Third Order Methods using slices of the Tensor and AD developments

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What's to come

- Third Order information can be used in practical nonlinear solvers
  - Automatic Differentiation (AD) methods that calculate third-order information at the same cost of the Hessian.
  - A family of third order methods that requires solving two linear systems.
  - Large-Scale tests comparing to Newton

Overview

Why not third order

Unconstrained minimization of $f : \mathbb{R}^n \to \mathbb{R}$.

First-order

$$d = -\alpha Df(x)$$

$$(Df(x) \equiv \text{The gradient})$$

Second-order

$$D^2 f(x) \cdot d + Df(x) = 0$$

$$(D^2 f(x) \equiv \text{The Hessian matrix})$$

$$n(x) = -(D^2 f(x))^{-1} Df(x).$$

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Why stop here? It's hard to solve these n

$$\frac{1}{2} D^3 f(x) \cdot (d, d) + D^2 f(x) \cdot d + Df(x) = 0.$$

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Why exactly these red pieces? Order 3 local convergence

Convex $\lambda \in [0,1]$ combinations Halley-Chebyshev family

$$(1-\lambda)\left(\tfrac{1}{2}D^3f(x)\cdot n(x) + D^2f(x)\right)\cdot d + Df(x)\Big) = 0$$

$$+$$

$$\lambda\left(D^2f(x)\cdot d + Df(x) + \tfrac{1}{2}D^3f(x)\cdot (n(x))^2\right) = 0$$

$$=$$

$$\left(D^2f(x) + \frac{(1-\lambda)}{2}D^3f(x)\cdot n(x)\right)\cdot d + Df(x) + \frac{\lambda}{2}D^3f(x)\cdot (n(x))^2 = 0$$

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- Halley-Chebyshev family [Gutierrez, 1997]
- Implicit form [Steihaug, 2012]
- Convex combination ⇒ Order-3 convergence (My homepage)
- Higher order generalizations possible!

Handling third order derivative

Problem: $D^3 f(x)$ is cube.

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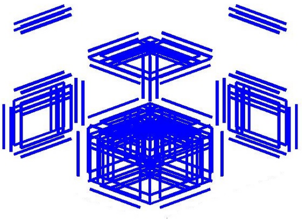

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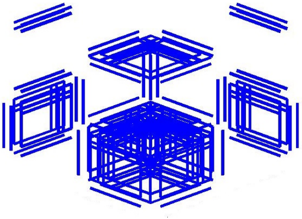

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- Data structures that balance Sparsity $\times$ Access time.
- Faster contractions $D^3 f(x) \cdot n(x)$.

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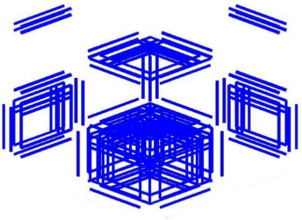

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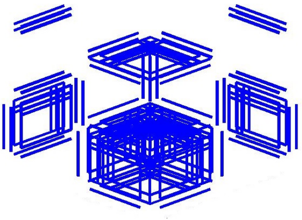

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Automatic **D**ifferentiation solution.

Why High Order AD?

- High order optimization methods
- Calculating quadratures (Vinay Kariwala 2012, G. F. Corliss, A. Griewank 1997)
- bifurcations and periodic orbits (J. Guckenheimer and B. Meloon 2000)
- Classifying Degenerate singularities and equilibria.

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

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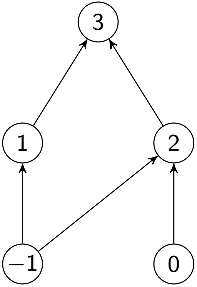

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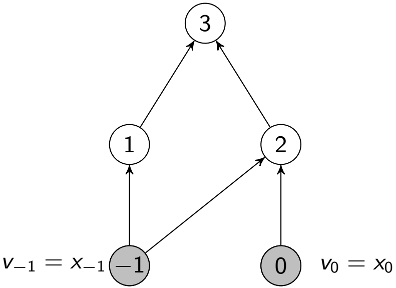

