Calculating Hessian matrices

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Motivation from nonlinear programming

- Second order Taylor approximations very common in nonlinear programming.
- Hessians desirable in interior-point and augmented Lagrangian methods.
- Sensitivity analysis

Function Representation

- Indices of matrices and vectors shifted by $-n$.
  $y \in \mathbb{R}^m$: $y = (y_{1-n}, \dots, y_{m-n})^T$

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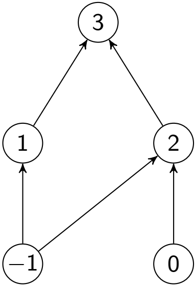

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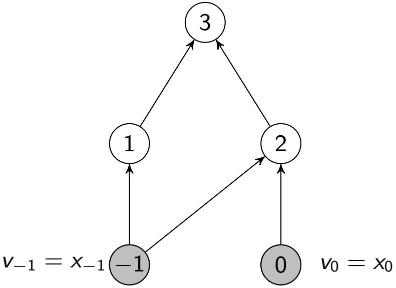

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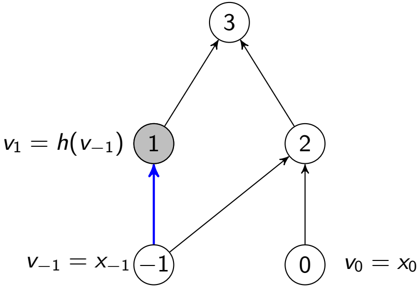

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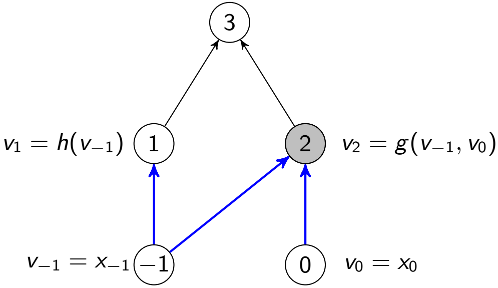

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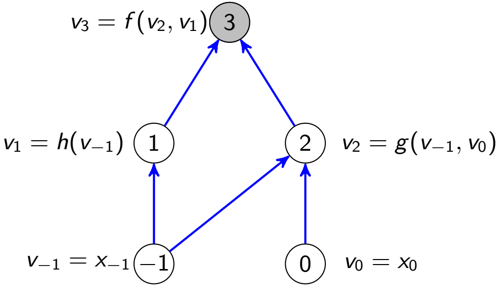

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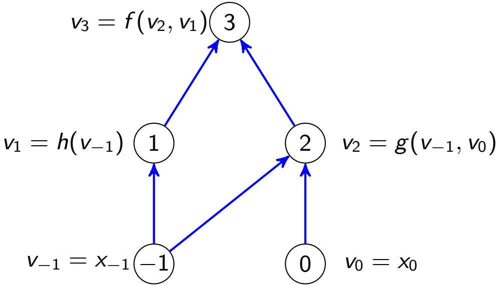

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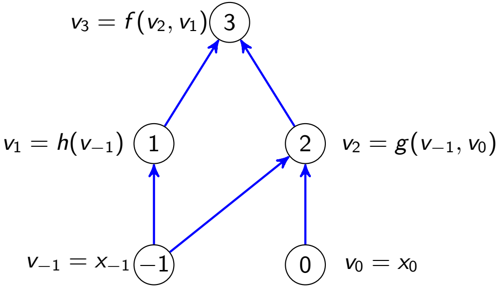

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TIME(eval$(f(x))$) $= O(\ell + n)$.

Forward Gradient: The first attempt

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$$\nabla v_i = \sum_{j \in P(i)} \frac{\partial \phi_i}{\partial v_j} \nabla v_j.$$

Each j passes on $\frac{\partial \phi_i}{\partial v_j} \nabla v_j$ to each sucessor i.

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- For each node visit, perform n-dimension vector arithmetic.
- **Time** complexity: $O(n\ell)$.
- **Storing and calculating all ∇v_i's is expensive and unnecessary.**

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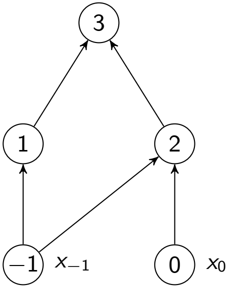

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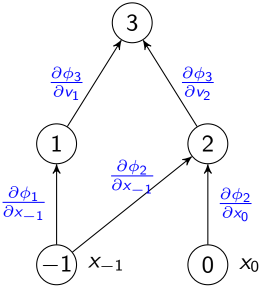

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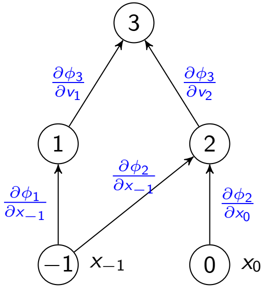

$$\frac{\partial f}{\partial x_0}$$

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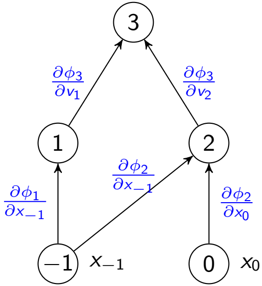

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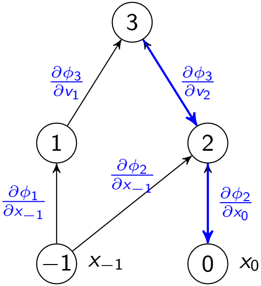

