Computing $F'(x)$ with AD

Observations:

- $F'(x)s$ can be computed in one forward pass.
  - A group of structurally ortogonal columns of $F'(x)$ can be obtained from the product $F'(x)s$ where s is initialized to the sum of the coordinate vectors for the columns in the group
- $w^T F'(x)$ can be computed in one reverse pass.
  - Apply CPR to $F'(x)^T$
  - A group of structurally orthogonal columns of $F'(x)^T$ is a group of structurally orthogonal rows of the Jacobian.
  - The group can be computed with one reverse pass by initiating w to be the columns of $F'(x)^T$ corresponding to structurally ortogonal columns

- A group of structurally orthogonal columns can be computed with one forward pass

- A group of structurally orthogonal rows can be computed with one reverse pass

Problem

Given a matrix $A \in \mathrm{R}^{m\times n}$ find the matrices $S \in \mathrm{R}^{n\times p}$ and $W \in \mathrm{R}^{m\times q}$ such that AS or $W^T A$ determines A uniquely with min$\{p, q\}$ groups.

Row OR column computation

$$\begin{pmatrix} \times & & & & \\ & \times & & & \\ & & \times & & \\ & & & \times & \\ \times & \times & \times & \times & \times \end{pmatrix}$$

Forward mode (**column computation**): $p = 5$

As_i, where $s_i = e_i$ for $i = 1, \ldots 5$

Reverse mode (**row computation**): $q = 2$

$w_1^T A$ and $w_2^T A$, $w_1^T = (1, 1, 1, 1, 0)$ and $w_2^T = (0, 0, 0, 0, 1)$

$$\begin{pmatrix} \times & & & & \times \\ & \times & & & \times \\ & & \times & & \times \\ & & & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix}$$

Forward mode (**column computation**): $p = 5$

As_i, where $s_i = e_i$ for $i = 1, \ldots, 5$

Reverse mode (**row computation**): $q = 5$

$w_i^T A$, where $w_i = e_i$ for $i = 1, \ldots, 5$.

Column OR row computation

Matrix	mxg	mxg'	min
abb313	10	26	10
ash219	4	9	4
ash292	8	10	8
ash331	6	12	6
ash608	6	12	6
ash958	6	13	6
curtis54	12	16	12
ibm32	8	7	7
will199	7	9	7
will57	11	11	11
will701	7	9	7
gent113	20	27	20
arc130	124	124	124
shl	422	4	4
shl200	440	4	4
shl400	426	4	4
str	34	35	34
str200	30	31	30
str400	33	36	33
str600	33	36	33
bp	266	20	20
bp200	283	21	21
bp400	295	21	21
bp600	302	21	21
bp800	304	21	21
bp1000	308	21	21
bp1200	311	21	21
bp1400	311	21	21
bp1600	304	21	21
fs541-1	13	541	13
fs541-2	13	541	13
eris	81	93	81
lundA	12	13	12
lubdB	12	13	12
Total	4462	1824	689

Row AND column computation

$$\begin{pmatrix} \times & & & & \times \\ & \times & & & \times \\ & & \times & & \times \\ & & & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix}$$

Set

$s_1^T = w_1^T = (0, 0, 0, 0, 1)$ and $s_2^T = (1, 1, 1, 1, 0)$.

Compute the nonzeros from

As_1 and As_2 by Forward mode and

$w_1^T A$ by Reverse mode.

Row-column consistent partition

Given a matrix $A \in \mathrm{R}^{m \times n}$ find the matrices $S \in \mathrm{R}^{n \times p}$ and $W \in \mathrm{R}^{m \times q}$ such that AS and $W^T A$ determines A uniquely with $p + q$ groups.

Partition the rows and columns of A into groups such that

- Each group consists entirely of either rows or columns.
- For every nonzero α_{ij} of A either

  - column a_j is in a group where no other column in its group has a nonzero in row position i

  or

  - row r_i is in a group where no other row has a nonzero in column position j.

Purpose:

Analyze this problem as a graph coloring problem.

Graph problem

p-coloring of $G = (V, E)$

$\phi : V \mapsto \{1, 2, \cdots p\}$, $\phi(v_i) \neq \phi(v_j)$, v_i and v_j are neighbors.