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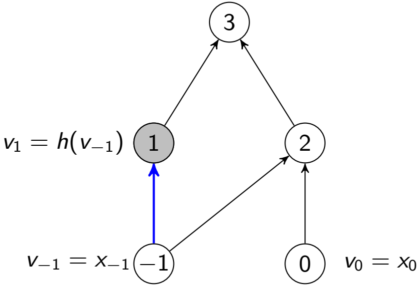

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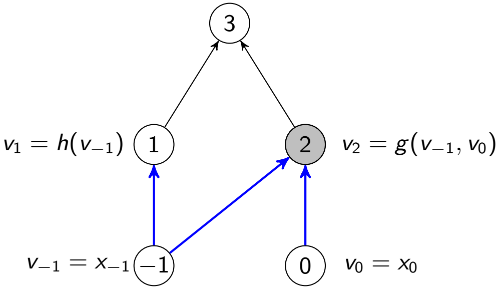

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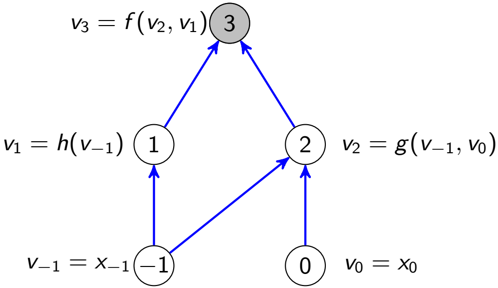

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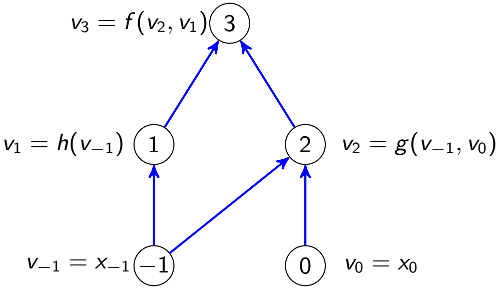

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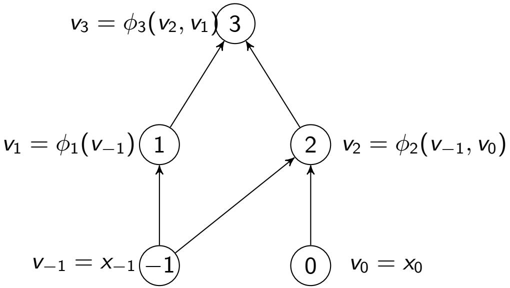
- Node numbering is in order of evaluation.
- (j is a predecessor of i) $\equiv j \in P(i)$.

Millions of nodes are common (This one has just 150)



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

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- Standardize function names ϕ_i
- In general case might have many *intermediate functions*

Standardized Function Evaluation

Input: $v_{i-n} = x_{i-n}$, for $i = 1, \dots n$
for $i = 1 \dots \ell$ **do**
$\quad v_i = \phi_i(v_{P(i)})$
end
Output: $f(x) = v_\ell$

- Nodes for *Independent variables:*
$$v_{i-n} = x_{i-n}, \quad \text{for } i = 1, \dots, n$$
- Nodes for *Intermediate variables:*
$$v_i = \phi_i(v_{P(i)}), \quad \text{for } i = 1, \dots, \ell.$$

Each ϕ_i a *elemental* function with derivatives coded.
AD packages transform users functions to standard form.

Differentiating standardized function

- How do we differentiate our Standardized function?
- How do we differentiate an algorithm?

Differentiating standardized function

- How do we differentiate our Standardized function?
- How do we differentiate an algorithm?
- Solution: represent as a composition of operators.
- We know how to differentiate operators.

