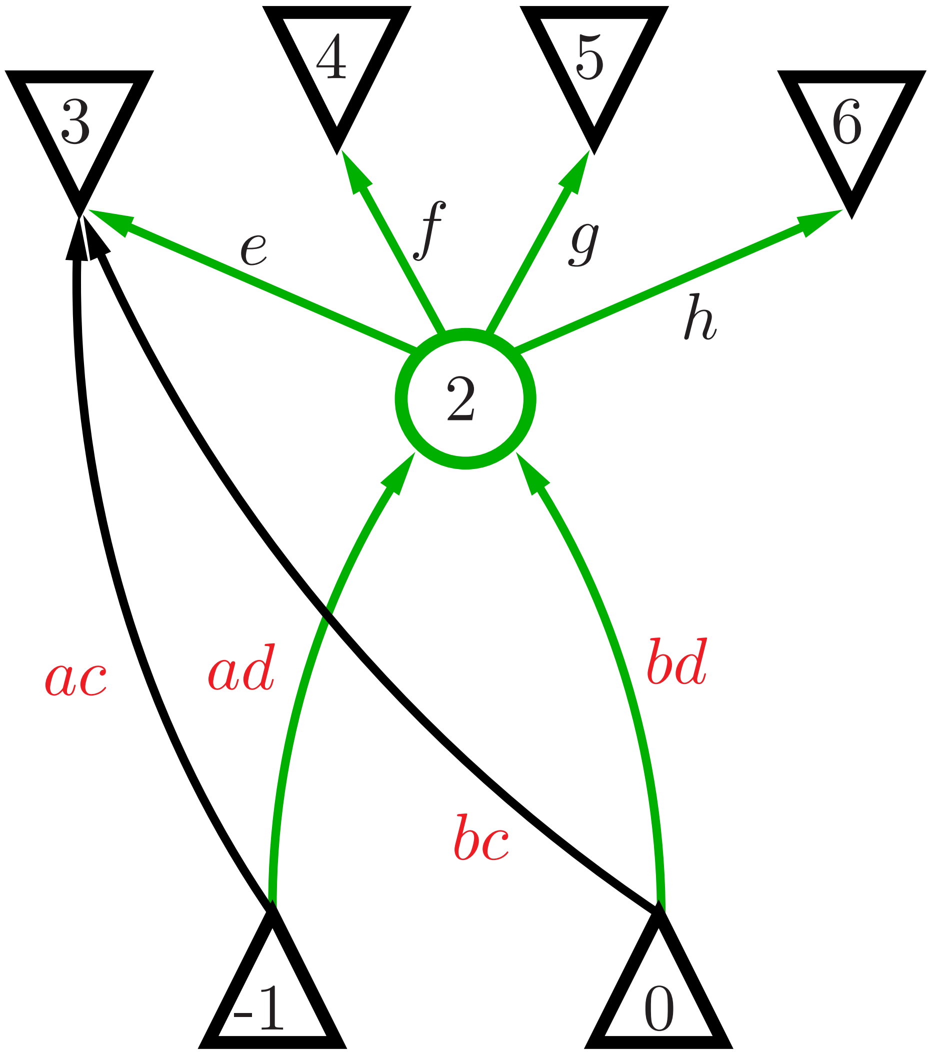


Vertex Elimination



$$ac = a * c$$
$$ad = a * d$$
$$bc = b * c$$
