Automatic Differentiation:
Exploiting Sparsity and Structure

Andrea Walther
Institute of Scientific Computing
Technische Universität Dresden

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Overview

1. Motivation

We have functions

$$F \; : \in \mathbb{R}^n \longrightarrow \mathbb{R}^m$$

and

$$f \; : \in \mathbb{R}^n \longrightarrow \mathbb{R}$$

We need

Jacobian matrix $\quad J(x) = F'(x) \in \mathbb{R}^{m \times n}$

and

Hessian matrix $\quad H(x) = f''(x) \in \mathbb{R}^{n \times n}$

Suppose, we have

$$J(x) = \begin{bmatrix} * & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & * & 0 & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & * & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * \end{bmatrix} \in \mathbb{R}^{m \times n}$$

Usual forward/reverse mode for $J(x) \Rightarrow$ many 0s computed!!

Same is true if $H(x)$ is sparse.

Alternatives?

Efficient computation of $J(x)$ and $H(x)$?

First order part $J(x)$:

$$F \xrightarrow{\;1\;} P_F \xrightarrow{\;2\;} S_F \xrightarrow{\;3\;} \tilde{J} = J(x)S_F$$

function — sparsity pattern — seed matrix — calculation of entries

Efficient computation of $J(x)$ and $H(x)$?

First order part $J(x)$:

$$F \xrightarrow{\;1\;} P_F \xrightarrow{\;2\;} S_F \xrightarrow{\;3\;} \tilde{J} = J(x)S_F$$

function → sparsity pattern → seed matrix → calculation of entries

Second-order part $H(x)$:

$$f \xrightarrow{\;1\;} P_f \xrightarrow{\;2\;} S_f \xrightarrow{\;3\;} \tilde{H} = H(x)S_f$$

function → sparsity pattern → seed matrix → calculation of entries

Remarks:

1. performed only once ➤ AD to compute sparsity pattern
   - propagation of bit patterns
   - propagation of appropriate index sets

2. performed only once ➤ coloring algorithms

3. evaluated for each x ➤ AD for derivative calculation
   - vector forward/reverse mode for Jacobian×matrix
   - new vector version of second order adjoint mode for Hessian×matrix.

General evaluation procedure:

v_{i-n}	$=$	x_i	for $i = 1, \ldots, n$
v_i	$=$	$\varphi_i(v_j)_{j \prec i}$	for $i = 1, \ldots, l$
y_{m-i}	$=$	v_{l-i}	for $i = m-1, \ldots, 0$

where

- v_i, $i \leq 0$, are the independents
- v_i, $i \geq l - m + 1$, are the dependents
- $\varphi_i \in \Phi$ is elemental function, $\Phi =$ set of elemental functions
- $j \prec i$ is dependence relation: v_i depends directly on v_j

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2. Computation of Sparsity Patterns

2.1. Sparsity Patterns of Jacobians

Use AD to compute the sparsity pattern itself!!

➤ propagation of booleans for dependency information
➤ all operations become a logical OR.

Tools:

- **ADOL-C:** AD by Operator Overloading
- **TAF:** AD by Source Trannsformation

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{aligned}
v_i &= x_i \\
v_7 &= \cos(v_1) \\
v_8 &= \sin(v_2) \\
v_9 &= v_7 * v_8 \\
v_{10} &= v_3 * v_9 \\
v_{11} &= \exp(v_3) \\
v_{12} &= \cos(v_4) \\
v_{13} &= \sin(v_5) \\
v_{14} &= v_{12} * v_{13} \\
v_{15} &= v_6 * v_{14} \\
v_{16} &= \exp(v_6) \\
y_1 &= v_{10} \\
y_2 &= v_{11} \\
y_3 &= v_{15} \\
y_4 &= v_{16}
\end{aligned}
$$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{aligned}
v_i &= x_i & \quad v_i &= \delta_{1i}\\
v_7 &= \cos(v_1)\\
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\begin{array}{lcl|lcl}
v_i & = & x_i & v_i & = & \delta_{1i} \\
v_7 & = & \cos(v_1) & v_7 & = & 1 \\
v_8 & = & \sin(v_2) & & & \\
v_9 & = & v_7 * v_8 & & & \\
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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$
$v_7 = \cos(v_1)$	$v_7 = 1$
$v_8 = \sin(v_2)$	$v_8 = 0$
$v_9 = v_7 * v_8$	
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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$		
$v_7 = \cos(v_1)$	$v_7 = 1$			
$v_8 = \sin(v_2)$	$v_8 = 0$			
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$			
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$			
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\begin{array}{lll|lll|ll|}
v_i & = & x_i & v_i & = & \delta_{1i} & = & \delta_{2i} \\
v_7 & = & \cos(v_1) & v_7 & = & 1 & = & 0 \\
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$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$	
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$	
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$	
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$	
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$		
$v_{11} = \exp(v_3)$	$v_{11} = 0$		
$v_{12} = \cos(v_4)$	$v_{12} = 0$		
$v_{13} = \sin(v_5)$	$v_{13} = 0$		
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$		
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$		
$v_{16} = \exp(v_6)$	$v_{16} = 0$		
$y_1 = v_{10}$	$y_1 = 1$		
$y_2 = v_{11}$	$y_2 = 0$		
$y_3 = v_{15}$	$y_3 = 0$		
$y_4 = v_{16}$	$y_4 = 0$		

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$=$	x_i	v_i	$=$	δ_{1i}	$=$	δ_{2i}
v_7	$=$	$\cos(v_1)$	v_7	$=$	1	$=$	0
v_8	$=$	$\sin(v_2)$	v_8	$=$	0	$=$	1
v_9	$=$	$v_7 * v_8$	v_9	$=$	$1 \vee 0 = 1$	$=$	1
v_{10}	$=$	$v_3 * v_9$	v_{10}	$=$	$0 \vee 1 = 1$	$=$	1
v_{11}	$=$	$\exp(v_3)$	v_{11}	$=$	0		
v_{12}	$=$	$\cos(v_4)$	v_{12}	$=$	0		
v_{13}	$=$	$\sin(v_5)$	v_{13}	$=$	0		
v_{14}	$=$	$v_{12} * v_{13}$	v_{14}	$=$	$0 \vee 0 = 0$		
v_{15}	$=$	$v_6 * v_{14}$	v_{15}	$=$	$0 \vee 0 = 0$		
v_{16}	$=$	$\exp(v_6)$	v_{16}	$=$	0		
y_1	$=$	v_{10}	y_1	$=$	1		
y_2	$=$	v_{11}	y_2	$=$	0		
y_3	$=$	v_{15}	y_3	$=$	0		
y_4	$=$	v_{16}	y_4	$=$	0		

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	
$v_{13} = \sin(v_5)$	$v_{13} = 0$	
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	
$v_{16} = \exp(v_6)$	$v_{16} = 0$	
$y_1 = v_{10}$	$y_1 = 1$	
$y_2 = v_{11}$	$y_2 = 0$	
$y_3 = v_{15}$	$y_3 = 0$	
$y_4 = v_{16}$	$y_4 = 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$	
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$	
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$	
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$	
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$	
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$	
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$	
$v_{13} = \sin(v_5)$	$v_{13} = 0$		
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$		
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$		
$v_{16} = \exp(v_6)$	$v_{16} = 0$		
$y_1 = v_{10}$	$y_1 = 1$		
$y_2 = v_{11}$	$y_2 = 0$		
$y_3 = v_{15}$	$y_3 = 0$		
$y_4 = v_{16}$	$y_4 = 0$		

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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lll|lll|l|l}
v_i & = & x_i & v_i & = & \delta_{1i} & = \delta_{2i} & \\
v_7 & = & \cos(v_1) & v_7 & = & 1 & = 0 & \\
v_8 & = & \sin(v_2) & v_8 & = & 0 & = 1 & \\
v_9 & = & v_7 * v_8 & v_9 & = & 1 \vee 0 = 1 & = 1 & \\
v_{10} & = & v_3 * v_9 & v_{10} & = & 0 \vee 1 = 1 & = 1 & \\
v_{11} & = & \exp(v_3) & v_{11} & = & 0 & = 0 & \\
v_{12} & = & \cos(v_4) & v_{12} & = & 0 & = 0 & \\
v_{13} & = & \sin(v_5) & v_{13} & = & 0 & = 0 & \\
v_{14} & = & v_{12} * v_{13} & v_{14} & = & 0 \vee 0 = 0 & & \\
v_{15} & = & v_6 * v_{14} & v_{15} & = & 0 \vee 0 = 0 & & \\
v_{16} & = & \exp(v_6) & v_{16} & = & 0 & & \\
y_1 & = & v_{10} & y_1 & = & 1 & & \\
y_2 & = & v_{11} & y_2 & = & 0 & & \\
y_3 & = & v_{15} & y_3 & = & 0 & & \\
y_4 & = & v_{16} & y_4 & = & 0 & &
\end{array}
$$

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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	
$v_{16} = \exp(v_6)$	$v_{16} = 0$	
$y_1 = v_{10}$	$y_1 = 1$	
$y_2 = v_{11}$	$y_2 = 0$	
$y_3 = v_{15}$	$y_3 = 0$	
$y_4 = v_{16}$	$y_4 = 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$		$= \delta_{2i}$
$v_7 = \cos(v_1)$	$v_7 = 1$		$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$		$= 1$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$		$= 1$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$		$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$		$= 0$
$v_{12} = \cos(v_4)$	$v_{12} = 0$		$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$		$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$		$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$		$= 0$
$v_{16} = \exp(v_6)$	$v_{16} = 0$		
$y_1 = v_{10}$	$y_1 = 1$		
$y_2 = v_{11}$	$y_2 = 0$		
$y_3 = v_{15}$	$y_3 = 0$		
$y_4 = v_{16}$	$y_4 = 0$		

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$
$v_7 = \cos(v_1)$	v_7	$= 1$	$= 0$
$v_8 = \sin(v_2)$	v_8	$= 0$	$= 1$
$v_9 = v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$
$v_{10} = v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$
$v_{11} = \exp(v_3)$	v_{11}	$= 0$	$= 0$
$v_{12} = \cos(v_4)$	v_{12}	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	v_{13}	$= 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$
$v_{15} = v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$
$v_{16} = \exp(v_6)$	v_{16}	$= 0$	$= 0$
$y_1 = v_{10}$	y_1	$= 1$	
$y_2 = v_{11}$	y_2	$= 0$	
$y_3 = v_{15}$	y_3	$= 0$	
$y_4 = v_{16}$	y_4	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lll|l|}
v_i = x_i & v_i & = \delta_{1i} & = \delta_{2i} \\
v_7 = \cos(v_1) & v_7 & = 1 & = 0 \\
v_8 = \sin(v_2) & v_8 & = 0 & = 1 \\
v_9 = v_7 * v_8 & v_9 & = 1 \vee 0 = 1 & = 1 \\
v_{10} = v_3 * v_9 & v_{10} & = 0 \vee 1 = 1 & = 1 \\
v_{11} = \exp(v_3) & v_{11} & = 0 & = 0 \\
v_{12} = \cos(v_4) & v_{12} & = 0 & = 0 \\
v_{13} = \sin(v_5) & v_{13} & = 0 & = 0 \\
v_{14} = v_{12} * v_{13} & v_{14} & = 0 \vee 0 = 0 & = 0 \\
v_{15} = v_6 * v_{14} & v_{15} & = 0 \vee 0 = 0 & = 0 \\
v_{16} = \exp(v_6) & v_{16} & = 0 & = 0 \\
y_1 = v_{10} & y_1 & = 1 & = 1 \\
y_2 = v_{11} & y_2 & = 0 & \\
y_3 = v_{15} & y_3 & = 0 & \\
y_4 = v_{16} & y_4 & = 0 &
\end{array}
$$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	$= 0$
$v_{16} = \exp(v_6)$	$v_{16} = 0$	$= 0$
$y_1 = v_{10}$	$y_1 = 1$	$= 1$
$y_2 = v_{11}$	$y_2 = 0$	$= 0$
$y_3 = v_{15}$	$y_3 = 0$	
$y_4 = v_{16}$	$y_4 = 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	$= 0$
$v_{16} = \exp(v_6)$	$v_{16} = 0$	$= 0$
$y_1 = v_{10}$	$y_1 = 1$	$= 1$
$y_2 = v_{11}$	$y_2 = 0$	$= 0$
$y_3 = v_{15}$	$y_3 = 0$	$= 0$
$y_4 = v_{16}$	$y_4 = 0$	