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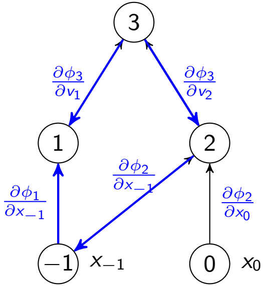

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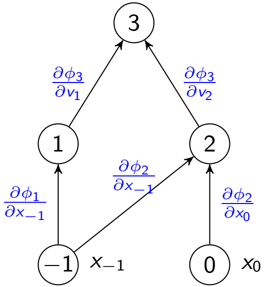

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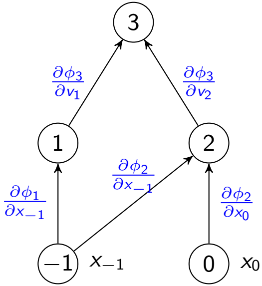

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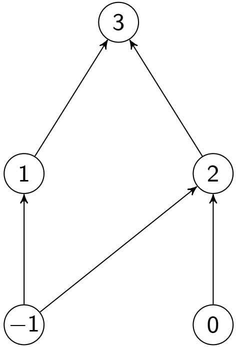
$$\frac{\partial f}{\partial x_i} = \sum_{p|\text{path from } i \text{ to } \ell} (\text{weight of path } p)$$

Reverse Gradient - Accumulating paths

$$f(x) = \phi_3(\phi_1(x_{-1}), \phi_2(x_{-1}, x_0))$$



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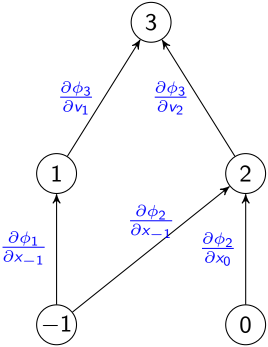

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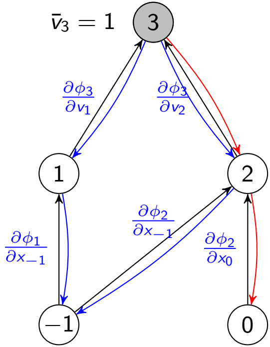

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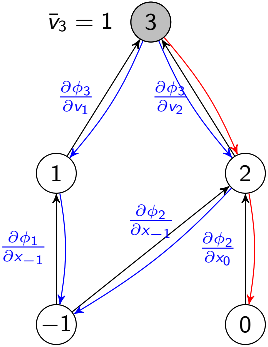

$$\bar{v}_i = \sum_{\text{path from } i \text{ to } \ell} (\text{path weight})$$

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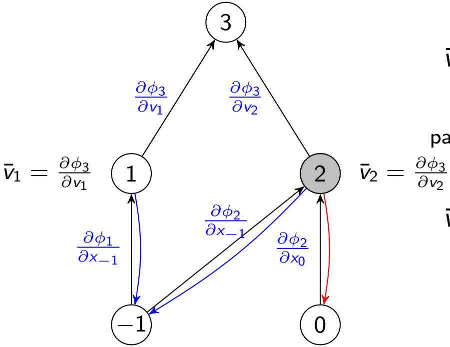

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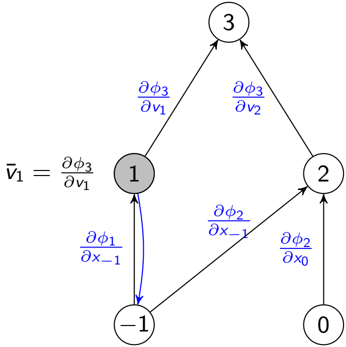

$$\bar{v}_{-1} = \frac{\partial \phi_2}{\partial x_{-1}} \bar{v}_2 \qquad \bar{v}_0 = \frac{\partial \phi_2}{\partial x_0} \bar{v}_2$$

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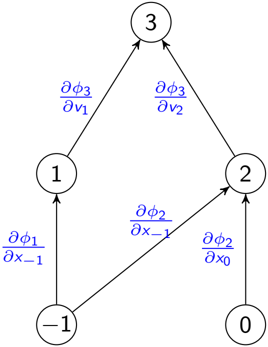

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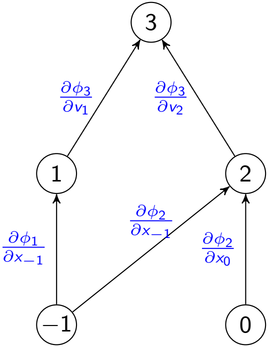

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$$\text{TIME}(\nabla f(x)) = \text{TIME}(f(x))$$

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Forward Hessian: McCormick and Jackson 1986

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$$\Downarrow$$

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$$\nabla v_i = \sum_{j \in P(i)} \frac{\partial \phi_i}{\partial v_j} \nabla v_j$$

$$\downarrow$$

$$v_i'' = \sum_{j,k \in P(i)} \nabla v_j \cdot \frac{\partial^2 \phi_i}{\partial v_j \partial v_k} \cdot \nabla v_k^T + \sum_{j \in P(i)} \frac{\partial \phi_i}{\partial v_j} \cdot v_j''$$

Forward Hessian resume

- For each node, store and calculate a $n \times n$ matrix.

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- For each node, store and calculate a $n \times n$ matrix.
- Is it necessary to calculate the gradient and Hessian of each node?
- Gain a deeper understanding on the problem using gradient graph.

Calculating the Hessian using the computational graph

- Function's computational graph + $\bar{v}_i$ nodes and dependencies = gradient computational graph.

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- Eliminate unnecessary symmetries on augmented graph.