$$bd = b * d$$

Vertex Elimination



$$ac = a * c$$
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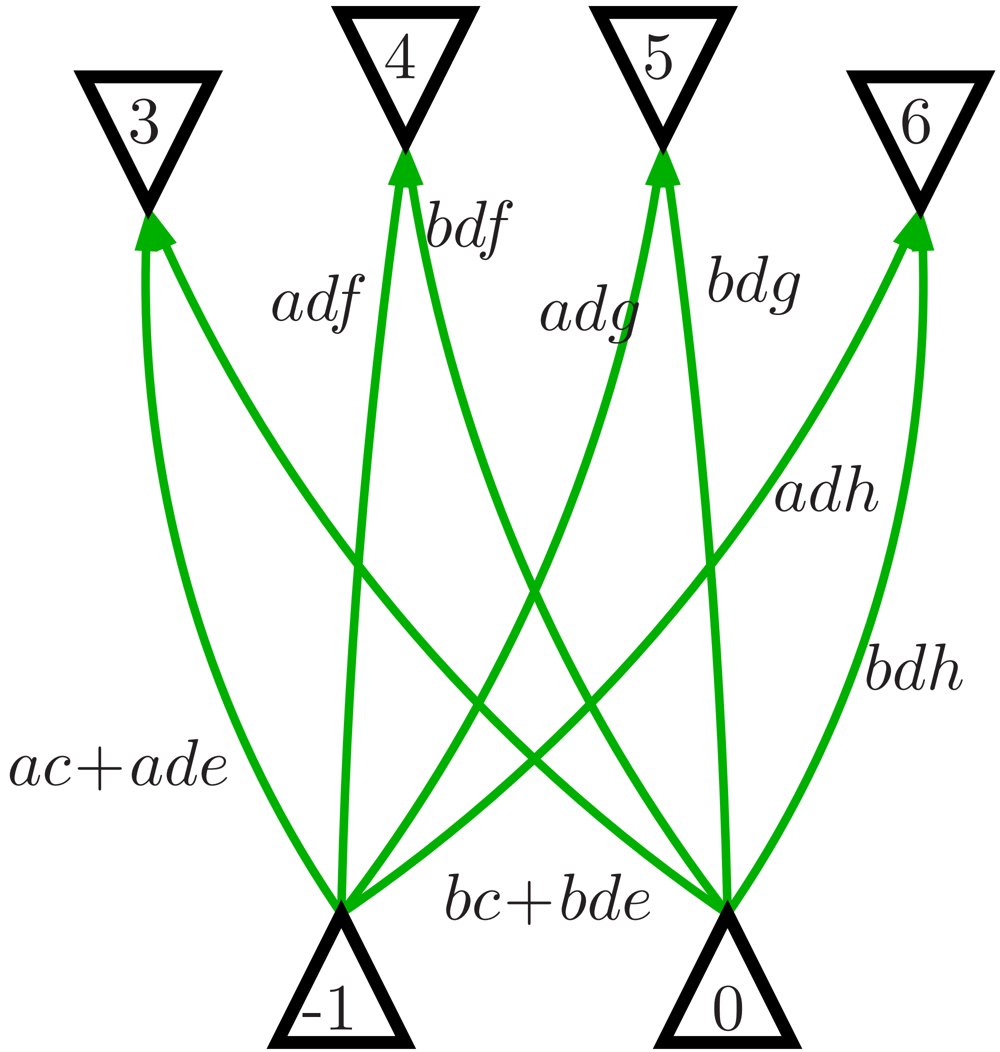
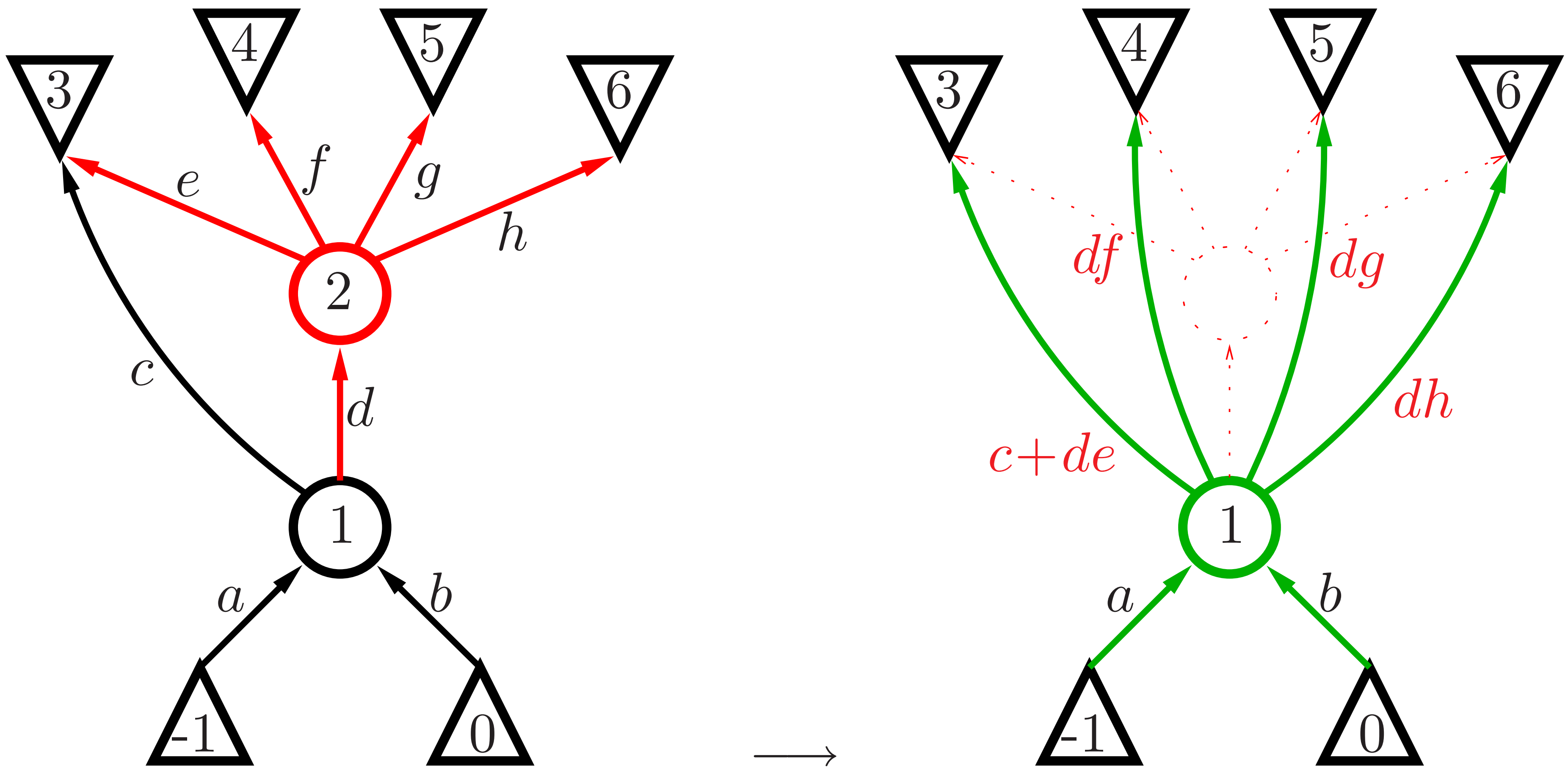
Vertex Elimination