A graph associated with $A \in \mathrm{R}^{m \times n}$:

$G_b(A) = (V_1 \cup V_2, E)$

$V_1 = \{a_1, a_2, \cdots a_n\}, V_2 = \{r_1, r_2, \cdots r_m\}$

$\{r_i, a_j\} \in E \Longleftrightarrow \alpha_{ij} \neq 0$

Path p-coloring of $G_b(A)$:

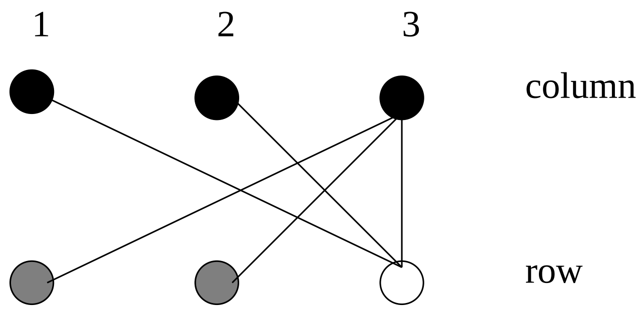
- ϕ is a p-coloring
- $\forall$ path (v_i, v_j, v_k, v_l) of length 3 uses at least 3 colors
- $\{\phi(u) : u \in V_1\} \cap \{\phi(v) : v \in V_2\} = \emptyset$

Result

The mapping ϕ induces a row-column consistent partition of the rows and column of A if and only if ϕ is a path p-coloring of $G_b(A)$

Example 1

$$\begin{pmatrix} & & \times \\ & & \times \\ \times & \times & \times \end{pmatrix}$$



- Need 3 colors
- Matrix can be estimated with

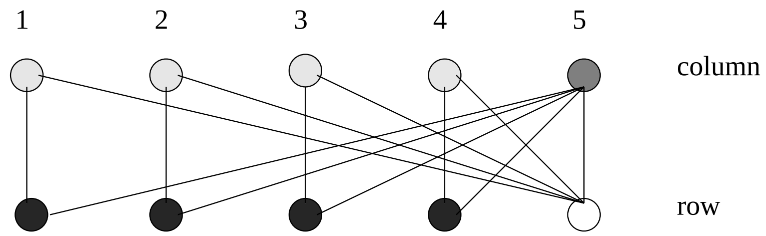
$s_1^T = (0, 0, 1)$ and $w_1^T = (0, 0, 1)$

Observation:

Zero sub row/sub column can be computed from either column group or row group

Example 2

$$\begin{pmatrix} \times & & & & \times \\ & \times & & & \times \\ & & \times & & \times \\ & & & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix}$$



- Need 4 colors
- Matrix can be computed with

$s_1^T = (0,0,0,0,1)$, $w_1^T = (0,0,0,0,1)$ and
$s_2^T = (1,1,1,1,0)$

Observation:

Diagonal matrix can be computed from either column group or row group

Cover

$\mathcal{S} =$ a group in a row-column consistent partition.

α_{ij} is **covered** by $\mathcal{S} \Longleftrightarrow a_j \in \mathcal{S}$ or $r_i \in \mathcal{S}$

Direct determination

Let α_{ij} be covered by $\mathcal{S}$

α_{ij} is **directly determined** by $\mathcal{S}$
$\Longleftrightarrow$
(if covered by a column) $\nexists\ a_q \in \mathcal{S}$ for which $\alpha_{iq} \neq 0$ or
(if covered by a row) $\nexists\ r_p \in \mathcal{S}$ for which $\alpha_{pj} \neq 0$

Complete direct cover

Let $\mathcal{S}_c$ be a collection of subsets of columns and $\mathcal{S}_r$ be be a collection of subsets of rows.

$\{S_c, S_r\}$ constitutes a **complete direct cover** for A if

- The intersection of any two subsets is empty
- For each nonzero element α_{ij}, there is a subset $\mathcal{S} \in \mathcal{S}_c \cup \mathcal{S}_r$ such that α_{ij} is directly determined by $\mathcal{S}$.

From cover to partition

Find a row-column consistent partition from a direct cover

Result

Given a complete direct cover $\{\mathcal{S}_c, \mathcal{S}_r\}$ for the matrix A, a row-column consistent partition of the rows and columns of A can be constructed that contains at most $|\mathcal{S}_c| + |\mathcal{S}_r| + 2$ groups

Intersection graphs

Column intersection graph: $A \in \mathrm{R}^{m \times n}$ $G(A) = (V, E)$,
$V = \{a_1, a_2, \cdots, a_n\}$
$\{a_i, a_j\} \in E$ if and only if $i \neq j$ and columns a_i and a_j have a nonzero in the same row position

Chromatic number: $\chi(G) = \min \, \{p : G$ has a p-coloring$\}$

Row intersection graph: $G(A^T)$

Results

- ϕ is a p-coloring of $G(A)$ ($G(A^T)$) if and only if ϕ induces a consistent partition of the columns (rows) of A
- $\chi_p(G_b(A)) \leq \min \, \{\chi(G(A^T)), \chi(G(A))\} + 1$
- Complete direct cover
  $|\mathcal{S}_c| + |\mathcal{S}_r| \leq \min \, \{\chi(G(A^T)), \chi(G(A))\}$

No Known Algorithms for

Exact path p-coloring

Heuristic Methods
T. Coleman and A. Verma 1998
S. Hossain and T. Steihaug, 1998 modifies an algorithm by M.J.D.Powell and Ph.L. Toint 1979
A.H.Gebremedhin,Manne and Pothen 2004