State transformation

Make an operator that calculates a single node

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Make an operator that calculates a single node
Big vector of all values

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$$v := (v_{1-n}, \ldots, v_{i-1}, v_i, v_{i+1}, \ldots, v_\ell)$$

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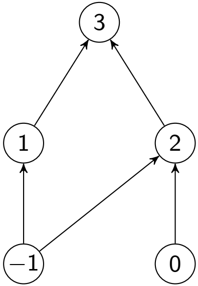
The ith State Transformation (Griewank)

$$\begin{aligned}\Phi^i : \mathbb{R}^{n+\ell} &\to \mathbb{R}^{n+\ell}, \\ v &\mapsto (v_{1-n}, \dots, v_{i-1}, \phi_i(v_{P(i)}), v_{i+1}, \dots, v_\ell),\end{aligned}$$



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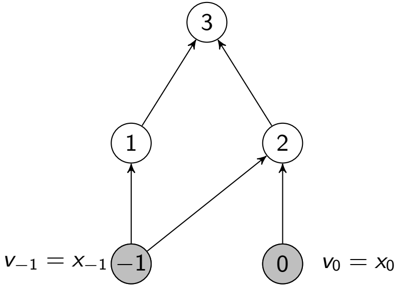

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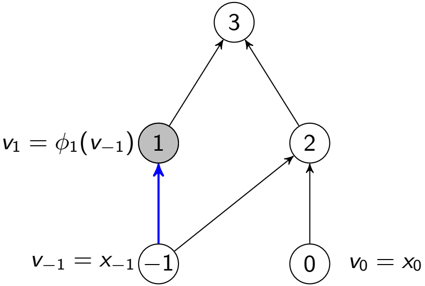
$$\mathcal{I}x$$

$$(v_{1-n}, v_0, 0, 0, 0)$$



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$$\Phi^1 \circ \mathcal{I}x$$

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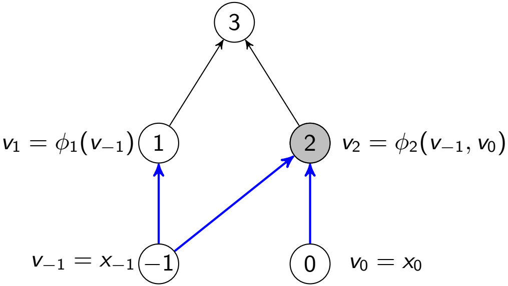

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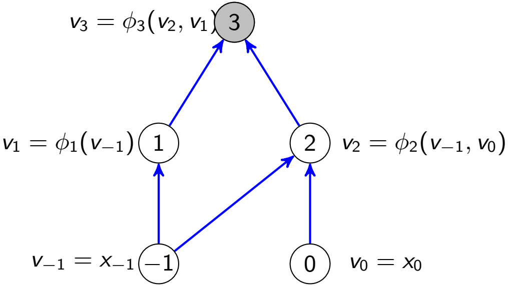
$$\Phi^2 \circ \Phi^1 \circ \mathcal{I}x$$

$$(v_{1-n}, v_0, v_1, v_2, 0)$$



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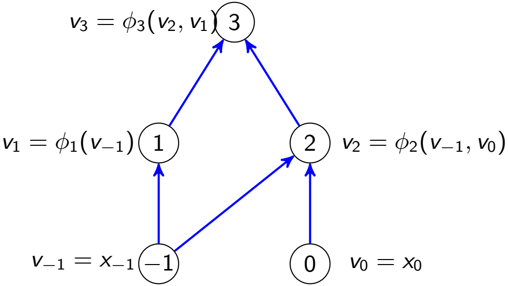

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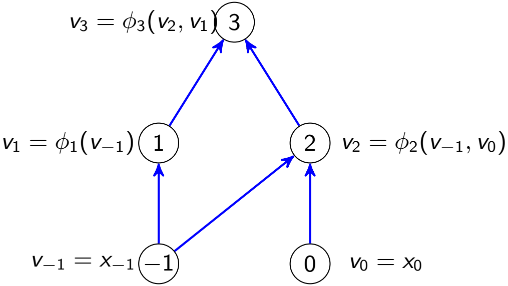

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We can differentiate compositions of operators

Reverse Gradient

$$f(x) = e_{\ell+n}^T \Phi^{\ell} \circ \Phi^{\ell-1} \circ \cdot \circ \Phi^1 \circ \mathcal{I} x$$

Chain-rule says:

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$$f(x) = e_{\ell+n}^T \Phi^\ell \circ \Phi^{\ell-1} \circ \cdot \circ \Phi^1 \circ \mathcal{I} x$$

Chain-rule says: Multiply the Jacobians

$$Df = e_{\ell+n}^T D\Phi^\ell \cdot D\Phi^{\ell-1} \cdots D\Phi^1 \cdot \mathcal{I}$$

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initialization: $\bar{v} = e^{\ell+n}$
for $i = \ell, \ldots, 1$ **do**
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Output: $Df(x) = \bar{v}$

- Implemented version $O(\text{eval}(f))$ **independent of** n!