$$ac = a * c$$
$$ad = a * d$$
$$bc = b * c$$
$$bd = b * d$$

$$\begin{aligned} ade &= ad * e \\ (ac + ade) &= ac + ade \\ adf &= ad * f \\ adg &= ad * g \\ adh &= ad * h \\ bde &= bd * e \\ (bc + bde) &= bc + bde \\ bdf &= bd * f \\ bdg &= bd * g \\ bdh &= bd * h \end{aligned}$$

Vertex Elimination



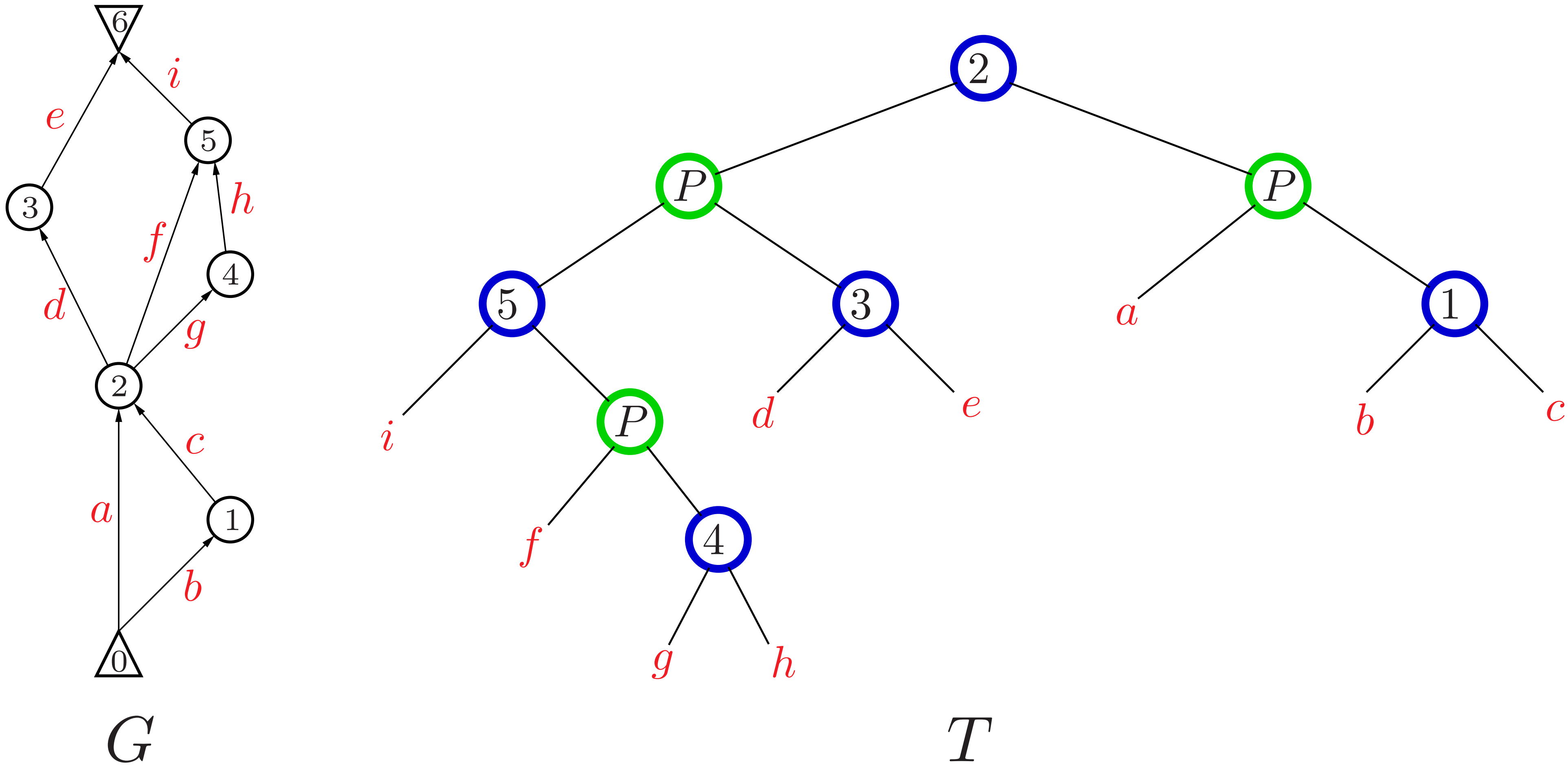
Vertex Elimination

$$\begin{array}{c} \mathtt{v}_2, \mathtt{v}_1 \\ \begin{pmatrix} a(c+de) & b(c+de) \\ a(df) & b(df) \\ a(dg) & b(dg) \\ a(dh) & b(dh) \end{pmatrix} \end{array} \qquad \begin{array}{c} \mathtt{v}_1, \mathtt{v}_2 \\ \begin{pmatrix} ac+(ad)e & bc+(bd)e \\ (ad)f & (bd)f \\ (ad)g & (bd)g \\ (ad)h & (bd)h \end{pmatrix} \end{array}$$