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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$= x_i$	v_i	$= \delta_{1i}$		$= \delta_{2i}$
v_7	$= \cos(v_1)$	v_7	$= 1$		$= 0$
v_8	$= \sin(v_2)$	v_8	$= 0$		$= 1$
v_9	$= v_7 * v_8$	v_9	$= 1 \vee 0 = 1$		$= 1$
v_{10}	$= v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$		$= 1$
v_{11}	$= \exp(v_3)$	v_{11}	$= 0$		$= 0$
v_{12}	$= \cos(v_4)$	v_{12}	$= 0$		$= 0$
v_{13}	$= \sin(v_5)$	v_{13}	$= 0$		$= 0$
v_{14}	$= v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$		$= 0$
v_{15}	$= v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$		$= 0$
v_{16}	$= \exp(v_6)$	v_{16}	$= 0$		$= 0$
y_1	$= v_{10}$	y_1	$= 1$		$= 1$
y_2	$= v_{11}$	y_2	$= 0$		$= 0$
y_3	$= v_{15}$	y_3	$= 0$		$= 0$
y_4	$= v_{16}$	y_4	$= 0$		$= 0$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	v_7	$= 1$	$= 0$	
$v_8 = \sin(v_2)$	v_8	$= 0$	$= 1$	
$v_9 = v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	
$v_{10} = v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	
$v_{11} = \exp(v_3)$	v_{11}	$= 0$	$= 0$	
$v_{12} = \cos(v_4)$	v_{12}	$= 0$	$= 0$	
$v_{13} = \sin(v_5)$	v_{13}	$= 0$	$= 0$	
$v_{14} = v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	
$v_{15} = v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	
$v_{16} = \exp(v_6)$	v_{16}	$= 0$	$= 0$	
$y_1 = v_{10}$	y_1	$= 1$	$= 1$	
$y_2 = v_{11}$	y_2	$= 0$	$= 0$	
$y_3 = v_{15}$	y_3	$= 0$	$= 0$	
$y_4 = v_{16}$	y_4	$= 0$	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lll|lll|l|l}
v_i & = & x_i & v_i & = & \delta_{1i} & = \delta_{2i} & = \delta_{3i} \\
v_7 & = & \cos(v_1) & v_7 & = & 1 & = 0 & = 0 \\
v_8 & = & \sin(v_2) & v_8 & = & 0 & = 1 & \\
v_9 & = & v_7 * v_8 & v_9 & = & 1 \vee 0 = 1 & = 1 & \\
v_{10} & = & v_3 * v_9 & v_{10} & = & 0 \vee 1 = 1 & = 1 & \\
v_{11} & = & \exp(v_3) & v_{11} & = & 0 & = 0 & \\
v_{12} & = & \cos(v_4) & v_{12} & = & 0 & = 0 & \\
v_{13} & = & \sin(v_5) & v_{13} & = & 0 & = 0 & \\
v_{14} & = & v_{12} * v_{13} & v_{14} & = & 0 \vee 0 = 0 & = 0 & \\
v_{15} & = & v_6 * v_{14} & v_{15} & = & 0 \vee 0 = 0 & = 0 & \\
v_{16} & = & \exp(v_6) & v_{16} & = & 0 & = 0 & \\
y_1 & = & v_{10} & y_1 & = & 1 & = 1 & \\
y_2 & = & v_{11} & y_2 & = & 0 & = 0 & \\
y_3 & = & v_{15} & y_3 & = & 0 & = 0 & \\
y_4 & = & v_{16} & y_4 & = & 0 & = 0 &
\end{array}
$$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$= x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
v_7	$= \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
v_8	$= \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
v_9	$= v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	
v_{10}	$= v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	
v_{11}	$= \exp(v_3)$	v_{11}	$= 0$	$= 0$	
v_{12}	$= \cos(v_4)$	v_{12}	$= 0$	$= 0$	
v_{13}	$= \sin(v_5)$	v_{13}	$= 0$	$= 0$	
v_{14}	$= v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	
v_{15}	$= v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	
v_{16}	$= \exp(v_6)$	v_{16}	$= 0$	$= 0$	
y_1	$= v_{10}$	y_1	$= 1$	$= 1$	
y_2	$= v_{11}$	y_2	$= 0$	$= 0$	
y_3	$= v_{15}$	y_3	$= 0$	$= 0$	
y_4	$= v_{16}$	y_4	$= 0$	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$= x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
v_7	$= \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
v_8	$= \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
v_9	$= v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	$= 0$
v_{10}	$= v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	
v_{11}	$= \exp(v_3)$	v_{11}	$= 0$	$= 0$	
v_{12}	$= \cos(v_4)$	v_{12}	$= 0$	$= 0$	
v_{13}	$= \sin(v_5)$	v_{13}	$= 0$	$= 0$	
v_{14}	$= v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	
v_{15}	$= v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	
v_{16}	$= \exp(v_6)$	v_{16}	$= 0$	$= 0$	
y_1	$= v_{10}$	y_1	$= 1$	$= 1$	
y_2	$= v_{11}$	y_2	$= 0$	$= 0$	
y_3	$= v_{15}$	y_3	$= 0$	$= 0$	
y_4	$= v_{16}$	y_4	$= 0$	$= 0$	

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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lll|ll|l|l}
v_i & = & x_i & v_i & = \delta_{1i} & = \delta_{2i} & = \delta_{3i} \\
v_7 & = & \cos(v_1) & v_7 & = 1 & = 0 & = 0 \\
v_8 & = & \sin(v_2) & v_8 & = 0 & = 1 & = 0 \\
v_9 & = & v_7 * v_8 & v_9 & = 1 \vee 0 = 1 & = 1 & = 0 \\
v_{10} & = & v_3 * v_9 & v_{10} & = 0 \vee 1 = 1 & = 1 & = 1 \\
v_{11} & = & \exp(v_3) & v_{11} & = 0 & = 0 & \\
v_{12} & = & \cos(v_4) & v_{12} & = 0 & = 0 & \\
v_{13} & = & \sin(v_5) & v_{13} & = 0 & = 0 & \\
v_{14} & = & v_{12} * v_{13} & v_{14} & = 0 \vee 0 = 0 & = 0 & \\
v_{15} & = & v_6 * v_{14} & v_{15} & = 0 \vee 0 = 0 & = 0 & \\
v_{16} & = & \exp(v_6) & v_{16} & = 0 & = 0 & \\
y_1 & = & v_{10} & y_1 & = 1 & = 1 & \\
y_2 & = & v_{11} & y_2 & = 0 & = 0 & \\
y_3 & = & v_{15} & y_3 & = 0 & = 0 & \\
y_4 & = & v_{16} & y_4 & = 0 & = 0 &
\end{array}
$$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$	
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$	
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$	
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	$= 0$	
$v_{16} = \exp(v_6)$	$v_{16} = 0$	$= 0$	
$y_1 = v_{10}$	$y_1 = 1$	$= 1$	
$y_2 = v_{11}$	$y_2 = 0$	$= 0$	
$y_3 = v_{15}$	$y_3 = 0$	$= 0$	
$y_4 = v_{16}$	$y_4 = 0$	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
$v_8 = \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	v_{11}	$= 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	v_{12}	$= 0$	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	v_{13}	$= 0$	$= 0$	
$v_{14} = v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	
$v_{15} = v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	
$v_{16} = \exp(v_6)$	v_{16}	$= 0$	$= 0$	
$y_1 = v_{10}$	y_1	$= 1$	$= 1$	
$y_2 = v_{11}$	y_2	$= 0$	$= 0$	
$y_3 = v_{15}$	y_3	$= 0$	$= 0$	
$y_4 = v_{16}$	y_4	$= 0$	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$=$	x_i	v_i	$=$	δ_{1i}	$=$	δ_{2i}	$=$	δ_{3i}
v_7	$=$	$\cos(v_1)$	v_7	$=$	1	$=$	0	$=$	0
v_8	$=$	$\sin(v_2)$	v_8	$=$	0	$=$	1	$=$	0
v_9	$=$	$v_7 * v_8$	v_9	$=$	$1 \vee 0 = 1$	$=$	1	$=$	0
v_{10}	$=$	$v_3 * v_9$	v_{10}	$=$	$0 \vee 1 = 1$	$=$	1	$=$	1
v_{11}	$=$	$\exp(v_3)$	v_{11}	$=$	0	$=$	0	$=$	1
v_{12}	$=$	$\cos(v_4)$	v_{12}	$=$	0	$=$	0	$=$	0
v_{13}	$=$	$\sin(v_5)$	v_{13}	$=$	0	$=$	0	$=$	0
v_{14}	$=$	$v_{12} * v_{13}$	v_{14}	$=$	$0 \vee 0 = 0$	$=$	0		
v_{15}	$=$	$v_6 * v_{14}$	v_{15}	$=$	$0 \vee 0 = 0$	$=$	0		
v_{16}	$=$	$\exp(v_6)$	v_{16}	$=$	0	$=$	0		
y_1	$=$	v_{10}	y_1	$=$	1	$=$	1		
y_2	$=$	v_{11}	y_2	$=$	0	$=$	0		
y_3	$=$	v_{15}	y_3	$=$	0	$=$	0		
y_4	$=$	v_{16}	y_4	$=$	0	$=$	0		

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lll|l|l|l}
v_i = x_i & v_i & = \delta_{1i} & = \delta_{2i} & = \delta_{3i} \\
v_7 = \cos(v_1) & v_7 & = 1 & = 0 & = 0 \\
v_8 = \sin(v_2) & v_8 & = 0 & = 1 & = 0 \\
v_9 = v_7 * v_8 & v_9 & = 1 \vee 0 = 1 & = 1 & = 0 \\
v_{10} = v_3 * v_9 & v_{10} & = 0 \vee 1 = 1 & = 1 & = 1 \\
v_{11} = \exp(v_3) & v_{11} & = 0 & = 0 & = 1 \\
v_{12} = \cos(v_4) & v_{12} & = 0 & = 0 & = 0 \\
v_{13} = \sin(v_5) & v_{13} & = 0 & = 0 & = 0 \\
v_{14} = v_{12} * v_{13} & v_{14} & = 0 \vee 0 = 0 & = 0 & = 0 \\
v_{15} = v_6 * v_{14} & v_{15} & = 0 \vee 0 = 0 & = 0 & \\
v_{16} = \exp(v_6) & v_{16} & = 0 & = 0 & \\
y_1 = v_{10} & y_1 & = 1 & = 1 & \\
y_2 = v_{11} & y_2 & = 0 & = 0 & \\
y_3 = v_{15} & y_3 & = 0 & = 0 & \\
y_4 = v_{16} & y_4 & = 0 & = 0 &
\end{array}
$$