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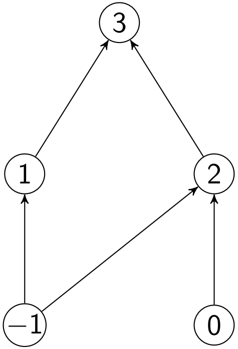
- Back on the graph (where calculations actually take place)

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



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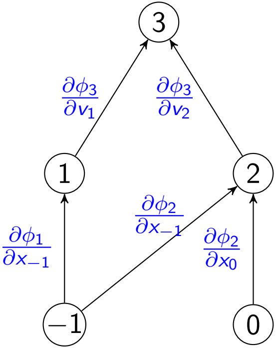

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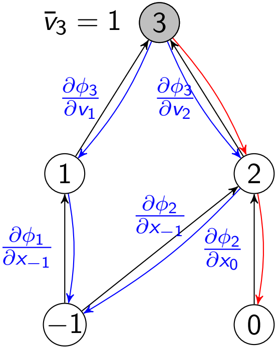

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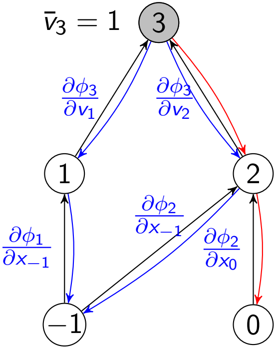

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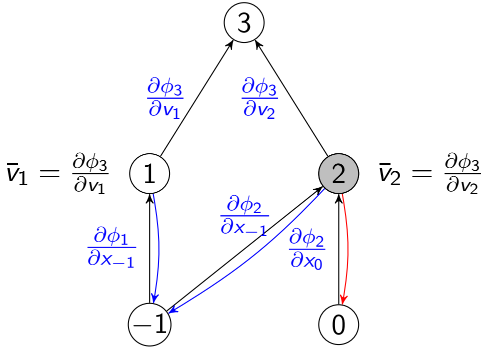

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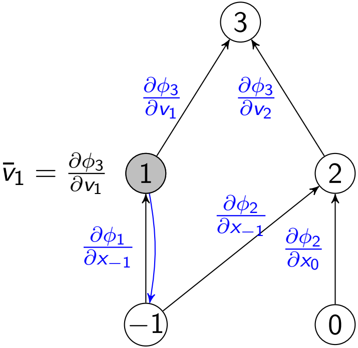

$$\bar{v}_{-1} = \frac{\partial \phi_2}{\partial x_{-1}} \bar{v}_2 \qquad \bar{v}_0 = \frac{\partial \phi_2}{\partial x_0} \bar{v}_2$$

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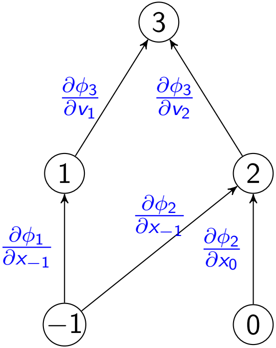

$$\bar{v}_{-1} = \frac{\partial \phi_1}{\partial x_{-1}} \bar{v}_1 + \frac{\partial \phi_2}{\partial x_{-1}} \bar{v}_2 \quad \bar{v}_0 = \frac{\partial \phi_2}{\partial x_0} \bar{v}_2$$

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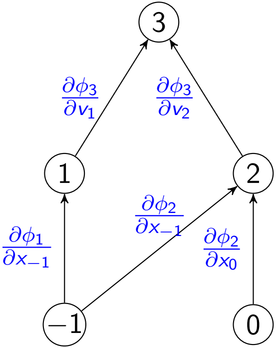

