CSE 6040
Computing for Data Analytics: Methods and Tools

Low-level matrix storage

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Recall: Tibbles

A tibble is a two-dimensional table of numerical values where:

- Each row is an observation, e.g., data point in $\mathbb{R}^n$.

- Columns are variables or features.

In Python, a Pandas DataFrame is a convenient way to store a tibble. In R, a dataframe is the equivalent.

depth	table	price	x	y	z
61.5	55.0	326	3.95	3.98	2.43
59.8	61.0	326	3.89	3.84	2.31
56.9	65.0	327	4.05	4.07	2.31
62.4	58.0	334	4.20	4.23	2.63
63.3	58.0	335	4.34	4.35	2.75
62.8	57.0	336	3.94	3.96	2.48
62.3	57.0	336	3.95	3.98	2.47
61.9	55.0	337	4.07	4.11	2.53
65.1	61.0	337	3.87	3.78	2.49
59.4	61.0	338	4.00	4.05	2.39
64.0	55.0	339	4.25	4.28	2.73
62.8	56.0	340	3.93	3.90	2.46
60.4	61.0	342	3.88	3.84	2.33
62.2	54.0	344	4.35	4.37	2.71
60.2	62.0	345	3.79	3.75	2.27
60.9	58.0	345	4.38	4.42	2.68
62.0	54.0	348	4.31	4.34	2.68
63.4	54.0	351	4.23	4.29	2.70

Matrices

The mathematical (linear algebraic) object of a *matrix* is also a two-dimensional table, with, say, *m* rows, *n* columns, and *m*n* values.

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{bmatrix}$$

A matrix might be stored as a tibble. There are two common scenarios:

- Rows are observations and columns are variables, i.e., the tibble *is* the matrix. This option is good when the matrix is *dense*, i.e., most or all entries are non-zero.

- Each entry of the matrix is a tuple (row, column, value), given by one (or more) observations. That is, the tibble *lists* the matrix entries. This option is best when the matrix is *sparse*, i.e., most values are zero and, therefore, need not be stored explicitly.

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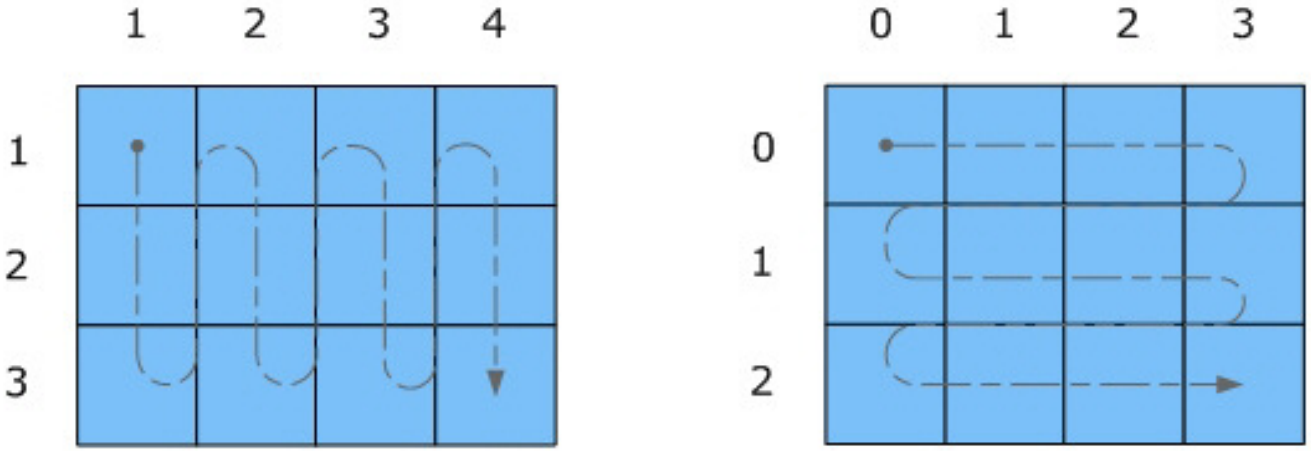
Dense matrix storage

Dense matrices in R and Matlab are stored in the **column-major** order: Entries in the same column are continuous in memory.