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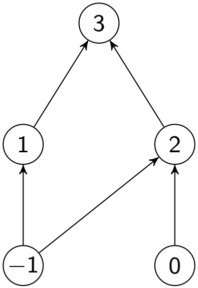
- node $\bar{\jmath} \longleftrightarrow \bar{v}_j$.

The adjoint variables of the Reverse Gradient satisfy

$$\bar{v}_j = \sum_{i \in S(j)} \bar{v}_i \frac{\partial \phi_i}{\partial v_j} \equiv \bar{\varphi}_j.$$

- Gradient's graph has $2(\ell + n)$ nodes: $(v_{1-n}, \ldots, v_\ell)$ and $(\bar{v}_{1-n}, \ldots, \bar{v}_\ell)$.
- node $\bar{\mathrm{j}} \longleftrightarrow \bar{v}_j$.
- $\bar{i} \in P(\bar{\mathrm{j}})$ iff $j \in P(i)$.

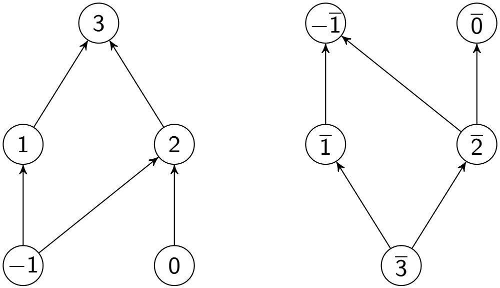
$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$



$$\begin{aligned} v_{-1} &= x_{-1} \\ v_0 &= x_0 \\ v_1 &= \sin(v_{-1}) \\ v_2 &= (v_{-1} + v_0) \\ v_3 &= v_1 v_2 \end{aligned}$$

$$\begin{aligned} \bar{v}_3 &= 1 \\ \bar{v}_2 &= \bar{v}_3 v_1 \\ \bar{v}_1 &= \bar{v}_3 v_2 \\ \bar{v}_0 &= \bar{v}_2 1 \\ \bar{v}_{-1} &= \bar{v}_2 1 + \bar{v}_1 \cos(v_{-1}) \end{aligned}$$

$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$



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\begin{aligned}
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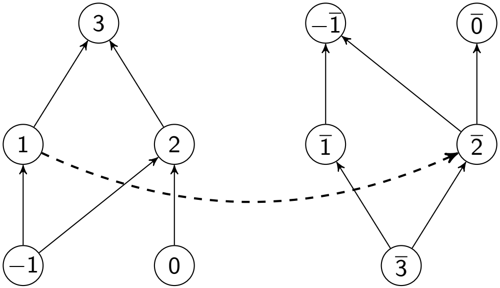

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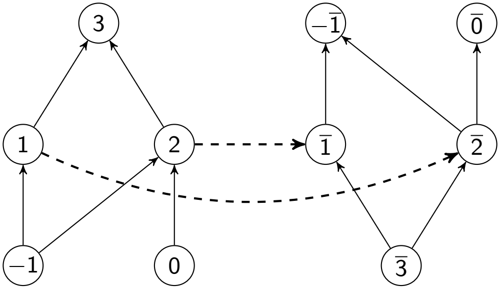

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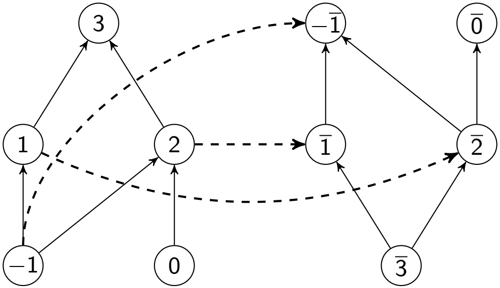

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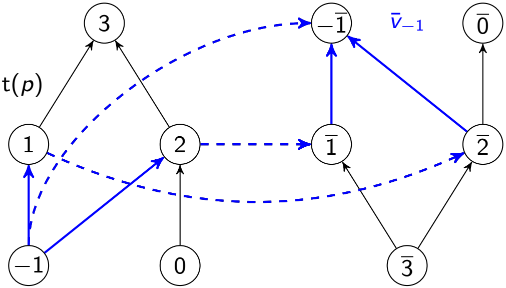
$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \sum_{p \text{ from } -1 \text{ to } -\bar{1}} \text{Weight}(p)$$



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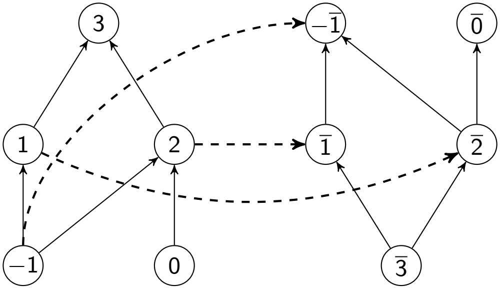

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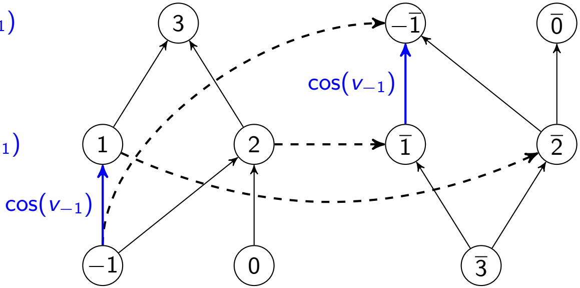
\end{aligned}$$