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Use induction instead

$$f(x) = e_{\ell+n}\Phi^2 \circ \Phi^1(x)$$

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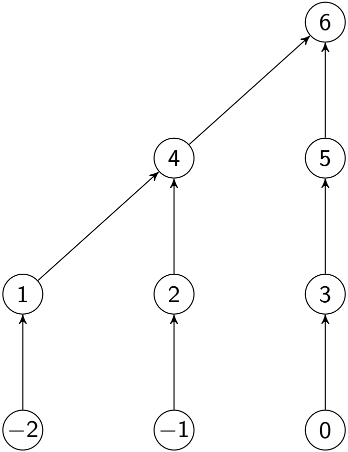
$$D^3 f \cdot d = e_{\ell+n}^T D^3\Phi^2 \cdot (D\Phi^1, D\Phi^1, D\Phi^1 d) + e_{\ell+n}^T D\Phi^2 \cdot D^3\Phi^1 d$$
$$+ e_{\ell+n}^T D^2\Phi^2 \cdot \left((D\Phi^1, D^2\Phi^1 d) + (D^2\Phi^1 d, D\Phi^1) + (D^2\Phi^1, D\Phi^1 d)\right)$$

Solve in reverse, apply inductively, solve a case with ℓ compositions.

Reverse Hessian on Graph



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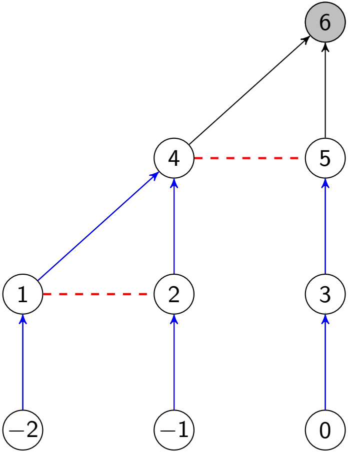

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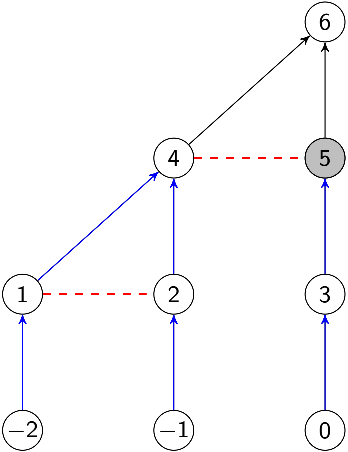

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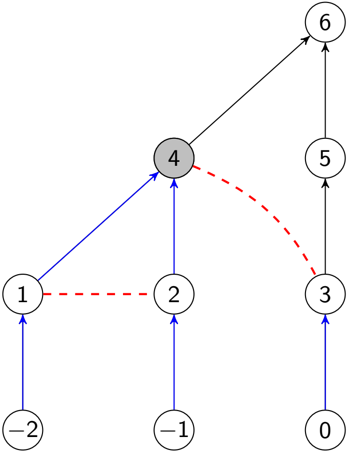

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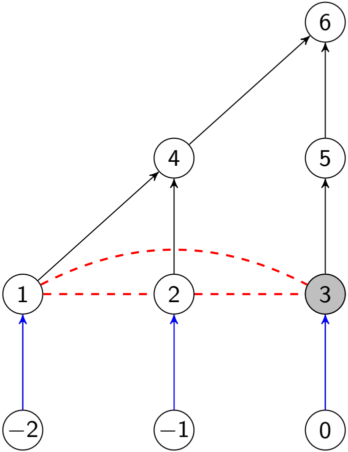

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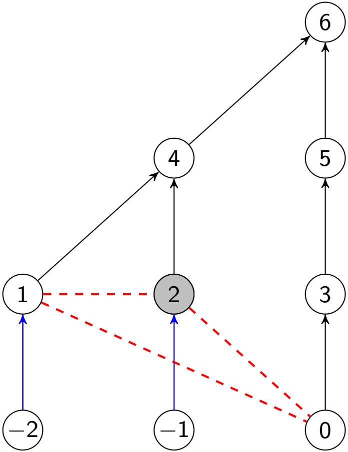