- Reason for column-major storage is historical: Numerical software developed in Fortran in the early days used the column-major order.

In Numpy:

- numpy.array([1, 2, 3], order='C') # row-major order; the default
- numpy.array([1, 2, 3], order='F') # column-major order



A: Column-major order (Fortran-style)

B: Row-major order (C-style)

Source: software.intel.com

Operating in the direction of major dimension

Accessing continuous memory is efficient.

Example: For matrices in the column-major order, scaling each column is fast, and scaling each row is slow.

```
> import numpy as np
> A = np.ones((10000, 10000), order='F')

> t0 = time.time()
> for i in range(10000):
>   A[:, i] *= 2.0          # scaling each column
> print time.time() - t0    # 0.119 second

> t0 = time.time()
> for i in range(10000):
>   A[i, :] *= 2.0          # scaling each row
> print time.time() - t0    # 1.574 seconds
```

Computational complexity of dense *matvec*

Complexity of a dense matrix $A \in \mathbb{R}^{n \times n}$ multiplying a vector $x \in \mathbb{R}^n$: $O(n^2)$

$$Ax = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n \\ A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n \\ \vdots \\ A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nn}x_n \end{bmatrix}$$

How to get this number?

n elements in the result vector, each requiring n scalar multiplications and $n-1$ scalar additions. Total count of flops (floating point operations): $(2n-1)n = 2n^2 - n$

What if the majority of A_{ij} are zero??

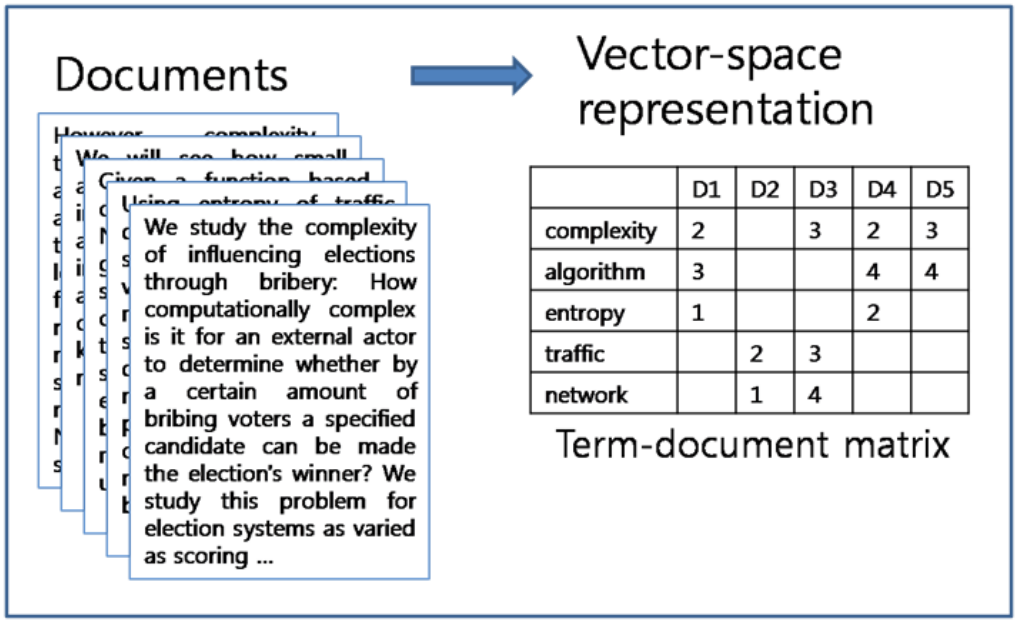
Sparse matrix: Term-document matrix

How to represent a text document?

We often ignore the ordering of words and keep only the counts of each unique word in a document, resulting in a *term-document matrix*.