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$= x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
v_7	$= \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
v_8	$= \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
v_9	$= v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	$= 0$
v_{10}	$= v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	$= 1$
v_{11}	$= \exp(v_3)$	v_{11}	$= 0$	$= 0$	$= 1$
v_{12}	$= \cos(v_4)$	v_{12}	$= 0$	$= 0$	$= 0$
v_{13}	$= \sin(v_5)$	v_{13}	$= 0$	$= 0$	$= 0$
v_{14}	$= v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
v_{15}	$= v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
v_{16}	$= \exp(v_6)$	v_{16}	$= 0$	$= 0$	
y_1	$= v_{10}$	y_1	$= 1$	$= 1$	
y_2	$= v_{11}$	y_2	$= 0$	$= 0$	
y_3	$= v_{15}$	y_3	$= 0$	$= 0$	
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$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
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$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{16} = \exp(v_6)$	$v_{16} = 0$	$= 0$	$= 0$
$y_1 = v_{10}$	$y_1 = 1$	$= 1$	
$y_2 = v_{11}$	$y_2 = 0$	$= 0$	
$y_3 = v_{15}$	$y_3 = 0$	$= 0$	
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$v_i = x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
$v_8 = \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	v_{11}	$= 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	v_{12}	$= 0$	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	v_{13}	$= 0$	$= 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{15} = v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{16} = \exp(v_6)$	v_{16}	$= 0$	$= 0$	$= 0$
$y_1 = v_{10}$	y_1	$= 1$	$= 1$	$= 1$
$y_2 = v_{11}$	y_2	$= 0$	$= 0$	
$y_3 = v_{15}$	y_3	$= 0$	$= 0$	
$y_4 = v_{16}$	y_4	$= 0$	$= 0$	

Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	$v_i = \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	$v_7 = 1$	$= 0$	$= 0$
$v_8 = \sin(v_2)$	$v_8 = 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	$v_9 = 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	$v_{10} = 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	$v_{11} = 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	$v_{12} = 0$	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	$v_{13} = 0$	$= 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	$v_{14} = 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{15} = v_6 * v_{14}$	$v_{15} = 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{16} = \exp(v_6)$	$v_{16} = 0$	$= 0$	$= 0$
$y_1 = v_{10}$	$y_1 = 1$	$= 1$	$= 1$
$y_2 = v_{11}$	$y_2 = 0$	$= 0$	$= 1$
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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

v_i	$=$	x_i	v_i	$=$	δ_{1i}	$=$	δ_{2i}	$=$	δ_{3i}
v_7	$=$	$\cos(v_1)$	v_7	$=$	1	$=$	0	$=$	0
v_8	$=$	$\sin(v_2)$	v_8	$=$	0	$=$	1	$=$	0
v_9	$=$	$v_7 * v_8$	v_9	$=$	$1 \vee 0 = 1$	$=$	1	$=$	0
v_{10}	$=$	$v_3 * v_9$	v_{10}	$=$	$0 \vee 1 = 1$	$=$	1	$=$	1
v_{11}	$=$	$\exp(v_3)$	v_{11}	$=$	0	$=$	0	$=$	1
v_{12}	$=$	$\cos(v_4)$	v_{12}	$=$	0	$=$	0	$=$	0
v_{13}	$=$	$\sin(v_5)$	v_{13}	$=$	0	$=$	0	$=$	0
v_{14}	$=$	$v_{12} * v_{13}$	v_{14}	$=$	$0 \vee 0 = 0$	$=$	0	$=$	0
v_{15}	$=$	$v_6 * v_{14}$	v_{15}	$=$	$0 \vee 0 = 0$	$=$	0	$=$	0
v_{16}	$=$	$\exp(v_6)$	v_{16}	$=$	0	$=$	0	$=$	0
y_1	$=$	v_{10}	y_1	$=$	1	$=$	1	$=$	1
y_2	$=$	v_{11}	y_2	$=$	0	$=$	0	$=$	1
y_3	$=$	v_{15}	y_3	$=$	0	$=$	0	$=$	0
y_4	$=$	v_{16}	y_4	$=$	0	$=$	0		

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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$v_i = x_i$	v_i	$= \delta_{1i}$	$= \delta_{2i}$	$= \delta_{3i}$
$v_7 = \cos(v_1)$	v_7	$= 1$	$= 0$	$= 0$
$v_8 = \sin(v_2)$	v_8	$= 0$	$= 1$	$= 0$
$v_9 = v_7 * v_8$	v_9	$= 1 \vee 0 = 1$	$= 1$	$= 0$
$v_{10} = v_3 * v_9$	v_{10}	$= 0 \vee 1 = 1$	$= 1$	$= 1$
$v_{11} = \exp(v_3)$	v_{11}	$= 0$	$= 0$	$= 1$
$v_{12} = \cos(v_4)$	v_{12}	$= 0$	$= 0$	$= 0$
$v_{13} = \sin(v_5)$	v_{13}	$= 0$	$= 0$	$= 0$
$v_{14} = v_{12} * v_{13}$	v_{14}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{15} = v_6 * v_{14}$	v_{15}	$= 0 \vee 0 = 0$	$= 0$	$= 0$
$v_{16} = \exp(v_6)$	v_{16}	$= 0$	$= 0$	$= 0$
$y_1 = v_{10}$	y_1	$= 1$	$= 1$	$= 1$
$y_2 = v_{11}$	y_2	$= 0$	$= 0$	$= 1$
$y_3 = v_{15}$	y_3	$= 0$	$= 0$	$= 0$
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Example:

Evaluation procedure for $F : \mathbb{R}^6 \mapsto \mathbb{R}^4$

$$
\begin{array}{lcl|lcl|cl|cl}
v_i & = & x_i & v_i & = & \delta_{1i} & = & \delta_{2i} & = & \delta_{3i} \\
v_7 & = & \cos(v_1) & v_7 & = & 1 & = & 0 & = & 0 \\
v_8 & = & \sin(v_2) & v_8 & = & 0 & = & 1 & = & 0 \\
v_9 & = & v_7 * v_8 & v_9 & = & 1 \vee 0 = 1 & = & 1 & = & 0 \\
v_{10} & = & v_3 * v_9 & v_{10} & = & 0 \vee 1 = 1 & = & 1 & = & 1 \\
v_{11} & = & \exp(v_3) & v_{11} & = & 0 & = & 0 & = & 1 \\
v_{12} & = & \cos(v_4) & v_{12} & = & 0 & = & 0 & = & 0 \\
v_{13} & = & \sin(v_5) & v_{13} & = & 0 & = & 0 & = & 0 \quad \cdots \\
v_{14} & = & v_{12} * v_{13} & v_{14} & = & 0 \vee 0 = 0 & = & 0 & = & 0 \\
v_{15} & = & v_6 * v_{14} & v_{15} & = & 0 \vee 0 = 0 & = & 0 & = & 0 \\
v_{16} & = & \exp(v_6) & v_{16} & = & 0 & = & 0 & = & 0 \\
y_1 & = & v_{10} & y_1 & = & 1 & = & 1 & = & 1 \\
y_2 & = & v_{11} & y_2 & = & 0 & = & 0 & = & 1 \\
y_3 & = & v_{15} & y_3 & = & 0 & = & 0 & = & 0 \\
y_4 & = & v_{16} & y_4 & = & 0 & = & 0 & = & 0
\end{array}
$$

Alternative:

Propagation of appropriate index sets

$$\mathcal{X}_i \equiv \{j \leq n \, : \, j - n \prec^* i\} \quad \text{for} \quad i = 1 - n, \ldots, l$$

One has:

$$\left\{ j \leq n \, : \, \frac{\partial v_i}{\partial x_j} \neq 0 \right\} \subseteq \mathcal{X}_i$$

➤ $\mathcal{X}_i$, $i = l - m + 1, \ldots, l$ yield sparsity pattern of Jacobian.

2.2. Sparsity Pattern of Hessians

So far: Only propagation of index sets

for sparse Hessians additionally:

Propagation of nonlinear interaction domains

$$\left\{ j \le n \; : \; \frac{\partial^2 y}{\partial x_i \partial x_j} \neq 0 \right\} \subseteq \mathcal{N}_i$$

for $i = 1, \ldots, n$.

➡ $\mathcal{N}_i$, $i = 1\,, \ldots, n$ yield sparsity pattern of Hessian.

Computation of $\mathcal{X}_i$ and $\mathcal{N}_i$?

Algorithm I: Computation of $\mathcal{X}_i$ and $\mathcal{N}_i$

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Algorithm I: Computation of $\mathcal{X}_i$ and $\mathcal{N}_i$

for $i = 1, \ldots, n$

$\mathcal{X}_{i-n} = \{i\}, \quad \mathcal{N}_i = \emptyset$

for $i = 1, \ldots, l$

$\mathcal{X}_i = \bigcup_{j \prec i} \mathcal{X}_j$

if φ_i **nonlinear then**

if $v_i = \varphi_i(v_j)$ **then**

$\forall k \in \mathcal{X}_j : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_j$

if $v_i = \varphi_i(v_j, v_l)$ **then**

$\forall k \in \mathcal{X}_j : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_l$

$\forall k \in \mathcal{X}_l : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_j$

Algorithm I: Computation of $\mathcal{X}_i$ and $\mathcal{N}_i$

for $i = 1, \ldots, n$
$\quad \mathcal{X}_{i-n} = \{i\}, \quad \mathcal{N}_i\ \emptyset$

for $i = 1, \ldots, l$
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Complexity ??

Algorithm I: Computation of $\mathcal{X}_i$ and $\mathcal{N}_i$

for $i = 1, \ldots, n$

$$\mathcal{X}_{i-n} = \{i\}, \quad \mathcal{N}_i = \emptyset$$

for $i = 1, \ldots, l$

$$\mathcal{X}_i = \bigcup_{j \prec i} \mathcal{X}_j \qquad (1)$$

if φ_i **nonlinear then**

if $v_i = \varphi_i(v_j)$ **then**

$$\forall k \in \mathcal{X}_j : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_j \qquad (2)$$

if $v_i = \varphi_i(v_j, v_l)$ **then**

$$\forall k \in \mathcal{X}_j : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_l \qquad (3)$$

$$\forall k \in \mathcal{X}_l : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_j \qquad (4)$$

Complexity ??