$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$

$$\frac{\partial \phi_1}{\partial v_{-1}} = \cos(v_{-1})$$

$$\frac{\partial \bar{\varphi}_{-1}}{\partial \bar{v}_1} = \cos(v_{-1})$$



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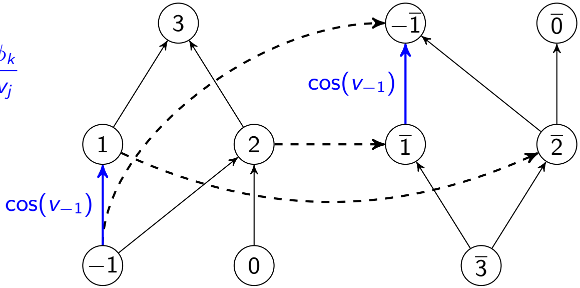
$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$

$$\frac{\partial \bar{\varphi}_j}{\partial \bar{v}_k} = c_{kj} = \frac{\partial \phi_k}{\partial v_j}$$



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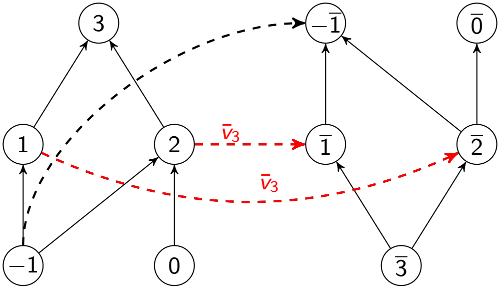
$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$



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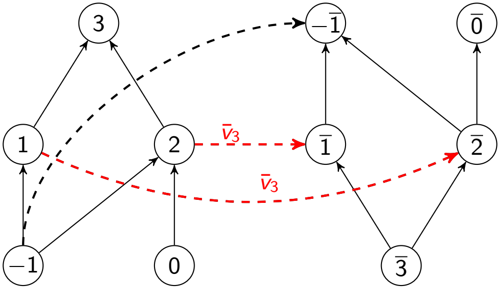
$$f(x) = \sin(x_{-1})(x_{-1} + x_0)$$

$$\frac{\partial \bar{\varphi}_1}{\partial v_2} = \bar{v}_3$$

$$\frac{\partial \bar{\varphi}_2}{\partial v_1} = \bar{v}_3$$



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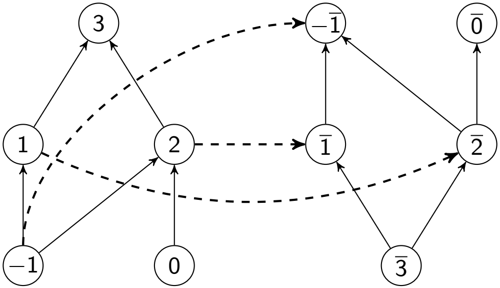
$$\frac{\partial \bar{\varphi}_j}{\partial \bar{v}_k} = \bar{c}_{kj} = \frac{\partial \bar{\varphi}_k}{\partial \bar{v}_j}$$



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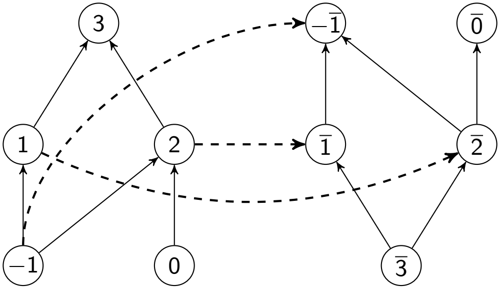
$$\bar{c}_{kj} = \sum_{i \in S(k) \cap S(j)} \bar{v}_i \frac{\partial^2 \phi_i}{\partial v_j \partial v_k}$$



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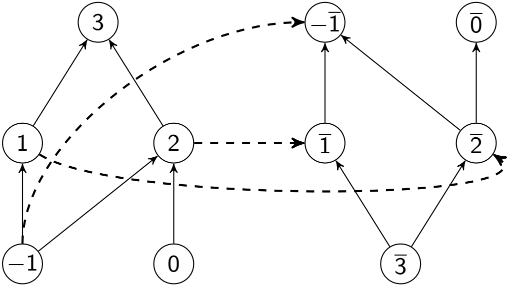
\end{aligned}$$

$$f(x) = \sin(x_{-1})(x_{-1} + x_0) = \phi_3(\phi_1(x_{-1}), \phi_2(x_{-1}, x_0))$$



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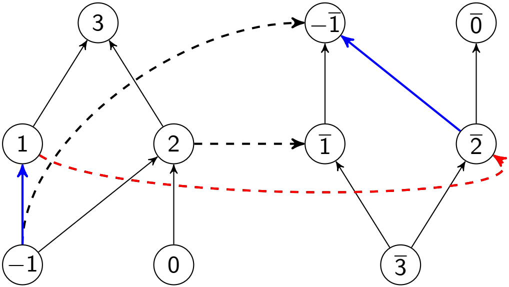

$$\frac{\partial^2 f}{\partial x_{-1}^2} = c_{1-1}\bar{c}_{21}c_{2-1}$$

$$\begin{aligned} v_{-1} &= x_{-1} \\ v_0 &= x_0 \\ v_1 &= \sin(v_{-1}) \\ v_2 &= (v_{-1} + v_0) \\ v_3 &= v_1 v_2 \end{aligned}$$

