Sparsity Detection in Matlab

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Outline

Introduction

- For a large sparse Jacobian compression techniques can greatly reduce the cost of determining a Jacobian's entries by AD [GW08, Chap.8].
- Such techniques require the Jacobian's sparsity pattern - or a tight over-estimate.
- Sophisticated approaches in ADOL-C [WG04] and TAF [GK06] for C/C++ and Fortran.
- By-product of use of sparse storage in forward mode AD [BKBC96, FK04].

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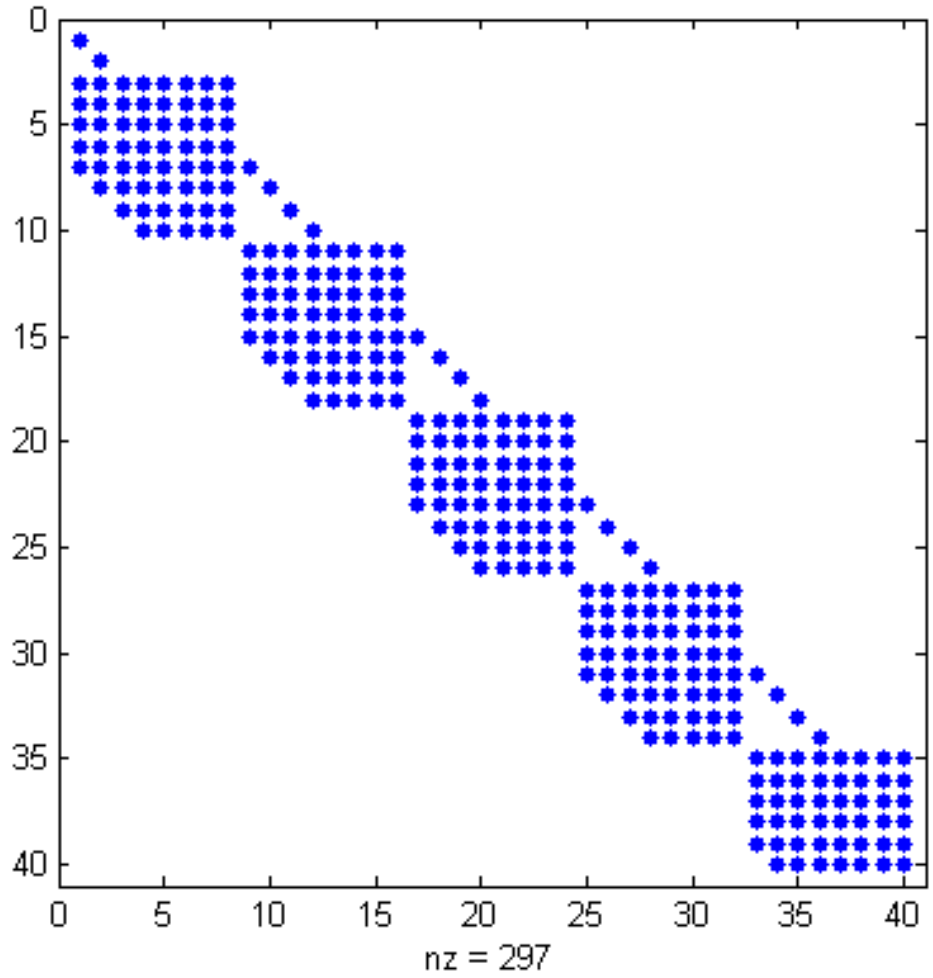
Example (Minpack FIC Sparsity Pattern [ACMX92])



Sparsity pattern = location of Jacobian entries

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Problem Definition

Definition (Sparsity Estimation)

Given a function $f : \mathbf{x} \in \mathbf{R}^{\mathbf{n}} \rightarrow \mathbf{y} \in \mathbb{R}^{\mathbf{m}}$ with Jacobian $\mathbf{Jf} \in \mathbb{R}^{\mathbf{m} \times \mathbf{n}}$ and **f** defined by a computer program then the sparsity estimation problem is to compute the locations (i, j) of all non-structurally zero elements (a.k.a. entries) of **Jf**.

- $\mathbf{Jf}_{i,j}$ is structurally zero if it is zero for all valid **x**.
- If the sparsity pattern is not valid for all valid independent variables **x** then this should be signalled.