Theorem: Complexity result for Algorithm I

Assume that the identity

$$\left\{ j \le n \, : \, \frac{\partial^2 y}{\partial x_i \partial x_j} \neq 0 \right\} = \mathcal{N}_i, \quad 1 \le i \le n,$$

holds for the given f. Then, one has

$$\mathrm{OPS}(\mathrm{NID}) \le c \left(\sum_{i=1}^{l} p_i + \bar{n}^2 * \mathrm{OPS}(f) \right),$$

with $p_i = |\mathcal{X}_i|$ and $\bar{n} =$ maximal #nonzeros per row in $H(x)$.

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with $p_i = |\mathcal{X}_i|$ and $\bar{n}$ = maximal #nonzeros per row in $H(x)$.

Proof: Analyse set operations:

- (1): $\text{OPS}(\mathcal{X}_i = \bigcup_{j \prec i} \mathcal{X}_j) = \mathcal{O}(p_i)$
- (2): $\text{OPS}(\forall k \in \mathcal{X}_j : \mathcal{N}_k = \mathcal{N}_k \cup \mathcal{X}_j) = \mathcal{O}(\bar{n}^2)$
- (3) + (4): same as (2)

Details see [W. 2005]

3. Compression Techniques

3.1. Row Compression for Jacobians

For a *seed matrix* $S \in \mathbb{R}^{n \times p}$ compute

$$\begin{aligned} B &= F'(x)S \in \mathbb{R}^{m\times p} \qquad \Rightarrow \\ b_i^T &= e_i^T B = e_i^T F'(x) S = \nabla F_i(x) S \end{aligned}$$

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Question: Choice of S such that

- $F'(x)$ can be reconstructed from B
- p as small as possible

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Question: Choice of S such that

- $F'(x)$ can be reconstructed from B
- p as small as possible

Possibilities:

1. direct methods: no arithmetic operations are required
2. substitution methods: only substractions are required
3. elimination methods: solution of general linear system

General setting:

Define

$$\mathcal{X}_k = \{j \le n : y_k \text{ depends on } x_j\}$$
$$\mathcal{Y}_k = \{i \le m : x_k \text{ impacts } y_i\}$$
$$p_k = |\mathcal{X}_k| \quad \hat{n} = \max_k p_k \quad q_k = |\mathcal{Y}_k| \quad \hat{m} = \max_k q_k$$

General setting:

Define

$$\begin{aligned}\mathcal{X}_k &= \{j \leq n : y_k \text{ depends on } x_j\}\\ \mathcal{Y}_k &= \{i \leq m : x_k \text{ impacts } y_i\}\\ p_k &= |\mathcal{X}_k| \quad \hat{n} = \max_k p_k \quad q_k = |\mathcal{Y}_k| \quad \hat{m} = \max_k q_k\end{aligned}$$

Then one has

$$b_i^T = e_i^T F'(x) S = \sum_{j \in \mathcal{X}_i} e_i^T F'(x) e_j e_j^T S = a_i^T S_i$$

where

$$a_i = (e_i^T F'(x) e_j)_{j \in \mathcal{X}_i} \in \mathbb{R}^{p_i} \quad S_i = (e_j^T S)_{j \in \mathcal{X}_i} \in \mathbb{R}^{p_i \times p}$$

1. **Direct methods:** Curtis-Powell-Reid Seeding (CPR)

Question:
Determine columns that can be combined
$\Rightarrow$ only 0-1 entries in S

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How?
Find mapping

$$c : \{1, \ldots, n\} \mapsto \{1, \ldots, p\} \qquad \text{such that}$$

$$\mathcal{Y}_j \cap \mathcal{Y}_k \neq \emptyset \Rightarrow c(j) \neq c(k)$$

$\Rightarrow$ images $c^{-1}(i)$ form the “column groups”.

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$\Rightarrow$ images $c^{-1}(i)$ form the "column groups".

Now: Determination of c?

Mapping c = Graph coloring of column incidence graph

$$G_c = (V_c, E_c), \qquad V_c = \{1, \ldots, n\}$$

$$(j,k) \in E_c \;\Leftrightarrow\; \mathcal{Y}_j \cap \mathcal{Y}_k \neq \emptyset$$

$\Rightarrow$ Two vertices have different colors if they are adjacent.

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Determination of $\chi(G_c)$ is NP-hard, but
efficient heuristics available yielding nearly optimal coloring

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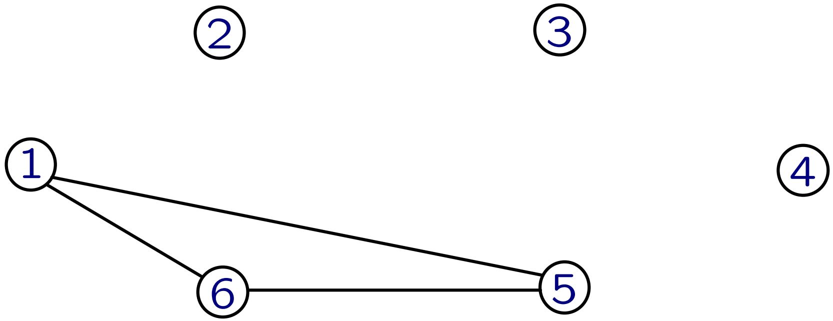

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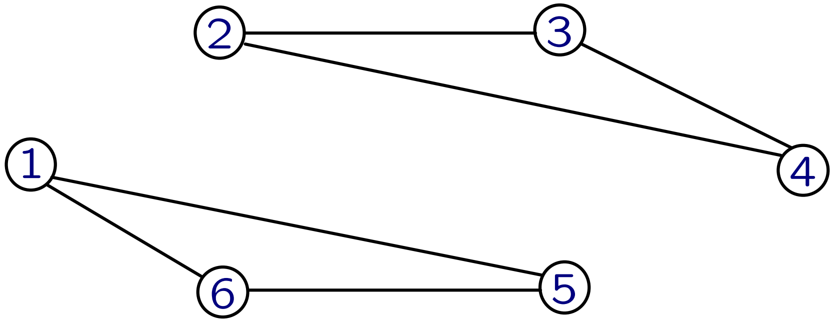

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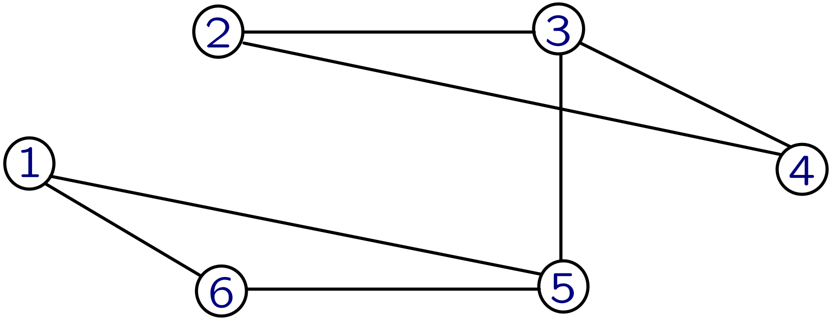

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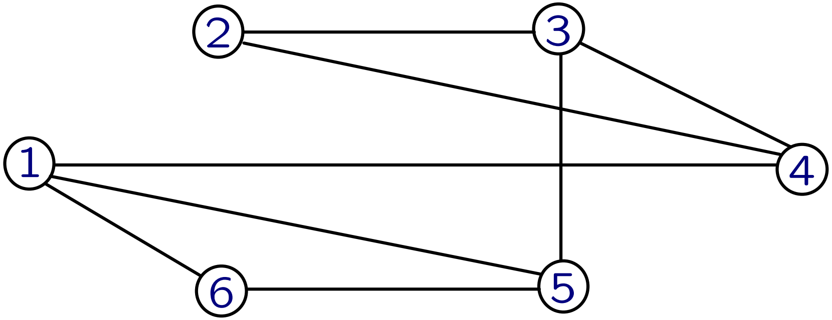

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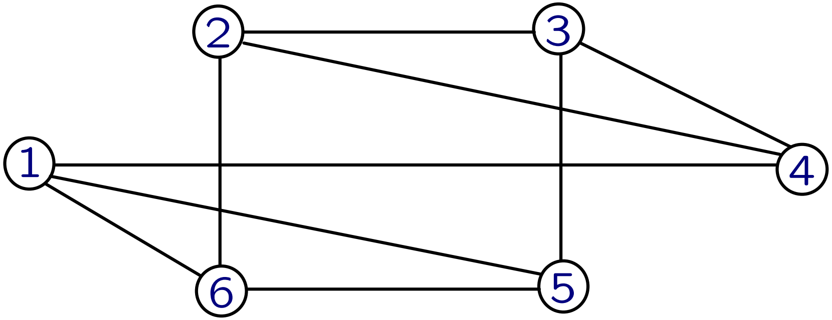

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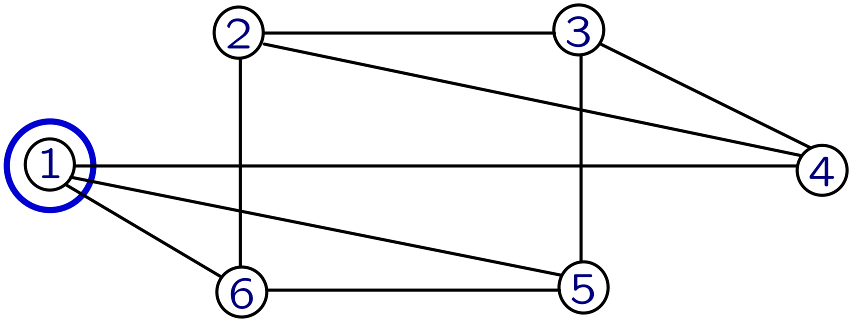

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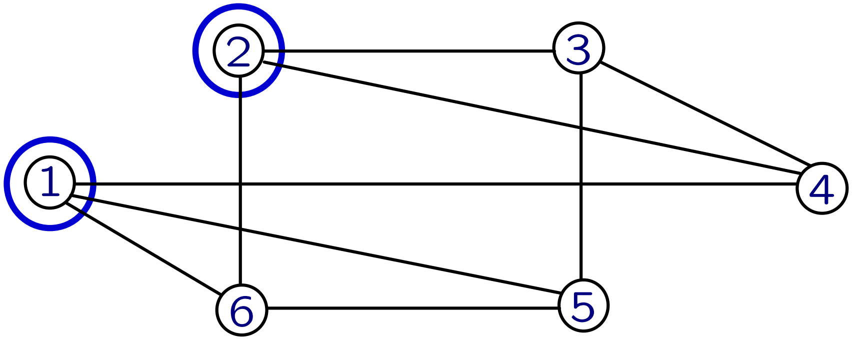

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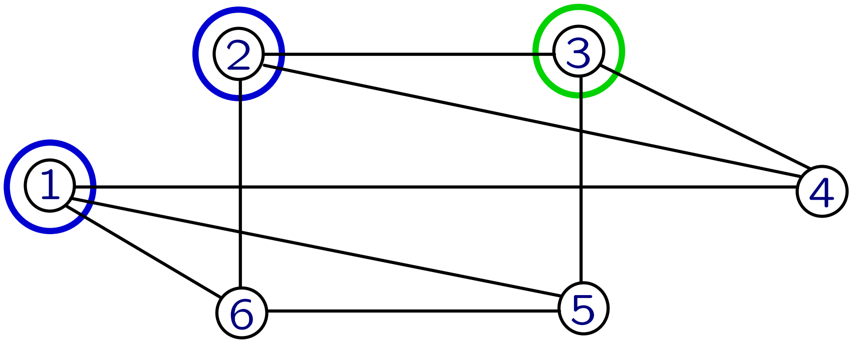