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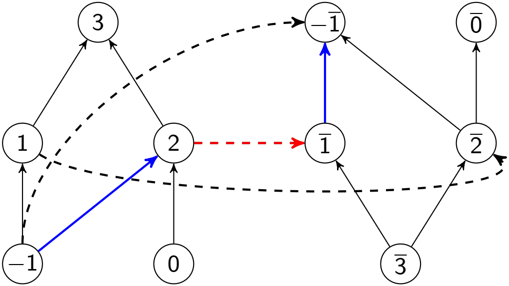

$$\frac{\partial^2 f}{\partial x_{-1}^2} = c_{1-1}\bar{c}_{21}c_{2-1} + c_{2-1}\bar{c}_{21}c_{1-1}$$

$$\begin{aligned} v_{-1} &= x_{-1} \\ v_0 &= x_0 \\ v_1 &= \sin(v_{-1}) \\ v_2 &= (v_{-1} + v_0) \\ v_3 &= v_1 v_2 \end{aligned}$$

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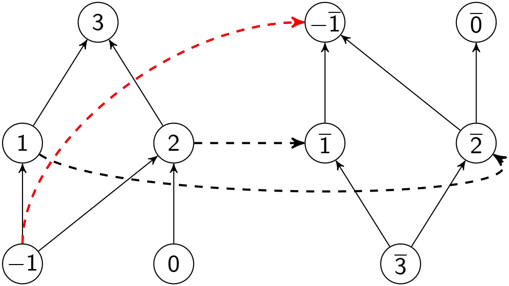
$$f(x) = \sin(x_{-1})(x_{-1} + x_0) = \phi_3(\phi_1(x_{-1}), \phi_2(x_{-1}, x_0))$$



$$\frac{\partial^2 f}{\partial x_{-1}^2} = c_{1-1}\bar{c}_{21}c_{2-1} + c_{2-1}\bar{c}_{21}c_{1-1} + \bar{c}_{-1-1}$$

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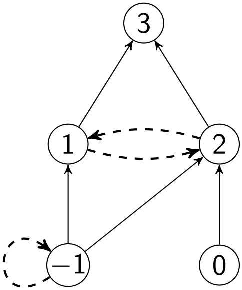
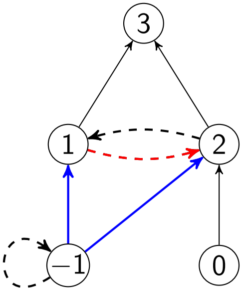
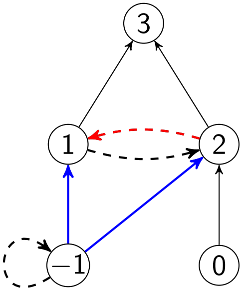


- Fold mirror subgraph.



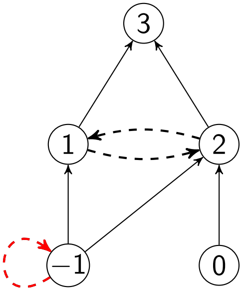
$$\frac{\partial^2 f}{\partial x_{-1}^2} = c_{1-1} \bar{c}_{21} c_{2-1}$$

- Fold mirror subgraph.



- Fold mirror subgraph.

$$\frac{\partial^2 f}{\partial x_{-1}^2} = c_{1-1}\bar{c}_{21}c_{2-1} + c_{2-1}\bar{c}_{21}c_{1-1}$$



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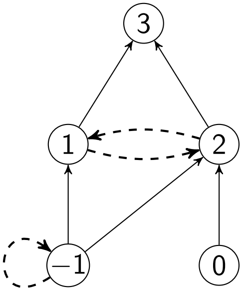
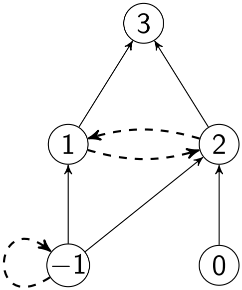
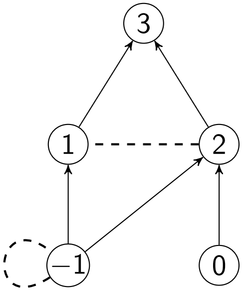


- Fold mirror subgraph.
- More symmetry



- Fold mirror subgraph.
- More symmetry
- $k \dashrightarrow j$ iff $k \dashleftarrow j$

$$\bar{c}_{kj} = \bar{c}_{jk}$$



- Fold mirror subgraph.
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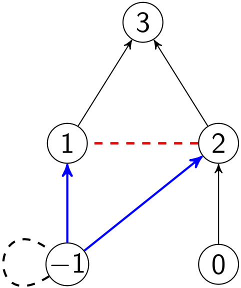

$$\frac{\partial^2 f}{\partial x_{-1}^2} = 2c_{1-1}\bar{c}_{21}c_{2-1}$$

- Fold mirror subgraph.
- More symmetry
- $k \dashrightarrow j$ iff $k \dashleftarrow j$

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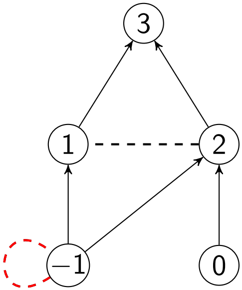
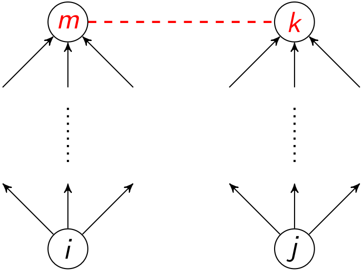
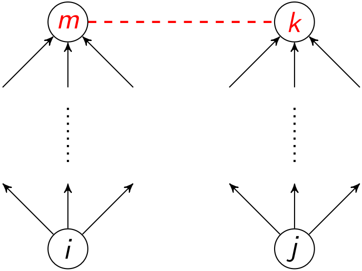


$$\frac{\partial^2 f}{\partial x_{-1}^2} = 2c_{1-1}\bar{c}_{21}c_{2-1} + \bar{c}_{-1-1}$$

- Fold mirror subgraph.
- More symmetry
- $k \dashrightarrow j$ iff $k \dashleftarrow j$

$$\bar{c}_{kj} = \bar{c}_{jk}$$


m
k
i
j



$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \sum_{\substack{\text{nonlinear} \\ \text{edge } \{m,k\}}} \sum_{\{p|\text{ from } i \text{ to } m\}} (\text{ weight of } p)\, \bar{c}_{mk} \sum_{\{p|\text{ from } j \text{ to } k\}} (\text{ weight of } p)\,.$$

Building shortcuts

- $P(m) = \{i, j\}$.