- Rows correspond to documents
- Columns correspond to terms

Example:



	D1	D2	D3	D4	D5
complexity	2		3	2	3
algorithm	3			4	4
entropy	1			2	
traffic		2	3		
network		1	4		

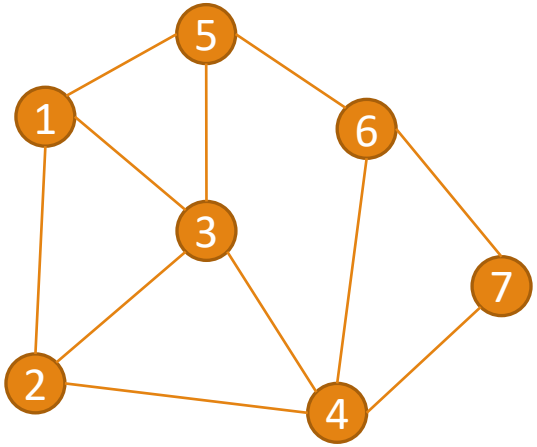
Term-document matrix

Note:
Lots of zeros because all the terms cannot appear in one document.

Source: mlg.postech.ac.kr/research/nmf

Sparse matrix: Graph adjacency matrix

How to represent a graph?



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

A node in a graph is typically connected to only a small fraction of nodes.

Source: www.cs.umn.edu/~metis

Sparse matrix is often very sparse

Term-document matrix for 4.5M English Wikipedia articles:

0.05% nonzeros

DBLP co-authorship network for 300,000 academic authors:

0.0007% nonzeros

We need efficient storage for sparse matrices.

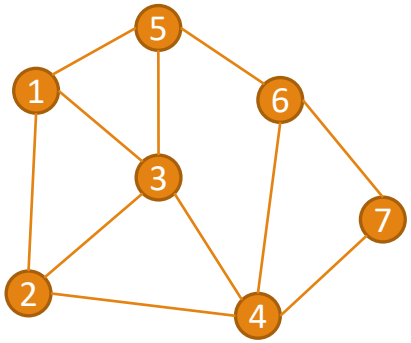
Storage of a sparse matrix

We store only the nonzeros and their positions

- (row, column, value)-triplet

Use the same example:

(1, 2, 1) (1, 3, 1) (1, 5, 1)
(2, 1, 1) (2, 3, 1) (2, 4, 1)
(3, 1, 1) (3, 2, 1) (3, 4, 1) (3, 5, 1)
(4, 2, 1) (4, 3, 1) (4, 6, 1) (4, 7, 1)
(5, 1, 1) (5, 3, 1) (5, 6, 1)
(6, 4, 1) (6, 5, 1) (6, 7, 1)
(7, 4, 1) (7, 6, 1)



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

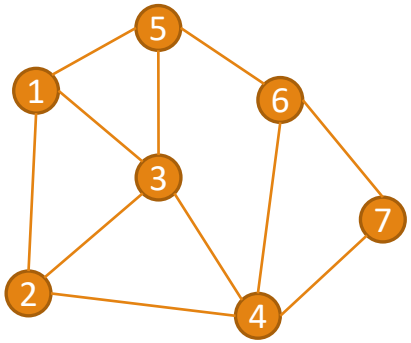
Viewing indices of the matrix as graph nodes, these triplets are edges.

Symmetric sparse matrix ($A = A^T$) ⇔ Undirected graph

Non-symmetric sparse matrix ⇔ Bipartite graph

Coordinate (COO) format

The triplets can be stored as 3 arrays: rows, cols, values.



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

`rows` = [0, 0, 0, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 5, 5, 5, 6, 6]

`cols` = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]

`values` = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]

Note: 0-based arrays

Compressed sparse row (CSR) format

Suppose a sparse matrix has `nnz` nonzero entries.

`rows` = [0, 0, 0, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 5, 5, 5, 6, 6]

`cols` = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]

`values` = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]

The COO format needs `3nnz` elements to store the matrix. Can we do better?

When the nonzeros are stored row by row, we can compress the above storage:

`rowptr` = [0, 3, 6, 10, 14, 17, 20, 22] Row pointer

`colind` = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5] Column index

`values` = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1] Values

This CSR format needs `2nnz+n` elements to store the matrix.

Similary, we have compressed sparse column (CSC) format.

Sparse formats in Scipy

```
> import scipy.sparse as sp
> rows = [0, 0, 0, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 5, 5, 5, 6, 6]
> cols = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]
> values = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
> A = sp.coo_matrix( (values, (rows, cols)) )
> A
<7x7 sparse matrix of type '<type 'numpy.int32'>'
        with 22 stored elements in COOrdinate format>
> B = A.tocsr()
> B
<7x7 sparse matrix of type '<type 'numpy.int32'>'
with 22 stored elements in Compressed Sparse Row format>
```

Typical and efficient way to construct a sparse matrix:
Initialize and fill in the three arrays (rows, cols, values), then call coo_matrix().