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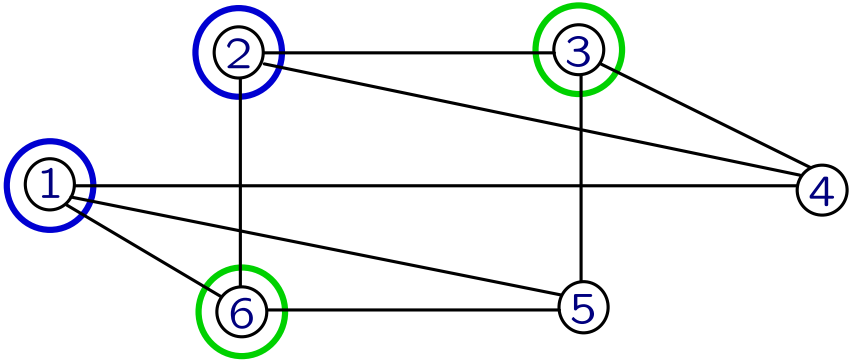

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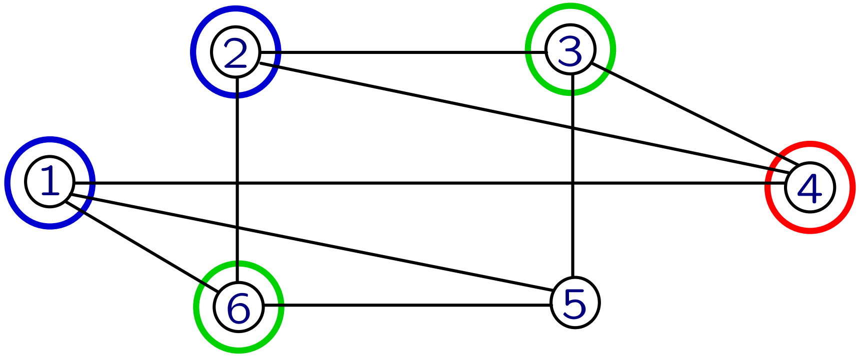

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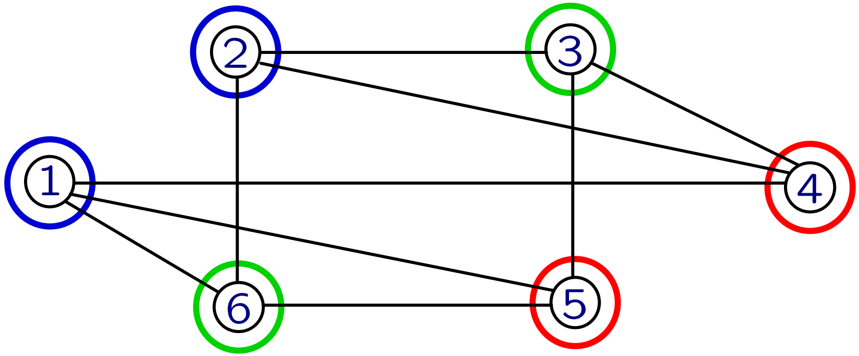


Define

$$S = \left[e^T_{c(j)} \right]_{j=1,\ldots,n} \in \mathbb{R}^{n\times p} \quad \Rightarrow \quad S_i = \left[e^T_{c(j)} \right]_{j\in\mathcal{X}_i} \in \mathbb{R}^{p_i\times p}$$

Hence

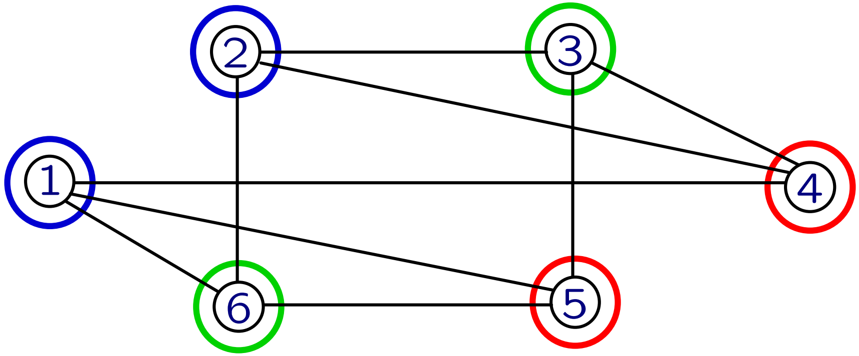
- each row and each column of S_i contains only one 1
- all other entries are zero

One obtains

$$a_i \;=\; e_i^T F'(x) e_j \;=\; e_i^T B e_{c(j)} = b_{ic(j)}$$

Example:

$$\begin{bmatrix} a & 0 & 0 & 0 & b & c \\ 0 & d & e & f & 0 & 0 \\ 0 & 0 & g & 0 & h & 0 \\ i & 0 & 0 & j & 0 & 0 \\ 0 & k & 0 & 0 & 0 & l \end{bmatrix}$$



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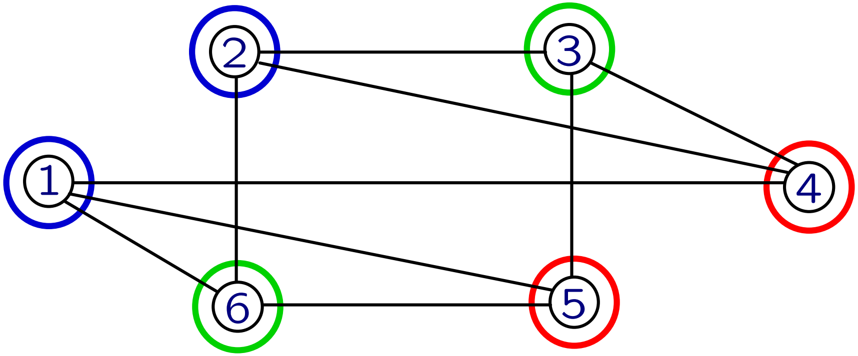

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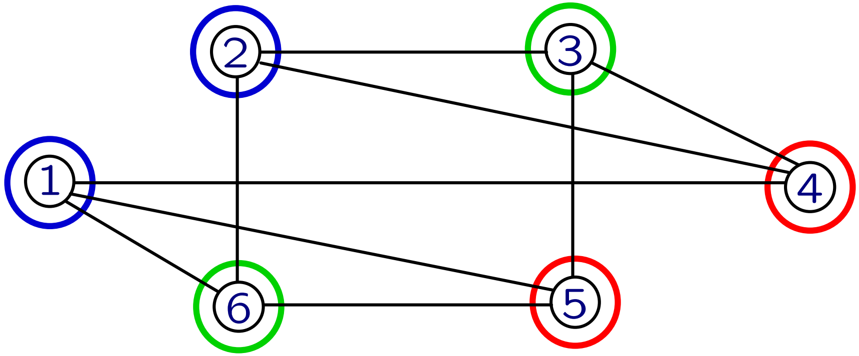

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2. Elimination methods:

Newsam-Ramsdell Seeding (NR): Use Vandermonde matrices

$$S = \left[\lambda_j^{k-1}\right]_{j=1,\ldots,n} \in \mathbb{R}^{n\times\hat{n}} \quad \Rightarrow \quad S_i = \left[\lambda_j^{k-1}\right]_{j\in\mathcal{X}_i} \in \mathbb{R}^{p_i\times\hat{n}}$$

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with same coloring c as before.

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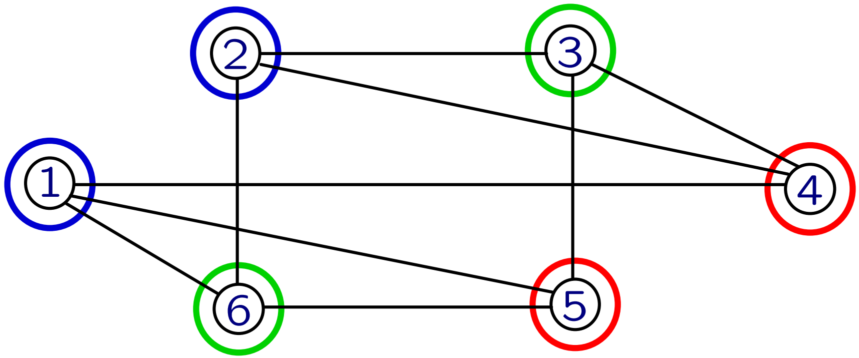
$\Rightarrow$ OPS(Solution of linear system) $\approx 2.5p_i^2$, but conditioning!!

Possible choice of λ_j:

$$\lambda_j = 2\frac{j-1}{n-1} - 1 \quad \text{or} \quad \lambda_{c(j)} = 2\frac{c(j)-1}{n-1} - 1$$

Example:

$$\begin{bmatrix} a & 0 & 0 & 0 & b & c \\ 0 & d & e & f & 0 & 0 \\ 0 & 0 & g & 0 & h & 0 \\ i & 0 & 0 & j & 0 & 0 \\ 0 & k & 0 & 0 & 0 & l \end{bmatrix}$$



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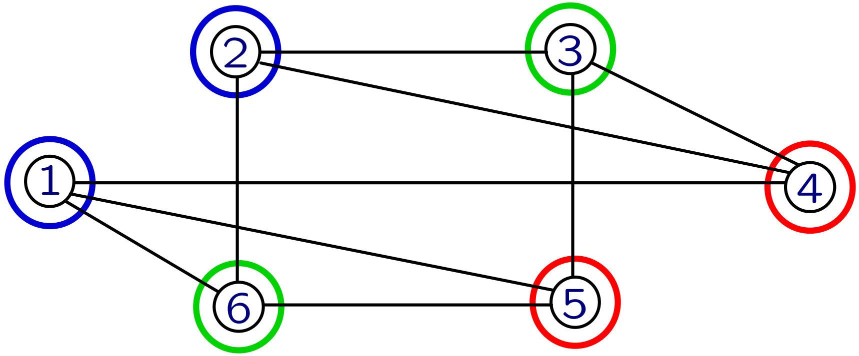

$$p = 3 \Rightarrow \lambda_1 = -1, \lambda_2 = 0, \lambda_3 = 1$$

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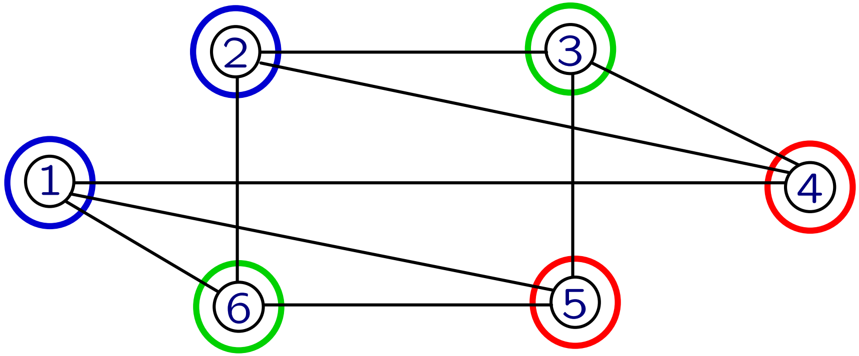

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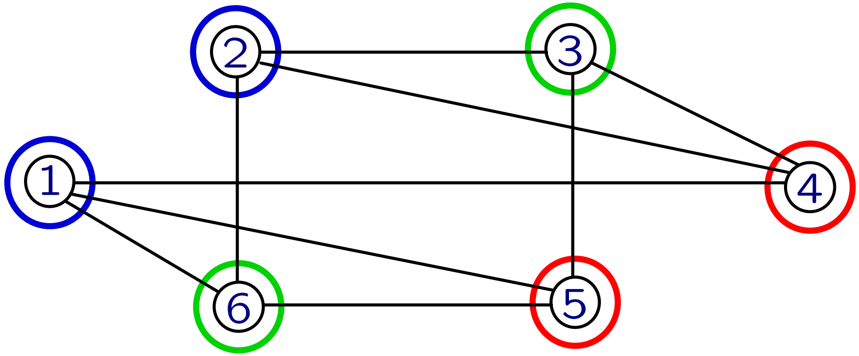

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Due to conditioning, other approaches are proposed:

- $S = [T_{k-1}(\lambda_{c(j)})]$, i.e. use Chebychev polynomials
  $\Rightarrow$ better condition, but expensive solution of linear systems
  Geitner, Utke, Griewank [96]

- Pascal seeding
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So far:

$F'(x)S =$ forward mode of AD or even finite differences

Can we use also $W^T F'(x) =$ reverse mode of AD?