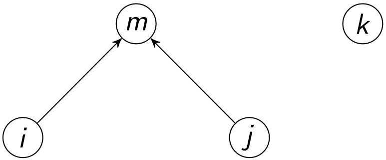


Figure: Pushing the edge $\{m, k\}$

Building shortcuts

- $P(m) = \{i, j\}$.
- $(m, k) \in$ Path

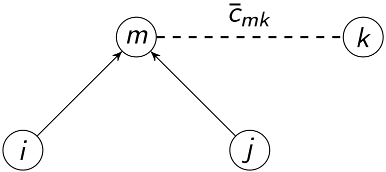


Figure: Pushing the edge $\{m, k\}$

Building shortcuts

- $P(m) = \{i, j\}$.
- $(m, k) \in$ Path
- $\Rightarrow$ path $\ni (i, m, k)$ or path $\ni (j, m, k)$

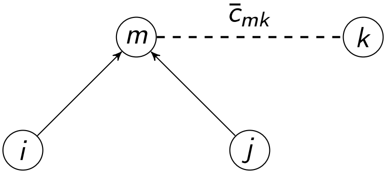


Figure: Pushing the edge $\{m, k\}$

Building shortcuts

- $P(m) = \{i, j\}$.
- $(m, k) \in$ Path
- $\Rightarrow$ path $\ni (i, m, k)$ or path $\ni (j, m, k)$

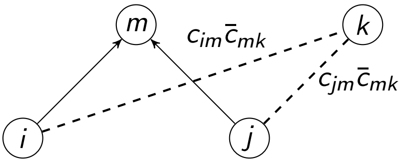
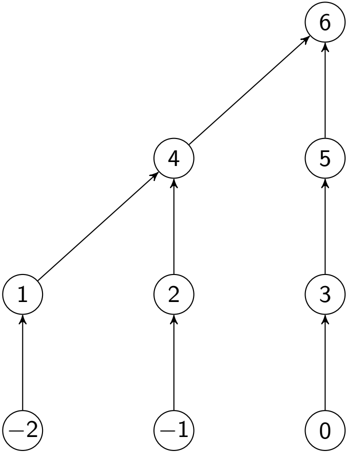


Figure: Pushing the edge $\{m, k\}$

Simple example of edge_pushing execution



$$f(x) = (x_{-2}+1)(x_{-1}+1)3(x_0+1)$$

$$v_1 = v_{-2} + 1$$
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$$v_3 = v_0 + 1$$
$$v_4 = v_1 v_2$$
$$v_5 = 3v_3$$
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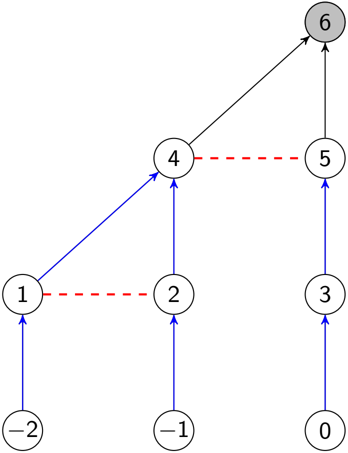

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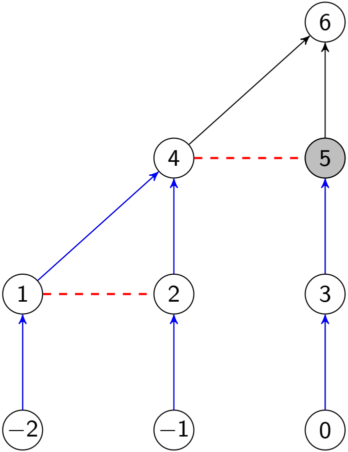

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$$\begin{aligned}
v_1 &= v_{-2}+1\\
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\end{aligned}$$

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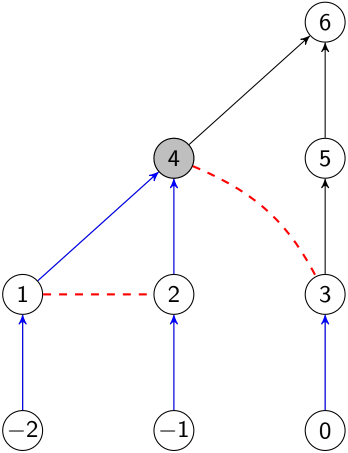

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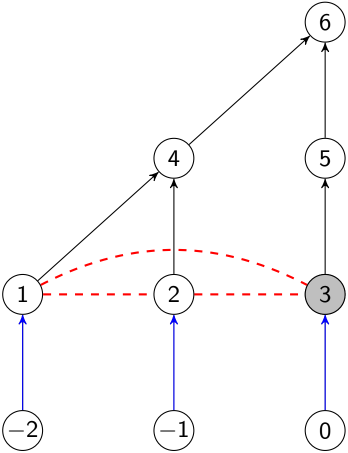