Sparse formats in Scipy

```
> import numpy as np
> import scipy.sparse as sp
> rowptr = [0, 3, 6, 10, 14, 17, 20, 22]
> colind = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]
> values = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
> A = sp.csr_matrix( (values, colind, rowptr), dtype=np.float64 )
> A
<7x7 sparse matrix of type '<type 'numpy.float64'>'
        with 22 stored elements in Compressed Sparse Row format>
> A.toarray()
array([[ 0.,  1.,  1.,  0.,  1.,  0.,  0.],
       [ 1.,  0.,  1.,  1.,  0.,  0.,  0.],
       [ 1.,  1.,  0.,  1.,  1.,  0.,  0.],
       [ 0.,  1.,  1.,  0.,  0.,  1.,  1.],
       [ 1.,  0.,  1.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.,  1.,  0.,  1.],
       [ 0.,  0.,  0.,  1.,  0.,  1.,  0.]])
```

Pitfall: `matrix` vs. `array`

‘array’ or ‘matrix’? Which should I use?

Historically, NumPy has provided a special matrix type, *np.matrix*, which is a subclass of ndarray which makes binary operations linear algebra operations. You may see it used in some existing code instead of *np.array*. So, which one to use?

Short answer

Use arrays.

- They are the standard vector/matrix/tensor type of numpy. Many numpy functions return arrays, not matrices.
- There is a clear distinction between element-wise operations and linear algebra operations.
- You can have standard vectors or row/column vectors if you like.

Until Python 3.5 the only disadvantage of using the array type was that you had to use `dot` instead of `*` to multiply (reduce) two tensors (scalar product, matrix vector multiplication etc.). Since Python 3.5 you can use the matrix multiplication `@` operator.

Given the above, we intend to deprecate `matrix` eventually.

https://numpy.org/devdocs/user/numpy-for-matlab-users.html#array-or-matrix-which-should-i-use

Sparse formats in Scipy

COO FORMAT

Facilitates fast conversion among sparse formats

Very fast conversion to and from CSR/CSC formats

Does not directly support arithmetic operations and slicing (indexing)

Intended usage:

- COO is a fast format for constructing sparse matrices
- Once a matrix has been constructed, convert to CSR or CSC format for fast arithmetic and matrix vector operations

CSR FORMAT

Efficient arithmetic operations CSR + CSR, CSR * CSR, etc.

efficient row slicing

Fast matrix vector products

Slow column slicing operations (consider CSC)

Changes to the sparsity structure (adding/deleting nonzeros) are expensive (consider LIL or DOK)

- **(Can you figure out why?)**

Source: docs.scipy.org

Sparse matrix operations

Operations involving two sparse matrices A, B yield a sparse matrix:

- Addition: `A+B`
- Multiplication: `A*B` or `A.dot(B)`
- Entrywise multiplication: `A.multiply(B)`

Operations involving a sparse matrix A and a dense matrix B (2D array in Numpy) yield a dense matrix:

- Addition: `A+B`
- Multiplication: `A*B` or `A.dot(B)`
- Entrywise multiplication: `A.multiply(B)`

Computational complexity of sparse *matvec*

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

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{bmatrix} = \begin{bmatrix} 1 \cdot x_2 + 1 \cdot x_3 + 1 \cdot x_5 \\ 1 \cdot x_1 + 1 \cdot x_3 + 1 \cdot x_4 \\ 1 \cdot x_1 + 1 \cdot x_2 + 1 \cdot x_4 + 1 \cdot x_5 \\ 1 \cdot x_2 + 1 \cdot x_3 + 1 \cdot x_6 + 1 \cdot x_7 \\ 1 \cdot x_1 + 1 \cdot x_3 + 1 \cdot x_6 \\ 1 \cdot x_4 + 1 \cdot x_5 + 1 \cdot x_7 \\ 1 \cdot x_4 + 1 \cdot x_6 \end{bmatrix}$$

Scalar multiplication is needed for nonzeros only.

Complexity: O(nnz)