3.2. Column Compression for Jacobians

For a *seed matrix* $W \in \mathbb{R}^{m \times q}$ compute

$$C^T = W^T F'(x) \in \mathbb{R}^{q \times n} \qquad \Rightarrow$$
$$c_j = C^T e_j = W^T F'(x) e_j = W_j^T a_j$$

where

$$a_j = (e_k^T F'(x) e_j)_{k \in \mathcal{Y}_j} \in \mathbb{R}^{q_i} \quad W_j = (e_k^T W)_{k \in \mathcal{Y}_j} \in \mathbb{R}^{q_i \times q}$$

Question: Choice of W such that

- $F'(x)$ can be reconstructed from C
- q as small as possible

1. **Direct methods:** Curtis-Powell-Reid Seeding (CPR)

Question:
Determine rows that can be combined
$\Rightarrow$ only 0-1 entries in W

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Determine rows that can be combined
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How?
Find mapping

$$d : \{1, \ldots, m\} \mapsto \{1, \ldots, q\} \qquad \text{such that}$$

$$\mathcal{X}_j \cap \mathcal{X}_k \neq \emptyset \Rightarrow d(j) \neq d(k)$$

$\Rightarrow$ images $d^{-1}(i)$ form the “row groups”.

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Mapping d = Graph coloring of row incidence graph

$$G_r = (V_r, E_r), \qquad V_r = \{1, \ldots, m\}$$

$$(j,k) \in E_r \;\Leftrightarrow\; \mathcal{X}_j \cap \mathcal{X}_k \neq \emptyset$$

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Define

$$W = \left[e_{d(i)}^T\right]_{i=1,\dots,m} \in \mathbb{R}^{m \times q} \quad \Rightarrow \quad W_j = \left[e_{d(i)}^T\right]_{i \in \mathcal{Y}_j} \in \mathbb{R}^{q_i \times q}$$

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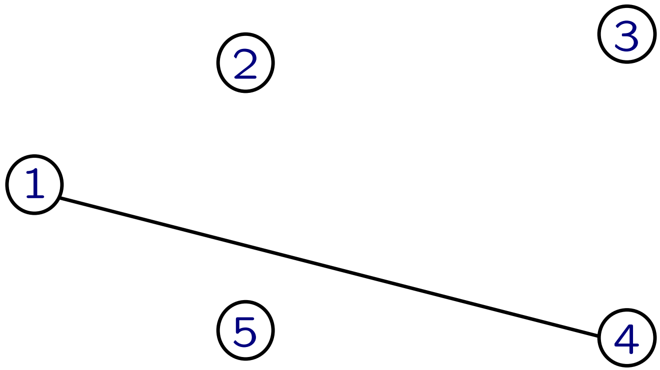

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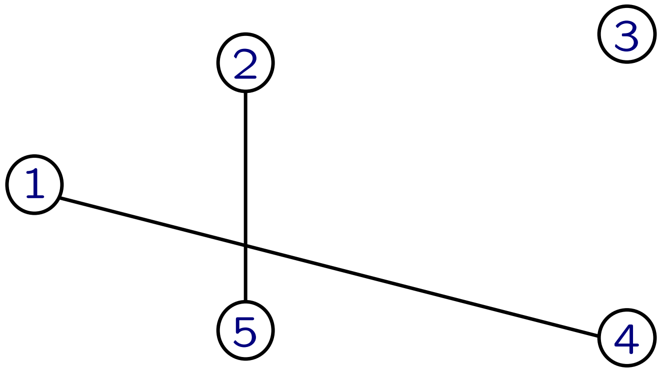

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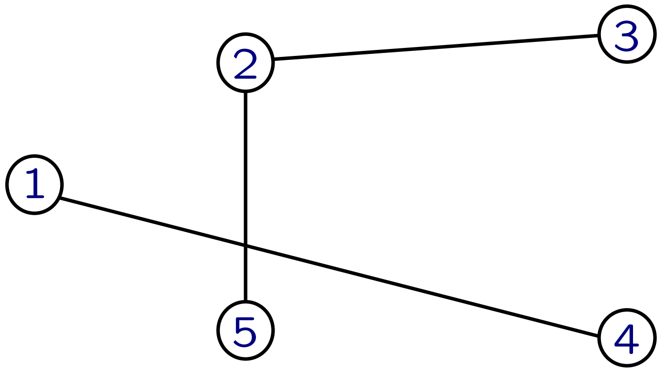

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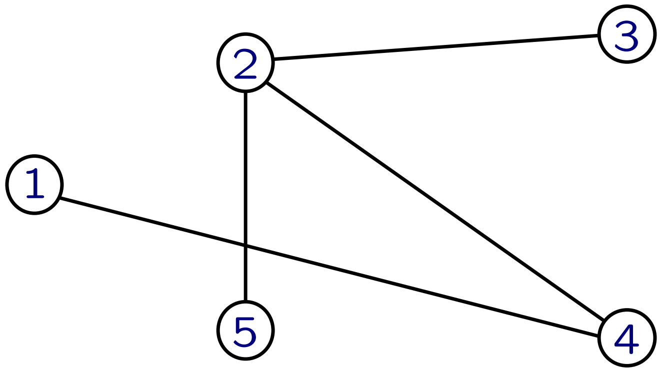

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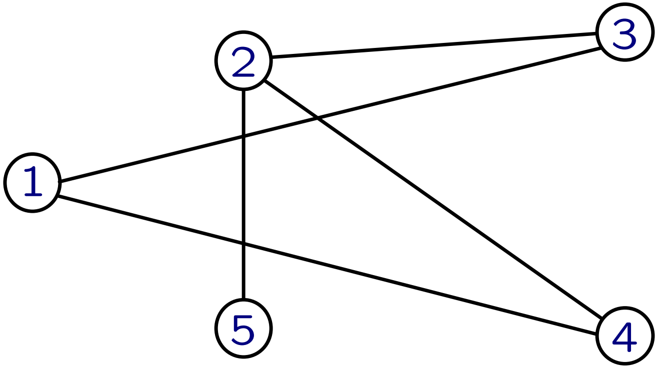

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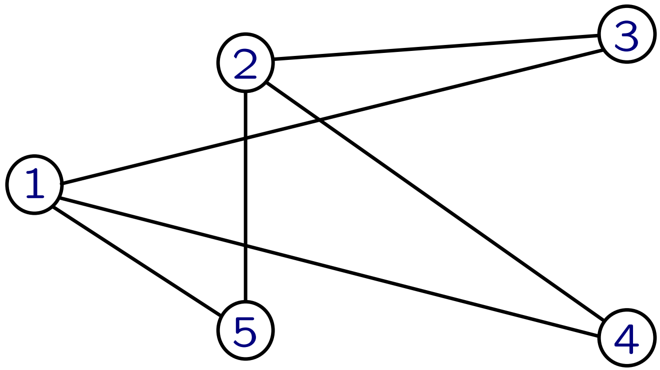

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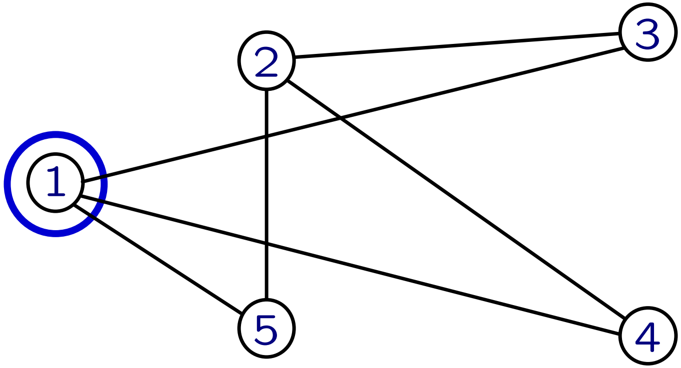

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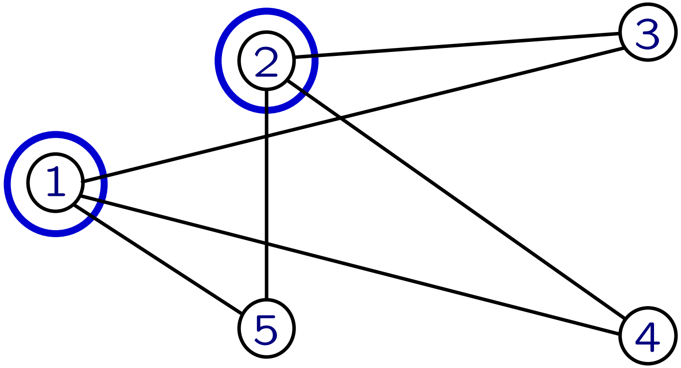

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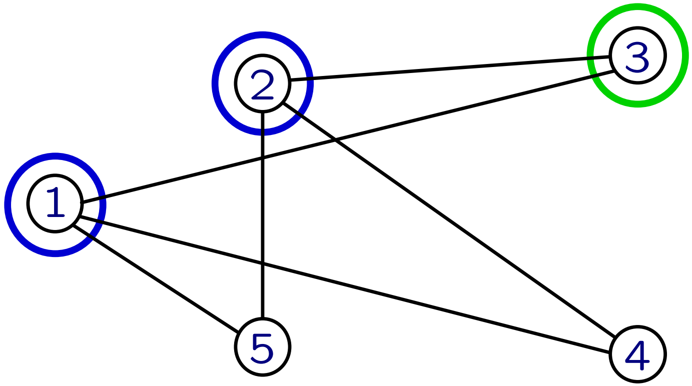