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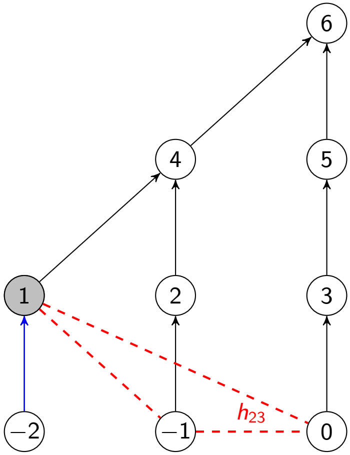

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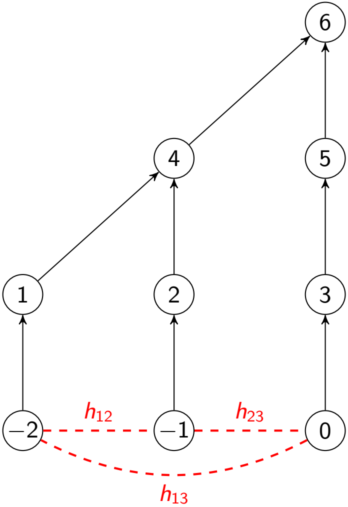

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\end{aligned}
$$

$$D^2 f = \begin{pmatrix} 0 & h_{12} & h_{13} \\ h_{12} & 0 & h_{23} \\ h_{13} & h_{12} & 0 \end{pmatrix}$$

Reverse Hessian Results

- Implemented version average 9s for Hessian matrices $10^6 \times 10^6$ from CUTE.
- Faster then state-of-the-art graph coloring based methods, Gebremedhin, Manne, Pothen, Walther, Tarafdar

$D^2 f(x)$ $D^2 f(x) S$

$\Rightarrow$

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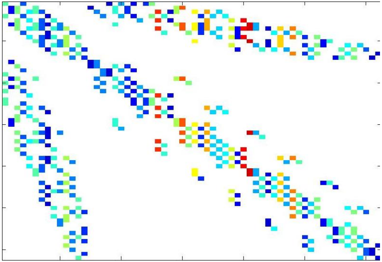

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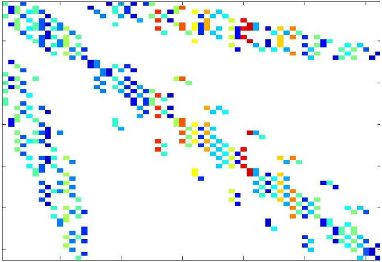

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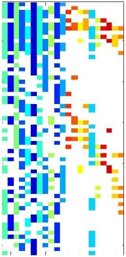

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Differentiating operators works for higher orders

Same induction technique, design reverse method for

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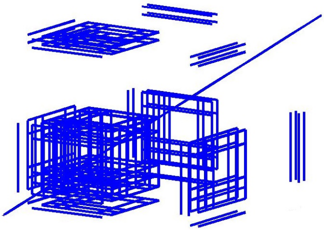
$D^3 f(x) =$



A sparse symmetric cube

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$$\frac{d}{dt} D^2 f(x+td)|_0 = D^3 f(x) \cdot d =$$

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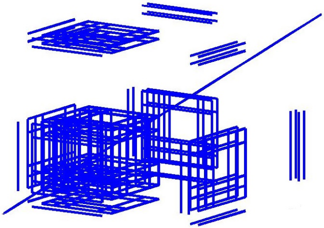

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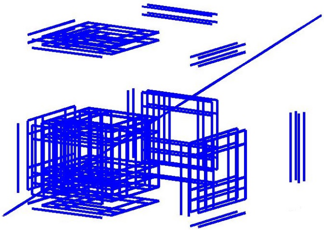

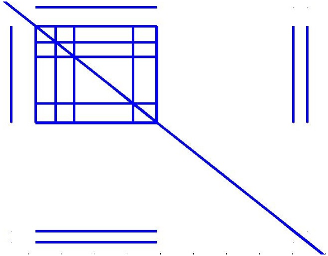

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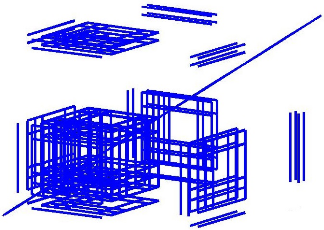