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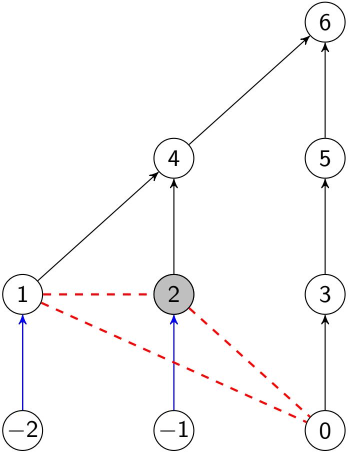

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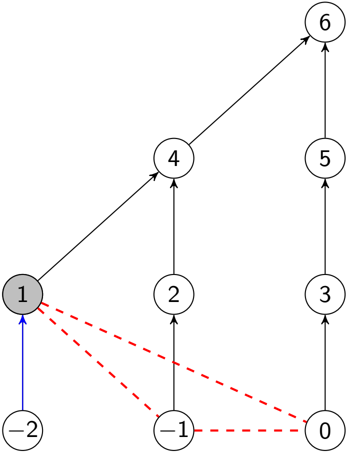

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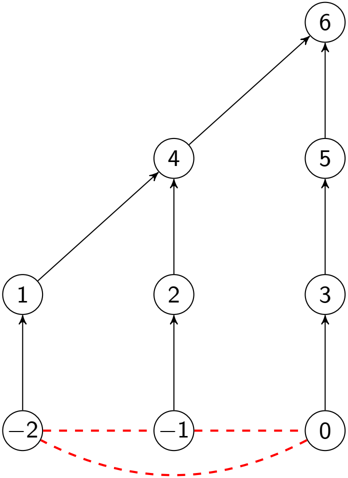

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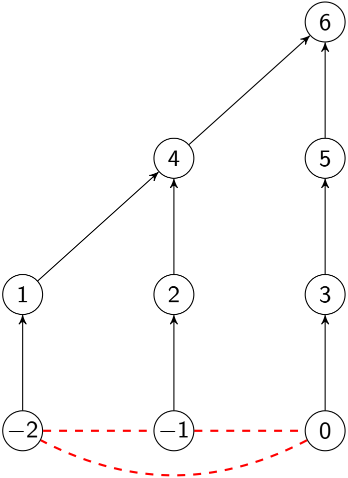

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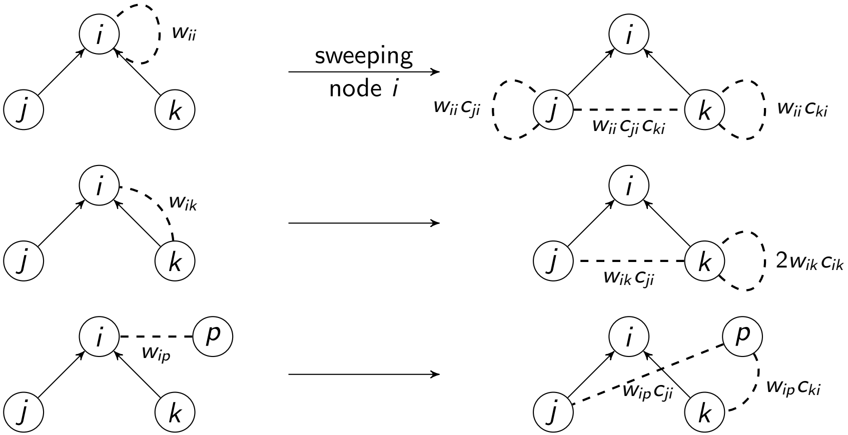
$$f'' = \begin{pmatrix} 0 & X & X \\ X & 0 & X \\ X & X & 0 \end{pmatrix}$$

pushing of nonlinear edges



The pseudo-code of `edge_pushing`

Input: $x \in \mathbb{R}^n$,

for $i = \ell, \dots, 1$ **do**

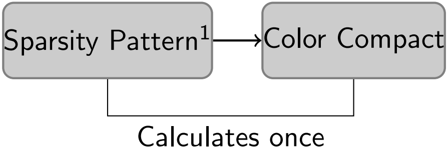
  `Create` nonlinear edges if ϕ_i is nonlinear ;

  `Push` nonlinear edges adjacent to i;

end

Competitor for `edge_pushing`: Graph coloring

- `edge_pushing` implementation aimed at large sparse Hessians.
- state-of-the-art competitor: graph coloring methods
  Gebremedhin, Manne, Pothen, Walther, Tarafdar
  - *Efficient Computation of Sparse Hessians Using Coloring and Automatic Differentiation*(2009)
  - *What Color Is Your Jacobian? Graph Coloring for Computing Derivatives*(2005)



$f''(x)$

$f''(x)S$

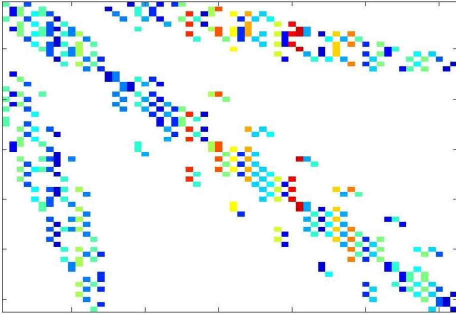
$\Rightarrow$

[1]Uses Walther's 2008 algorithm

Sparsity Pattern[1] $\longrightarrow$ Color Compact

Calculates once

$f''(x)$



$\Rightarrow$

$f''(x)S$

---

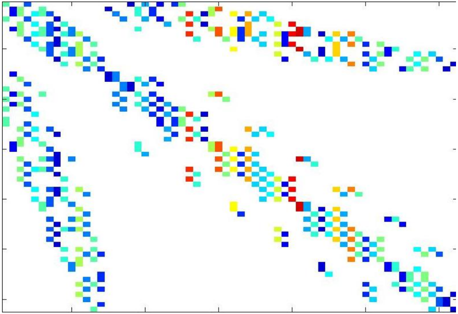
[1] Uses Walther's 2008 algorithm

Sparsity Pattern[1] → Color Compact → Derive Compact → Recover

Calculates once (Sparsity Pattern, Color Compact)