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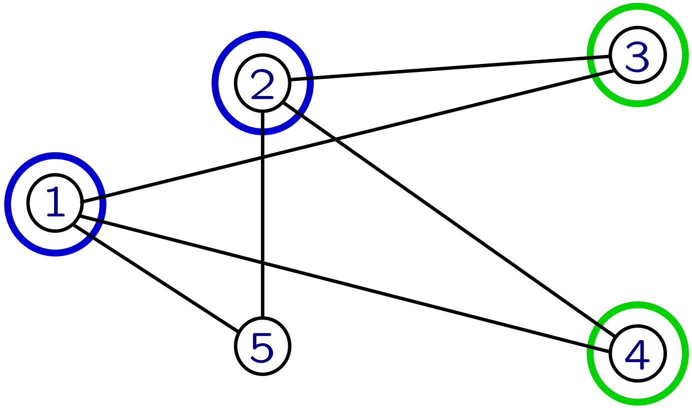

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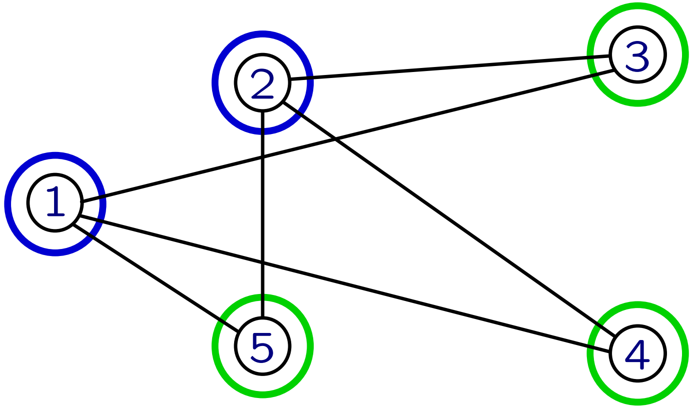

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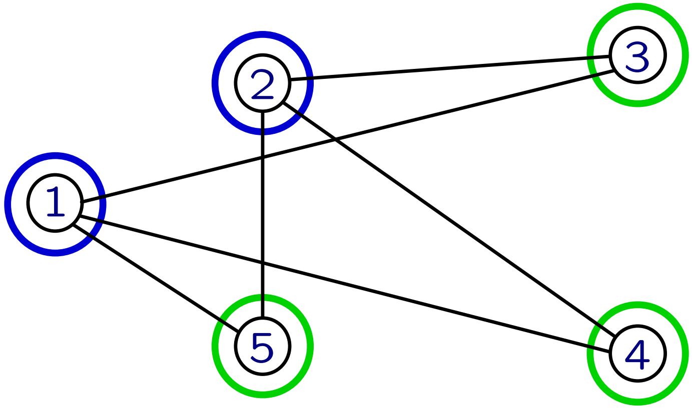

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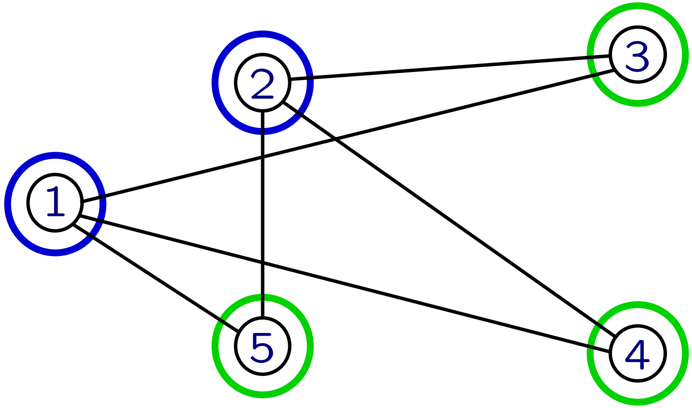

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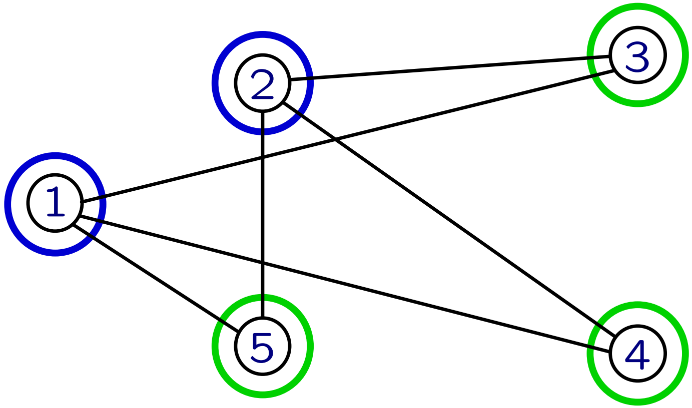

$$W = \left[e_{d(j)}^T \right] = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \Rightarrow C^T = W^T F'(x) = \begin{bmatrix} a & d & e & f & b & c \\ i & k & g & j & h & l \end{bmatrix}$$

2. Elimination methods:

Newsam-Ramsdell Seeding (NR):

$$W = \left[\mu_i^{k-1}\right]_{i=1,\ldots,m} \in \mathbb{R}^{m\times\hat{m}} \quad \text{or} \quad W = \left[\mu_{d(i)}^{k-1}\right]_{i=1,\ldots,m} \in \mathbb{R}^{m\times\hat{m}}$$

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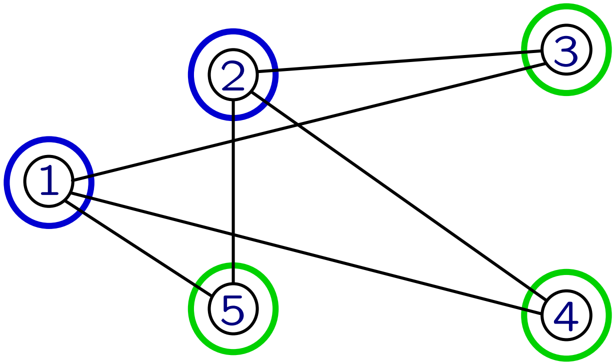

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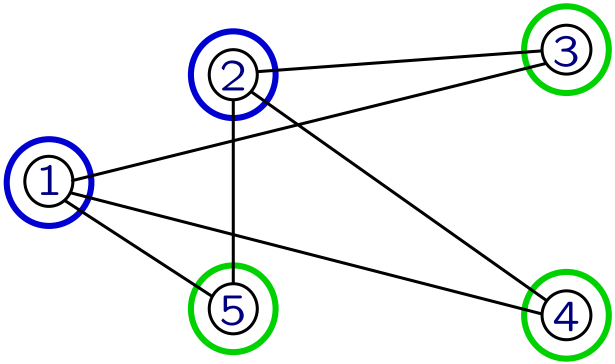

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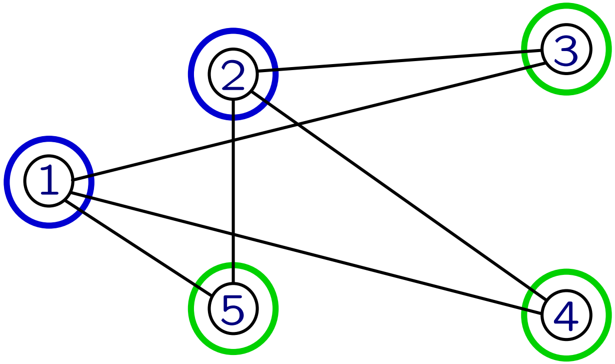

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3.3. Column and Row Compression

Suppose, we have

$$A \equiv F'(x) = \begin{bmatrix} \delta_1 & \alpha_2 & \cdots & \alpha_{n-1} & \alpha_n \\ \beta_2 & \delta_2 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \beta_{n-1} & \vdots & \ddots & \delta_{n-1} & 0 \\ \beta_n & 0 & \cdots & 0 & \delta_n \end{bmatrix} \in \mathbb{R}^{n \times n}$$

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G_r "full" $\Rightarrow n = \hat{n} = p$ and G_c "full" $\Rightarrow m = \hat{m} = q$

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Alternatives?

Observe for

$$A \equiv F'(x) = \begin{bmatrix} \delta_1 & \alpha_2 & \cdots & \alpha_{n-1} & \alpha_n \\ \beta_2 & \delta_2 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \beta_{n-1} & \vdots & \ddots & \delta_{n-1} & 0 \\ \beta_n & 0 & \cdots & 0 & \delta_n \end{bmatrix} \in \mathbb{R}^{n\times n}$$

that

$$A \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ \vdots & \vdots \\ 1 & 0 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \sum_{i=2}^{n} \alpha_i & \delta_1 \\ \delta_2 & \beta_2 \\ \vdots & \vdots \\ \delta_{n-1} & \beta_{n-1} \\ \delta_n & \beta_n \end{bmatrix}$$

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⇒ Find S and W with $p + q$ small such that B and C allow reconstruction of A

See Colemann, Verma [96]

3.4. Remarks

Sparse Jacobians:

- So far assumed that sparsity pattern is known correctly!
  Cheap consistency check:

$$S \;\rightarrow\; [S, s] \quad \Rightarrow \quad F'(x)[S, s] = [B, b]$$

  Verify that $F'(x)s = b$ holds for reconstructed $F'(x)$.

- S and W also to compute sparse second derivatives:

$$S^T F''(x) S \quad \text{or} \quad W^T F''(x) S$$

  to reconstruct second order tensor $F''(x) \in \mathbb{R}^{m \times n \times n}$

Sparse Hessians:

- Similar coloring techniques also for Hessians
  - star coloring (direct method)
    acyclic coloring (elimination method)

- Subsequently:
  Second order adjoint mode to compute compressed derivative matrix.

4. Compressed Derivative Matrices

Sparse Jacobians

How to reduce overhead in forward and reverse mode?
Propagate a bundle of vectors instead of a single vector!

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Sparse Jacobians

How to reduce overhead in forward and reverse mode?
Propagate a bundle of vectors instead of a single vector!

Forward mode:

$$\text{Instead of } \dot{y} \;=\; F'(x)\dot{x} \in \mathbb{R}^m \qquad \text{for} \qquad \dot{x} \in \mathbb{R}^n$$

compute

$$\dot{Y} \;=\; F'(x)\dot{X} \in \mathbb{R}^{m\times p} \qquad \text{for} \qquad \dot{X} \in \mathbb{R}^{n\times p}$$

- Replace $\dot{v}_j \in \mathbb{R}$ by $\dot{V}_j \in \mathbb{R}^p$ in tangent procedure
- Everything else remains unchanged
- $\dot{X} = S$

Reverse mode:

$$\text{Instead of } \bar{x} = \bar{y}F'(x) \in \mathbb{R}^n \qquad \text{for} \qquad \bar{y} \in \mathbb{R}^m$$

compute

$$\bar{X} = \bar{Y}F'(x) \in \mathbb{R}^{q\times n} \qquad \text{for} \qquad \bar{Y} \in \mathbb{R}^{q\times m}$$

Implementation:

- Replace $\bar{v}_i \in \mathbb{R}$ by $\bar{V}_i \in \mathbb{R}^q$ in adjoint recursion
- Everything else remains unchanged
- $\bar{Y} = W$

Sparse Hessians

Second order adjoints computed with AD:

$$y = f(x) \xrightarrow[\text{diff.}]{\text{reverse}} \bar{x} = \bar{y} f'(x) \xrightarrow[\text{diff.}]{\text{forward}} \dot{\bar{x}} = \bar{y} f''(x)\dot{x} + \dot{\bar{y}} f'(x)$$

Sparse Hessians

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Complexity [Griewank 2000]:

$$\text{TIME}(H(x)\dot{x}) \leq \omega_{soad}\text{TIME}(f(x)) \qquad \text{with} \quad \omega_{soad} \in [7, 10]$$

$$\text{TIME}(H(x)S) \leq \omega_{soad}\, p\, \text{TIME}(f(x)) \qquad \text{with} \quad \omega_{soad} \in [7, 10].$$

Reduction possible ??