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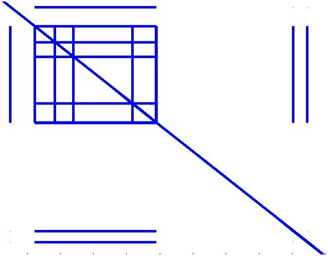

A sparse symmetric matrix. **No cube ever formed**. Pseudocode

Tests calculating $D^3 f(x) \cdot v$ is fast

Average 10 seconds for dimension $= 10^6 \times 10^6$

Costs 1.08% of $D^2 f(x)$, on average

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name	Pattern	nnz/n	$D^3 f(x) \cdot v + D^2 f(x)$
cosine	B 3	3.0000	5.25
chainwood	B 3	1.4999	7.22
morebv	B 3	3.0000	9.44
scon1dls	B 3	0.7002	8.12
bdexp	B 5	0.0004	3.86
pspdoc	B 5	4.9999	5.97
augmlagn	5×5 diagonal blocks	4.9998	9.28
brybnd	B 11	12.9996	38.79
chainros_trigexp	B 3 + D 6	4.4999	12.87
toiqmerg	B 7	6.9998	8.89
arwhead	arrow	3.0000	6.78
nondquar	arrow + B 3	4.9999	5.61
sinquad	frame + diagonal	4.9999	10.01
bdqrtic	arrow + B 7	8.9998	19.62
noncvxu2	irregular	6.9998	9.55
ncvxqp3	irregular	6.9997	6.48
heavey_band	B 39	38.9995	61.27

Large dimensional tests become possible

Sometimes Newton is faster

$$\text{Arrow head}(x) = \sum_{i=1}^{n-1} \left(-4x_i + 3.0 + (x_i^2 + x_{n-1}^2)^2\right)$$

n	Newton	HallC $\lambda = 0$	HallC $\lambda = 0.5$	HallC $\lambda = 1.0$
$2 \cdot 10^5$	5 (7s)	5(14s)	5(11s)	5(11s)

$$\text{Broyden banded}(x) = \sum_{i=1}^{n} \left(x_i(2 + 5x_i^2) + 1 - \sum_{j \in J_i} x_j(1 + x_j) \right)^2$$

$J_i = \{j \in 1 \cdots n : \max(1, i-1) \leq j \leq \min(n, i+5)\}$, for $i = 1, \ldots, n$.

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Sometimes Halley-Chebyshev is better

λ makes a difference

$$\text{Chain Wood}(x) = \sum_{i=1}^{n/2-2} \Big(100(x_{2i} - x_{2i-1}^2)^2 + (1.0 - x_{2i-1})^2 \\ + 90(x_{2i+2} - x_{2i+1}^2)^2 + (1.0 - x_{2i+1})^2 \\ + 10(x_{2i} + x_{2i+2} - 2.0)^2 + (x_{2i} - x_{2i+2})^2/10\Big)$$

n	Newton	HallC $\lambda = 0$	HallC $\lambda = 0.5$	HallC $\lambda = 1.0$
$2 \cdot 10^5$	NC	NC	NC	18 (54.7s)

$$\text{bdqrtic}(x) = \sum_{i=1}^{n-4} \left((-4x_i + 3.0)^2 + (x_i^2 + 2x_{i+1}^2 + 3x_{i+2}^2 + 4x_{i+3}^2 + 5x_n^2)^2\right)$$

n	Newton	HallC $\lambda = 0$	HallC $\lambda = 0.5$	HallC $\lambda = 1.0$
100	2683(2.6s)	62 (0.2 s)	62 (0.2s)	51 (0.2s)
10^4	$10^5 >$ (20min)	94 (40s)	94 (40s)	93 (40s)

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Conclusions & Contributions

- method for designing high order AD algorithms
- new third-order methods for large-scale

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  submitted www.maths.ed.ac.uk/ERGO/

- Automatic derivatives $\Rightarrow$ Empirical comparisons of high order methods possible.
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- What is possible if high order information is not so expensive?