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Example (Structurally Zero)

Consider the trivial problem $\mathbf{y} = \mathbf{f}(\mathbf{x})$ with,

$$f_i = x_i^2,$$

and

$$\mathbf{Jf}_{i,j} = \begin{cases} 2x_i, & i = j, \\ 0, & i \neq j. \end{cases}$$

- Sparsity pattern is clearly the identity matrix.
- But if $x_i \equiv 0$ then $\mathbf{Jf}_{i,i} = 0$.
- Element $\mathbf{Jf}_{i,j}, i \neq j$ is structurally zero.
- Element $\mathbf{Jf}_{i,i}$ is not structurally zero.
- Element $\mathbf{Jf}_{i,i}$ may *accidentally* be zero when $x_i \equiv 0$.

n.b. Branching can give similar effects.

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Approaches to Sparsity Detection

- By-Product of Sparse Forward Mode AD
- Using Bit Operations
- Verma's Matlab Implementation

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By-Product of Sparse Forward Mode AD

ADiFor, MAD, ADO2 [BKBC96, FK04, PR98] may propagate derivative vectors using sparse storage.

- For each active variable's derivatives ∇v_k store only the non-zeros as a data structure[1],

$$\nabla v_k = \left\{ \left(j, \frac{\partial v_k}{\partial x_j} \right) : \frac{\partial v_k}{\partial x_j} \neq 0 \right\}.$$

- Such methods typically do not store a derivative if it is *accidentally* zero.
- Sparsity pattern may be an underestimate - unsafe.
- Work-around: randomize **x** to reduce likelihood of *accidents* [FK04] - resulting **Jf** of no practical use.

[1] or similar!

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Using Bit Operations

The sparsity pattern $\hat{v}_k$ for any variable v_k may be defined by a bit pattern,

$$\hat{v}_k = \left\{ \hat{v}_k{}^j, j = 1, \ldots, n \in \{0,1\}^n \right\},$$

with

$$\hat{v}_k{}^j = \begin{cases} 0 & \text{if } \frac{\partial v_k}{\partial x_j} \text{ structurally zero} \\ 1 & \text{if } \frac{\partial v_k}{\partial x_j} \text{ not structurally zero} \end{cases}.$$

e.g. for $n = 3$ then

$$\begin{aligned} \hat{x}_1 &= \{1,0,0\} \\ \hat{x}_2 &= \{0,1,0\} \\ \hat{x}_3 &= \{0,0,1\} \\ \hat{v}_1 : v_1 = x_1 + x_2 &= \{1,1,0\} \end{aligned}$$

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Using Bit Operations (ctd.)

For active scalars x, y and constant a [GK06],

- If $v = x \circ y$ with $\circ = +, -, *, /$ then,

$$\hat{v} = \hat{x}|\hat{y},$$

with $|$ the bit-wise or operation

$$\hat{v}^j = \begin{cases} 1 & \text{if } \hat{x}^j = 1 \text{ or } \hat{y}^j = 1, \\ 0 & \text{otherwise.} \end{cases}$$

- For $v = a \circ x$, or $x \circ a$, $a \neq 0$,

$$\hat{v} = \hat{x}.$$

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Using Bit Operations (ctd.)

- Such bit-wise operations exist in C, C++, Fortran and Matlab for (unsigned) integer types.
- With 32 bit (4 byte) integers the sparsity pattern for up to 32 directional derivatives may be stored in a single integer.
- For n independent variables a vector of length $n/32$ can hold the entire sparsity pattern for a scalar.
- Just $n/32$ bit-wise or operations are required to combine such patterns in $\hat{x}|\hat{y}$.
- For 64 bit integers (8 bytes) use $n/64$ in above!
- TAF can produce sparsity patterns 2 orders of magnitude faster than Jacobians [GK06].

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Verma's Matlab Implementation

Verma [Ver98] realised that sparsity propagation rules must be adapted to vector/matrix operations.

Example ($\mathbf{z} = \mathbf{I_n x}$)

- In Matlab `z = eye(n)*x`.
- If we don't account for zeros in $\mathbf{I_n}$ then Jacobian sparsity pattern is the overestimate,

$$\hat{\mathbf{J}}_{\mathbf{z}} = \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & \cdots & 1 \end{bmatrix}$$

- In operation $\mathbf{z} = \mathbf{A x}$ account for sparsity of $\mathbf{A}$.