Algorithm II: Computation of $H(x)\dot{x} \in \mathbb{R}^n$

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for $i = 1, \ldots, n$

$$v_{i-n} = x_i, \qquad \dot{v}_{i-n} = \dot{x}_i, \quad \bar{v}_{i-n} = 0, \quad \dot{\bar{v}}_{i-n} = 0$$

for $i = 1, \ldots, l$

$$v_i = \varphi_i(v_j)_{j \prec i}, \quad \dot{v}_i = \sum_{j \prec i} \frac{\partial}{\partial v_j} \varphi_i(v_j)_{j \prec i}\, \dot{v}_j,$$

$$\bar{v}_i = 0 \qquad \dot{\bar{v}}_i = 0$$

$$y = v_l, \quad \dot{y} = \dot{v}_l, \quad \bar{v}_l = \bar{y}$$

for $i = l, \ldots, 1$

$$\bar{v}_j \mathrel{+}= \bar{v}_i \frac{\partial}{\partial v_j} \varphi_i(v_j)_{j \prec i} \qquad \text{for} \quad j \prec i$$

$$\dot{\bar{v}}_j \mathrel{+}= \bar{v}_i \sum_{k \prec i} \frac{\partial^2}{\partial v_j \partial v_k} \varphi_i(v_j)_{j \prec i}\, \dot{v}_k \qquad \text{for} \quad j \prec i$$

for $i = 1, \ldots, n$

$$\bar{x}_i = \bar{v}_{i-n}, \qquad \dot{\bar{x}}_i = \dot{\bar{v}}_{i-n}$$

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for $i = 1, \ldots, n$

$$\bar{x}_i = \bar{v}_{i-n}, \qquad \dot{\bar{X}}_i = \dot{\bar{V}}_{i-n}$$

Complexity ?

$$\mathrm{TIME}(\dot{\bar{X}}) \leq \omega_{soadp} \mathrm{TIME}(f(x))$$

with

$$\omega_{soadp} \in [4 + 3p, 4 + 6p].$$

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Reduction of run time complexity:

$$\text{From } [7p, 10p] \text{ to } [4+3p, 4+6p]$$

due to reduced number of recalculations.

For details see [W. 2005]

5. Partial Separability

Two kinds of partial separability:

The function $F : \mathbb{R}^n \mapsto \mathbb{R}^m$ is called

- *partially value separable* if for at least one $y_i = \Phi_i(v_j, v_k)$
  - $\Phi_i(v_j, v_k)$ is an addition or subtraction
  - $|\mathcal{X}_j| < n$ and $|\mathcal{X}_k| < n$

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  - $\Phi_i(v_j, v_k)$ is an addition or subtraction
  - $|\mathcal{X}_j| < n$ and $|\mathcal{X}_k| < n$

- *partially argument separable* if for at least one x_j
  - at least two intermediates depend on x_j
  - $|\mathcal{Y}_k| < m$ for all k with $j \prec k$

Value separability:

Define for $y_i = v_j + v_k$

$$y_{i-1/2} = v_j, \quad y_{i+1/2} = v_k$$

$$\tilde{F}(x) \equiv (y_1, \ldots, y_{i-1}, y_{i-1/2}, y_{i+1/2}, y_{i+1}, \ldots, y_m)$$

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Then one has

$$\nabla F_k(x) = \nabla \tilde{F}_k(x) \qquad k = 1, \ldots, i-1, i+1, \ldots, m$$

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- ith row of $\nabla F(x)$ splitted into two rows
- $\widehat{n}(\tilde{F}(x)) \leq \widehat{n}(F(x))$

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- good for row compression, bad for column compression

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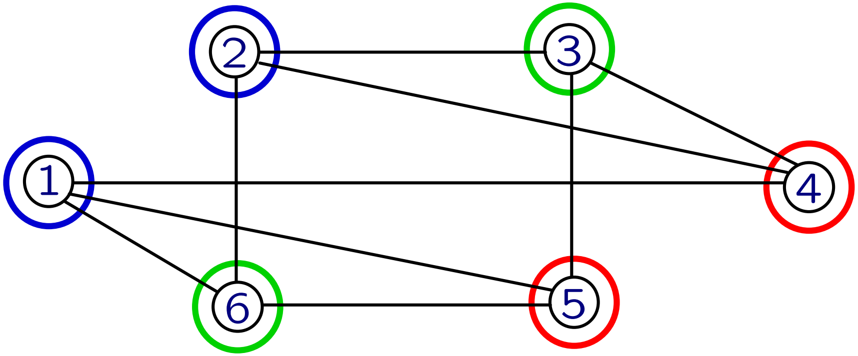
Then one has

$$\nabla F_k(x) = \nabla \tilde{F}_k(x) \qquad k = 1, \ldots, i-1, i+1, \ldots, m$$
$$\nabla F_i(x) = \nabla \tilde{F}_{i-1/2}(x) + \nabla \tilde{F}_{i+1/2}(x)$$

- ith row of $\nabla F(x)$ splitted into two rows
- $\hat{n}(\tilde{F}(x)) \leq \hat{n}(F(x))$ and $\hat{m}(\tilde{F}(x)) \geq \hat{m}(F(x))$
- good for row compression, bad for column compression
- Implementation: LANCELOT

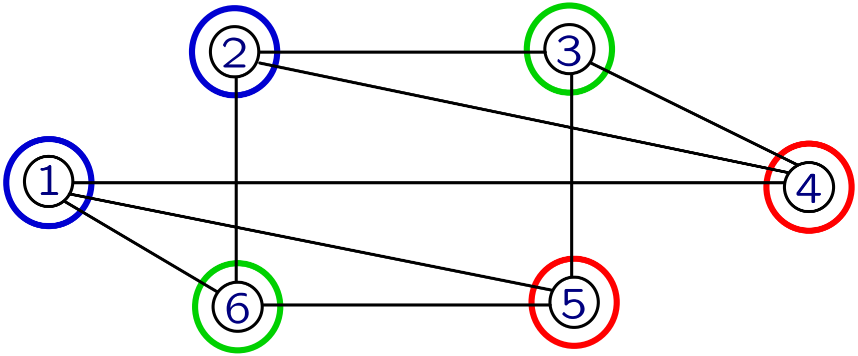
Example:

$$\begin{bmatrix} \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & 0 & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & 0 & 0 & 0 & \times \end{bmatrix}$$

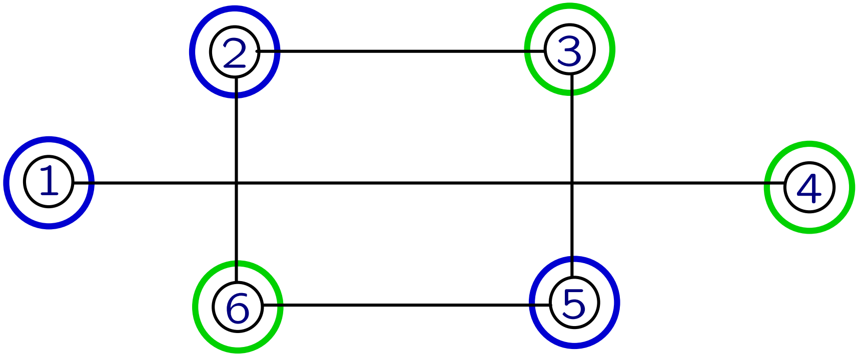


Example:

$$\begin{bmatrix} \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & 0 & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & 0 & 0 & 0 & \times \end{bmatrix}$$



$$\begin{bmatrix} \times & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & 0 & 0 & 0 \\ 0 & 0 & \times & \times & 0 & 0 \\ 0 & 0 & \times & 0 & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & 0 & 0 & 0 & \times \end{bmatrix}$$



Argument separability:

Define for x_j

$$x_{j,k} \;=\; x_j \quad \text{for all } v_k \text{ that depend on } x_j$$

$$\tilde{F}(x) : \mathbb{R}^{\tilde{n}} \mapsto \mathbb{R}^m, \qquad v_k = \Phi_k(\ldots, x_{j,k}, \ldots)$$

Then one has

$$\frac{\partial F(x)}{\partial x_j} = \sum_k \frac{\partial F(x)}{\partial x_{j,k}}$$

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- jth column of $\nabla F(x)$ splitted into columns
- $\hat{m}(\tilde{F}(x)) \leq \hat{m}(F(x))$

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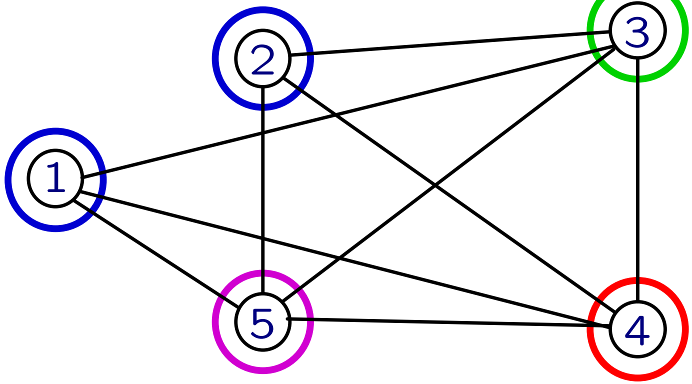
- good for column compression, bad for row compression

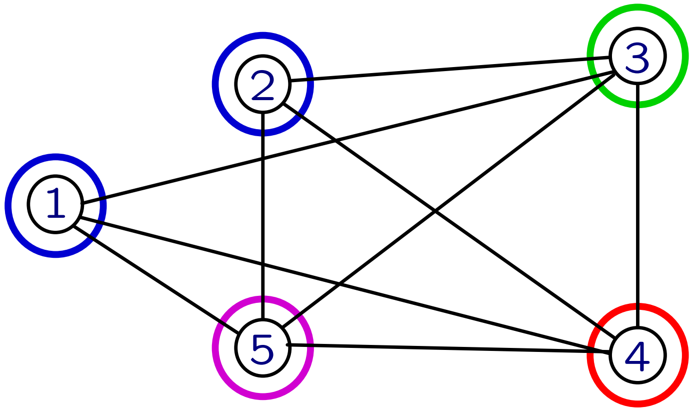
Example:

$$\begin{bmatrix} \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & y & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & 0 & y & 0 & \times \end{bmatrix}$$



Example:

$$\begin{bmatrix} \times & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & y & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & 0 & y & 0 & \times \end{bmatrix}$$



$$\begin{bmatrix} \times & 0 & 0 & 0 & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & \times & 0 & 0 \\ 0 & 0 & \times & 0 & 0 & y & \times & 0 \\ \times & 0 & 0 & \times & 0 & 0 & 0 & 0 \\ 0 & \times & 0 & 0 & y & 0 & 0 & \times \end{bmatrix}$$