

Graph Learning Sparse Matrices

Thomas Bonald

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Motivation

Large graphs are typically **sparse**

Dataset	#nodes	#edges	Density
Flights	2,939	30,500	$\approx 10^{-3}$
Amazon products	335k	925k	$\approx 10^{-5}$
Actors	382k	33M	$\approx 10^{-4}$
Wikipedia (en)	12M	378M	$\approx 10^{-6}$
Twitter	42M	1.5G	$\approx 10^{-6}$
Friendster	68M	2.5G	$\approx 10^{-7}$

Sparse matrices

$$\begin{bmatrix} 5 & 6 & 9 & 0 & 2 & 2 & 0 & 4 \\ 5 & 0 & 0 & 0 & 7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 1 & 3 \\ 0 & 0 & 5 & 0 & 0 & 0 & 9 & 0 \end{bmatrix}$$

Efficient coding in Python

```
> from scipy import sparse
```

Coordinate format

$$\begin{bmatrix} 5 & 6 & 9 & 2 & 2 & & 4 \\ 5 & & & 7 & & & \\ & 5 & & & 3 & & \\ 6 & & & & & 1 & 3 \\ & & 5 & & & 9 & \end{bmatrix}$$

with vector v , we can do $A \cdot \text{dot}(v)$

`shape = (6, 8)`

`data = (5, 6, 9, 2, 2, 4, 5, 7, 5, 3, 6, 1, 3, 5, 9)`

`row = (0, 0, 0, 0, 0, 0, 1, 1, 3, 3, 4, 4, 4, 5, 5)`

`col = (0, 1, 2, 4, 5, 7, 0, 4, 1, 5, 0, 6, 7, 2, 6)`

the entry 4 is in row 0, col 7

Compressed Sparse Row

$$\begin{bmatrix} 5 & 6 & 9 & 2 & 2 & & 4 \\ 5 & & & 7 & & & \\ & 5 & & & 3 & & \\ 6 & & & & & 1 & 3 \\ & & 5 & & & 9 & \end{bmatrix}$$

$$\text{shape} = (6, 8)$$

$$\text{data} = (5, 6, 9, 2, 2, 4, 5, 7, 5, 3, 6, 1, 3, 5, 9)$$

$$\text{col} = \text{indices} = (0, 1, 2, 4, 5, 7, 0, 4, 1, 5, 0, 6, 7, 2, 6)$$

$$\text{index pointer} = \text{indptr} = (0, 6, 8, 8, 10, 13, 15)$$

[0, 6] 6 non-zero entries in row 1 (0,1,2,4,5,7)

[8 - 6] 2 entries in row 2 (0,4)

[8, 8] 0 entries in row 3

[10 - 8] 2 entries in row 4 (1,5)

Compressed Sparse Row

$$\begin{bmatrix} 5 & 6 & 9 & 2 & 2 & & 4 \\ 5 & & & 7 & & & \\ & 5 & & & 3 & & \\ 6 & & & & & 1 & 3 \\ & & 5 & & & 9 & \end{bmatrix}$$

$$\text{shape} = (6, 8)$$

$$\text{data} = (5, 6, 9, 2, 2, 4, 5, 7, 5, 3, 6, 1, 3, 5, 9)$$

$$\text{indices} = (0, 1, 2, 4, 5, 7, 0, 4, 1, 5, 0, 6, 7, 2, 6)$$

$$\text{indptr} = (0, 6, 8, 8, 10, 13, 15)$$

$$\text{row} = (0, 0, 0, 0, 0, 0, 1, 1, 3, 3, 4, 4, 4, 5, 5)$$

Matrix-vector multiplication (CSR format)

```
> matrix.dot(vector)
```

$$\begin{bmatrix} 5 & 6 & 9 & 2 & 2 & 4 \\ 5 & & & 7 & & \\ & 5 & & 3 & & \\ 6 & & & & 1 & 3 \\ & 5 & & 9 & & \end{bmatrix} \begin{bmatrix} 3 \\ 6 \\ 1 \\ 2 \\ 0 \\ 3 \\ 0 \\ 1 \end{bmatrix}$$

```
data = (5, 6, 9, 2, 2, 4, 5, 7, 5, 3, 6, 1, 3, 5, 9)
```

```
indices = (0, 1, 2, 4, 5, 7, 0, 4, 1, 5, 0, 6, 7, 2, 6)
```

```
indptr = (0, 6, 8, 8, 10, 13, 15)
```

Matrix-vector multiplication (CSR format)

$$\begin{bmatrix} 5 & 6 & 9 & 2 & 2 & 4 \\ 5 & & & 7 & & \\ & 5 & & & 3 & \\ 6 & & & & & 1 & 3 \\ & & 5 & & & 9 & \end{bmatrix} \begin{bmatrix} 3 \\ 6 \\ 1 \\ 2 \\ 0 \\ 3 \\ 0 \\ 1 \end{bmatrix}$$

$\text{vector}[\text{indices}] = (3, 6, 1, 0, 3, 1, 3, 0, 6, 3, 3, 0, 1, 1, 0)$

$\text{data} = (5, 6, 9, 2, 2, 4, 5, 7, 5, 3, 6, 1, 3, 5, 9)$
 $\text{indices} = (0, 1, 2, 4, 5, 7, 0, 4, 1, 5, 0, 6, 7, 2, 6)$
 $\text{indptr} = (0, 6, 8, 8, 10, 13, 15)$

Compressed Sparse Column

CSC = CSR^T

$$\begin{bmatrix} 5 & 6 & 9 & & 2 & 2 & & 4 \\ 5 & & & & 7 & & & \\ & 5 & & & & 3 & & \\ 6 & & & & & & 1 & 3 \\ & & 5 & & & & 9 & \end{bmatrix}$$

shape = (8, 6)

data = (5, 5, 6, 6, 5, 9, 5, 2, 7, 2, 3, 1, 9, 4, 3)
indices = (0, 1, 4, 0, 3, 0, 5, 0, 1, 0, 3, 4, 5, 0, 4)
indptr = (0, 3, 5, 7, 7, 9, 11, 13, 15)

List of Lists

5	6	9	2	2	4
5			7		
	5			3	
6					1 3
		5			9

```
data = [[5, 6, 9, 2, 2, 4], [5, 7], [], [5, 3], [6, 1, 3], [5, 9]]
```

```
rows = [[0, 1, 2, 4, 5, 7], [0, 4], [], [1, 5], [0, 6, 7], [2, 6]]
```

Choosing the right format

	COO	CSR	CSC	LIL
Arithmetic		✓	✓	
Row slicing		✓		
Column slicing			✓	
Modification				✓
Loading	✓			

Loading a graph

Data		Adjacency matrix (COO format)	
From	To		
12	38	→	row = (12, 71, 25, 12, ...) col = (38, 98, 21, 38, ...) data = (1, 1, 1, 1, ...)
71	98		
25	21		
12	38		
...	...		

Coding in Python

```
> adjacency = sparse.coo_matrix((data, (row, col)))  
> adjacency.sum_duplicates()
```