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Verma's Matlab Implementation (ctd.)

- What if matrix is active $\mathbf{z} = \mathbf{Y}\mathbf{x}$? Verma used sparsity of $\mathbf{Y}$'s value - but this might have entries that are accidentally zero.
- Verma stored sparsities using full arrays - performance overhead.

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Preliminary MAD Implementations

- Account for Sparsity of Intermediate Variables
- Logical Arrays for Derivative Sparsity
- Bitwise Storage for Derivative Sparsity
- Branch Detection

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Account for Sparsity of Intermediate Variables

Both our implementations have three components/properties:

- `value` - stores an object's numerical value.
- `entries` - a logical array indicating the location of structural non-zeros.
- `sparsity` - storage of derivative sparsity pattern - see later.

The `entries` component is updated as one might expect:

operation	entries operation
`z = x + y`	`z.entries = x.entries | y.entries`
`z = x .* y`	`z.entries = x.entries & y.entries`
`z = x * y`	`z.entries = logical(x.entries*y.entries)`

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Logical Matrices for Derivative Sparsity

- MAD's `derivvec` class stores pattern for an object `v` of size $d_1 \times d_2 \times \cdots \times d_D$ as a $(d_1 \cdot d_2 \cdots d_D) \times n$ logical matrix.
- The logical matrix may be full or sparse.
- Storage requirement is
  - full: $4 \cdot d_1 \cdot d_2 \cdots d_D \cdot n$ bytes
  - sparse: $< 12n$ `nnz(v.entries)` bytes (underlying CSC).
- Sparsity propagation a la Verma but using an object's `entries` and not its `value`.

operation	entries operation
`z = x + y`	`z.sparsity = x.sparsity | y.sparsity`
`z = x .* y`	`z.sparsity = x.entries & y.sparsity` `| x.sparsity & y.entries`

Conformability - `derivvec` *replicates* `entries` n times.

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Bitwise Storage for Derivative Sparsity

- `bitvec` class stores pattern for a $d_1 \times d_2 \times \cdots \times d_D$ object `v` as a $(d_1 \cdot d_2 \cdots d_D) \times \text{ceil}(n/32)$ `uint32` matrix.
- The integer matrix must be full - no sparse support.
- Storage requirement is $4 \cdot d_1 \cdot d_2 \cdots d_D \cdot \text{ceil}(n/32)$ bytes.
- Matlab R2010a has insufficient support for `uint64`.
- Sparsity propagation as for logical arrays.
- Conformability - `bitvec` *replicates* `entries` to ceil(n/32) `uint32` integers as required.

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Branch Detection

Basic facility [Men10].

- Logs results of logical operations on active variables expected to control branching.
- Logs can be examined or successive logs compared for changes in control flow.
- Not fully tested.

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Results

All test cases from the Minpack Collection [ACMX92].

- Flow in Channel - FIC
- Swirling Flow between Disks - SFD
- Combustion of Propane - CPF/CPR

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Flow in Channel - FIC

	problem size n		
technique	8	64	2400
fmad	0.5	1.4	120.3
logical derivvec	0.5	1.4	65.6
bitvec	0.5	1.4	42.4

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Swirling Flow between Disks - SFD

	problem size n			
technique	14	700	1400	2800
fmad	0.9	26.3	67.5	257.5
logical derivvec	0.9	24.6	51.8	110.7
bitvec	0.9	24.5	48.6	100.5

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Combustion of Propane - CPF/CPR

	problem and size *n*	
	CPR	CPF
technique	5	11
fmad	0.31	0.33
logical derivvec	0.26	0.28
bitvec	0.25	0.28

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Conclusions & Further Work

- It is possible to forward propagate sparsity patterns about 2.5 to 4 times faster than derivatives for moderate sized problems in Matlab.
- Presently, bitwise operations are slightly faster.
- Robustness requires:
  - Storage of an objects entries as well as its derivative sparsity pattern.
  - Branch detection.
- Scope for further improvements:
  - For efficiency of indexing and `|` and `&` operations logical `derivvec` internal storage should be transposed.
  - Improved Matlab support for `uint64`.
  - Hybrid approach using sparse bitwise storage - C/C++/Fortran coding?

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