The heuristic by Coleman and Verma, see Page 149 in Griewank's book on AD

An algorithm for complete direct cover

	$k := 0$
	edgecount $:= 0$
	$G[V_1^k \cup V_2^k] = G[V_1 \cup V_2]$
	while edgecount $< \|E\|$ do
Ordering:	Order the uncolored vertices V_1^k and V_2^k in nonincreasing degree in $G[V_1^k \cup V_2^k]$
Initialize:	Let w be the vertex that has maximum degree in $G[V_1^k \cup V_2^k]$ Let $V = V_1^k$ if $w \in V_1^k$ otherwise let $V = V_2^k$ Include w in W^k
Compute group:	Examine each vertex in V in the above order and include in W^k if it does not create a path of length 2 with other vertices in W^k
Assign new color:	$k := k + 1$ Assign the color k to the vertices in W^k Let E^k be the edges that has end points in W^k edgecount := edgecount $+\|E^k\|$
	endwhile

Numerical Results

Static information:

n - Number of columns
m - Number of rows
nnz - Number of nonzeros
mxr - Maximum number of nonzeros in any row
mxc - Maximum number of nonzeros in any column
mng - A lower bound on the number of column groups
mng' - A lower bound on the number of row groups

Coloring information:

mxg - Number of groups found by dsm on A
mxg' - Number of groups found by dsm on A^T
rg - Row groups in the complete direct cover
cg - Column groups in the complete direct cover
tg - $rg + cg$

Harwell Matrices (Static Information)

Matrix	n	m	nnz	*mxr*	mng	mxc	mng'
abb313	176	313	1557	6	10	26	26
ash219	85	219	438	2	3	9	9
ash292	292	292	1250	8	8	10	10
ash331	104	331	662	2	6	12	12
ash608	188	608	1216	2	5	12	12
ash958	292	958	1916	2	6	13	13
curtis54	54	54	291	12	12	16	16
ibm32	32	32	126	8	8	7	7
will199	199	199	701	6	7	9	9
will57	57	57	281	11	11	11	11
will701	199	199	701	6	7	9	9
gent113	113	113	655	20	20	27	27
arc130	130	130	1282	124	124	124	124
shl	663	663	1687	422	422	4	4
shl200	663	663	1726	440	440	4	4
shl400	663	663	1712	426	426	4	4
str	363	363	2454	34	34	34	34
str200	363	363	3068	30	30	26	26
str400	363	363	3157	33	33	34	36
str600	363	363	3279	33	33	34	36
bp	822	822	3276	266	266	20	20
bp200	822	822	3802	283	283	21	21
bp400	822	822	4028	295	295	21	21
bp600	822	822	4172	302	302	21	21
bp800	822	822	4534	304	304	21	21
bp1000	822	822	4661	308	308	21	21
bp1200	822	822	4726	311	311	21	21
bp1400	822	822	4790	311	311	21	21
bp1600	822	822	4841	304	304	21	21
fs541-1	541	541	4285	11	11	541	541
fs541-2	541	541	4285	11	11	541	541
eris	1176	1176	9864	81	81	93	93
lundA	147	147	1298	12	12	12	12
lubdB	147	147	1294	12	12	12	12

Complete Direct Cover

	dsm		*Complete direct cover*		
Matrix	mxg	mxg'	cg	rg	tg
abb313	10	26	13	0(1)	13
ash219	4	9	5	0(1)	5
ash292	8	10	3(1)	7	10
ash331	6	12	6	0(1)	6
ash608	6	12	7	0(1)	7
ash958	6	13	6	0(1)	6
curtis54	12	16	1(1)	9	10
ibm32	8	7	8	0(1)	8
will199	7	9	6	1(1)	7
will57	11	11	2(1)	7	9
will701	7	9	6	1(1)	7
gent113	20	27	10(1)	8	18
arc130	124	124	16(1)	10	26
shl	422	4	0(1)	4	4
shl200	440	4	0(1)	4	4
shl400	426	4	0(1)	4	4
str	34	35	18	6(1)	24
str200	30	31	0(1)	31	31
str400	33	36	1(1)	35	36
str600	33	36	26	9(1)	35
bp	266	20	2(1)	14	16
bp200	283	21	6(1)	12	18
bp400	295	21	7(1)	12	19
bp600	302	21	7	11(1)	18
bp800	304	21	0(1)	21	21
bp1000	308	21	0(1)	22	22
bp1200	311	21	0(1)	22	22
bp1400	311	21	0(1)	22	22
bp1600	304	21	0(1)	21	21
fs541-1	13	541	15	0(1)	15
fs541-2	13	541	15	0(1)	15
eris	81	93	10(1)	70	80
lundA	12	13	0(1)	14	14
lubdB	12	13	0(1)	14	14
Total	4462	1824			587