- Makes *poor* use of common subexpressions $(df), (dg), (dh)$
- Exploits distributivity effectively $a(c+de),\ b(c+de)$

- Makes good use of common subexpressions $(ad), (bd)$
- *Doesn't* exploit distributivity $ac+ade,\ bc+bde$

Vertex Elimination in TTSP Dags



Vertex Elimination in TTSP Dags

Every binary decomposition tree corresponds to a collection of vertex elimination sequences

$\Rightarrow$ OJA $=$ OVE for TTSP dags

Each vertex eliminated at $|\underline{P_v}| = |\underline{S_v}| = 1$

Generalizing to Scalar Valued Functions

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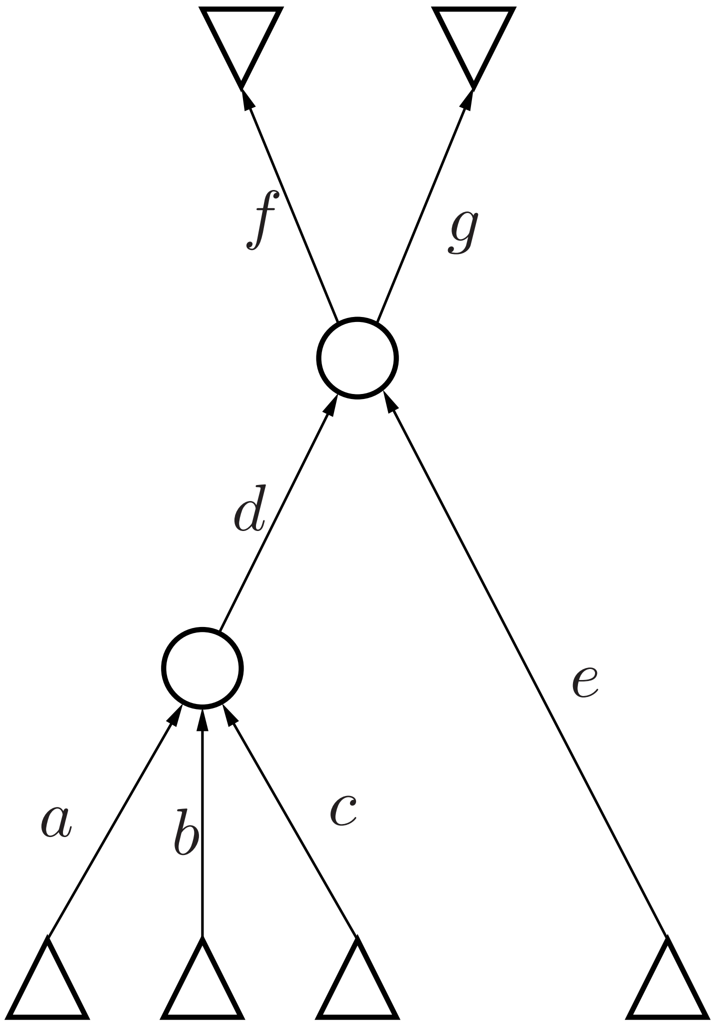
SP Tree NOT Optimal for General Jacobians



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Generalizing the decomposition: Modules

$G = (V, E) \to P = (E, \leq)$

($a \leq b \Leftrightarrow a$ and b lie on a common path)

Module M:

every $e \in E \setminus M$ is either comparable or incomparable to every $m \in M$

Future Work

- Extracting SP subgraphs from General graphs
- Generalize to modular decomposition
  (prove modules can be accumulated in isolation)
- Complexity of OJA by vertex, edge, face elimination (still!)
- Complexity of OJA in general (= face elimination??)