Repeat for each $x \in \mathbb{R}^n$ (Derive Compact, Recover)

$f''(x)$



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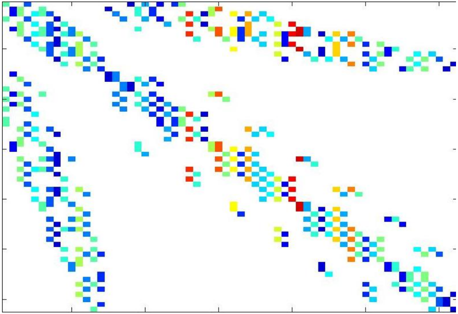

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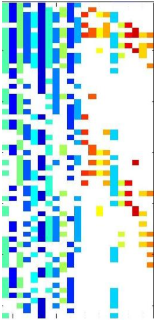


[1] Uses Walther's 2008 algorithm

- Invests a large initial time in 1st run $\Rightarrow$ fast subsequent runs.

- Invests a large initial time in 1st run $\Rightarrow$ fast subsequent runs.
- Two different coloring methods with different recoveries: Star and Acyclic.

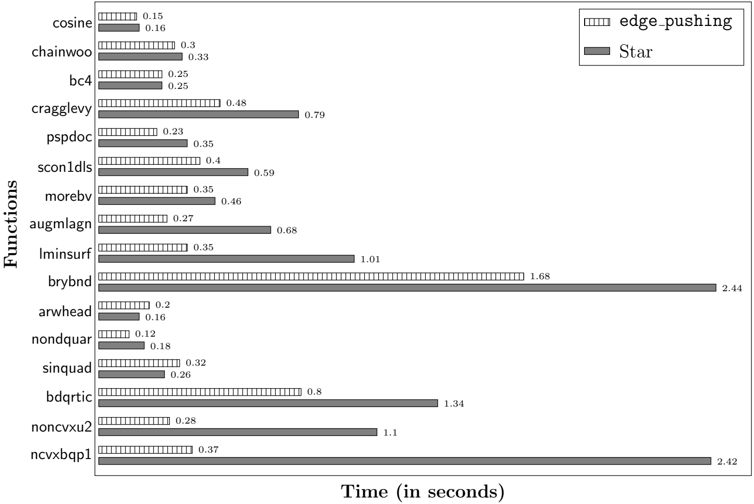
Test set chosen from CUTE

	$n = 50'000.$		
		# colors	
Name	Pattern	Star	Acyclic
cosine	B 1	3	2
chainwoo	B 2	3	3
bc4	B 1	3	2
cragglevy	B 1	3	2
pspdoc	B 2	5	3
scon1dls	B 2	5	3
morebv	B 2	5	3
augmlagn	5×5 diagonal blocks	5	5
lminsurf	B 5	11	6
brybnd	B 5	13	7
arwhead	arrow	2	2
nondquar	arrow + B 1	4	3
sinquad	frame + diagonal	3	3
bdqrtic	arrow + B 3	8	5
noncvxu2	irregular	12	7
ncvxbqp1	irregular	12	7

Numeric Results edge_pushing × Colouring methods

Name	Star 1st	Star 2nd	Acyclic 1st	Acyclic 2nd	e_p
cosine	9.93	0.16	9.68	2.52	0.15
chainwoo	35.07	0.33	33.24	5.08	0.30
bc4	10.02	0.25	10.00	2.56	0.25
cragglevy	28.17	0.79	28.15	2.60	0.48
pspdoc	10.31	0.35	10.27	4.39	0.23
scon1dls	11.00	0.59	10.97	4.96	0.40
morebv	10.36	0.46	10.33	4.49	0.35
augmlagn	15.99	0.68	8.36	16.74	0.27
lminsurf	9.30	1.01	9.24	3.89	0.35
brybnd	11.87	2.44	11.73	12.63	1.68
arwhead	176.50	0.16	45.86	0.24	0.20
nondquar	166.59	0.18	28.64	2.57	0.12
sinquad	606.72	0.26	888.57	1.51	0.32
bdqrtic	262.64	1.34	96.87	7.80	0.80
noncvxu2	29.69	1.10	29.27	7.76	0.28
ncvxbqp1	13.51	2.42	–	–	0.37
Averages	87.98	0.78	82.08	5.32	0.41
Variances	25 083.44	0.54	50 313.10	19.32	0.14

Graphical comparison: Star 2nd run versus edge_pushing.



Summing up

- Graph representation:

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    - New algorithm.

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    - New perspective.

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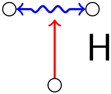
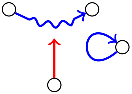
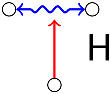
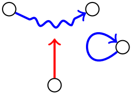
  - Promising test results.
  - Lives up to Griewank 16th rule.

The calculation of gradients by nonincremental reverse makes the corresponding computational graph symmetric, a property that should be exploited and maintained in accumulating Hessians.

 HANK

 U

 HANK  U

QUESTIONS?