References

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On diagonally structured problems in unconstrained optimization using an inexact super Halley method
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W. Hock and K. Schittkowski (1980)
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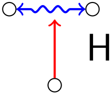
Journal of Optimization Theory and Applications, 30, pp. 127–129.

Ladislav Luksan and Jan Vlcek (2003)
Test problems for unconstrained optimization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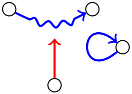
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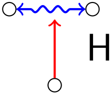
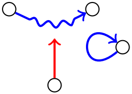
 HANK  U

QUESTIONS?

We have hand-picked sixteen problems from the CUTE collection, augm- lagn from [Hock, 1980], toiqmerg (Toint Quadratic Merging problem) and chainros trigexp (Chained Rosenbrook function with Trigonometric and exponential constraints) from [Vlcek, 2003] for the experiments. We have also created a function

$$\text{heavey\_band}(x, band) = \sum_{i=0}^{n-band} \sin\left(\sum_{j=0}^{band} x_{i+j}\right)$$

For our experiments, we tested heavey band(x, 20). Back

Preliminary tests Halley-Chebychev $\times$ Newton

Halley-Chebyshev iteration costs 2 to 3 X Newton step

- Large dimensional tests become possible
- Some cases Halley-Chebyshev better
- Some cases Newton is better
- λ makes a difference!

Name:dimension	Newton	HallC $\lambda = 0$	HallC $\lambda = 0.5$	HallC $\lambda = 1.0$
cosine:30	FAIL	74	74	74
cragglevy:10	FAIL	218	218	225
chainwood:2.10^5	FAIL	FAIL	FAIL	18
brybnd:10^5	125	117	117	118
arwhead:2.10^5	5	5	5	5
sinquad:2.10^5	29	18	18	20
bdqrtic:100	2683	62	62	51
bdqrtic:10^4	$10^5 >$	94	94	93

Table for time

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bdqrtic:10^4	$10^5 >$	94	94	93

Table for time

Name:dimension	Newton	HallC $\lambda = 0$	HallC $\lambda = 0.5$	HallC $\lambda = 1.0$
cosine:30	FAIL	0.03	0.02	0.02
cragglevy:10	FAIL	0.05	0.03	0.04
chainwood:$2 \cdot 10^5$	FAIL	FAIL	FAIL	54.7
brybnd:10^5	289.96	767.51	769.36	790.02
arwhead:$2 \cdot 10^5$	6.31	13.54	10.79	10.98
sinquad:$2 \cdot 10^5$	22.67	39.56	39.65	44.07
bdqrtic:100	2.58	0.18	0.16	0.14
Bdqrtic:10^4	$1492 >$	39.57	39.78	39.34

Back

Algorithm 1: Reverse Hessian Directional Derivative

initialization: $\dot{\mathrm{v}}^1 = d, \overline{\mathrm{v}} = y, W = Td = 0 \in \mathbb{R}^{m_\ell \times m_\ell}$

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

  $\dot{\mathrm{v}}^i \leftarrow D\Phi^i \cdot \dot{\mathrm{v}}^{i-1}$

end

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

  $Td \leftarrow Td \cdot (D\Phi^i, D\Phi^i)$

  $Td \leftarrow Td + W \cdot \big((D\Phi^i, D^2\Phi^i 1{,}1dot \dot{\mathrm{v}}^{i-1}) + (D^2\Phi^i \cdot \dot{\mathrm{v}}^{i-1}, D\Phi^i)\big)$

  $Td \leftarrow Td + W \cdot (D^2\Phi^i, D\Phi^i \cdot \dot{\mathrm{v}}^{i-1})$

  $Td \leftarrow Td + \overline{\mathrm{v}}^T D^3\Phi^i \cdot \dot{\mathrm{v}}^{i-1}$

  $W \leftarrow W \cdot (D\Phi^i, D\Phi^i) + \overline{\mathrm{v}}^T D^2\Phi^i$

  $\overline{\mathrm{v}}^T \leftarrow \overline{\mathrm{v}}^T D\Phi^i$

end

Output: $y^T D^3F(x) \cdot d \leftarrow Td,\ y^T D^2F \leftarrow W,\ y^T DF \leftarrow \overline{\mathrm{v}}^T$

Back