

# Scientific computing

Kylie A. Bemis

Northeastern University  
Khoury College of Computer Sciences



Northeastern University

# Goals for today

- Representing numbers
- Matrices and arrays
- Introduction to NumPy

# REPRESENTING NUMBERS

# Storing numbers

- We represent numbers using a **base 10** system
  - ◆ 1, 10, 100, 1000, etc.
- Computers only store **bits** (0s and 1s)
- How to store *integers* and *real numbers* using only patterns of *bits*?

# Patterns of bits

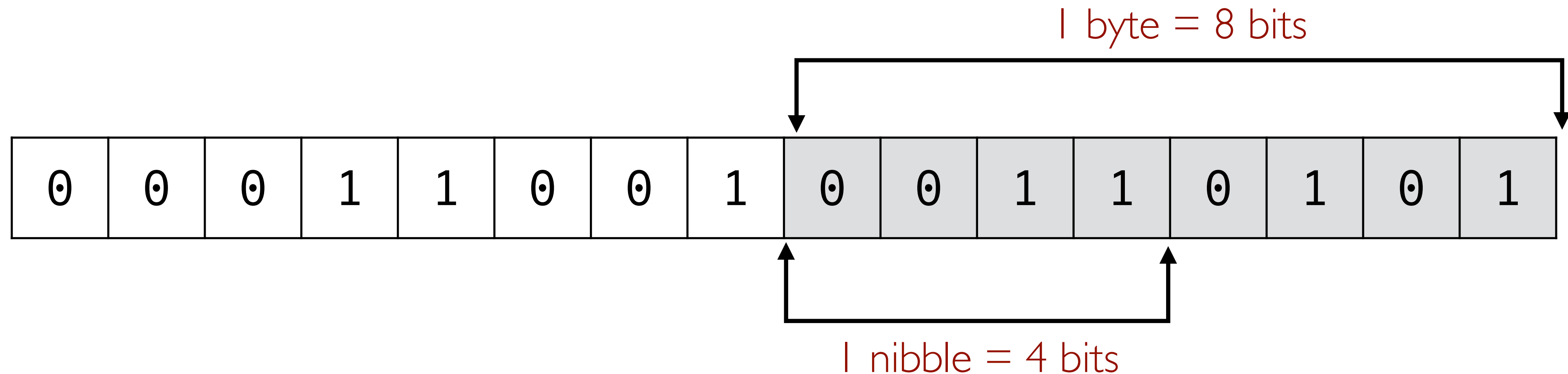
- All computer data is a sequence of bits
- How many unique values can be stored?

# of bits	Possible sequences	# of sequences
1	0, 1	2
2	00, 01, 10, 11	4
3	000, 001, 010, 011 100, 101, 110, 111	8

N bits can store  $2^N$  possible values!

# Bits and bytes

- Computers rarely work on individual bits
- Instead, operate on *chunks of bits*
- Typically, operate on **bytes** of 8 bits



# Bytes and storage

- Bytes are the building blocks of data types
- How many values can be stored per byte?

# of bytes	# of bits	# of values
1	8	256
2	16	65,536
4	32	4,294,967,296
8	64	$1.844674 \times 10^{19}$
16	128	$3.402823 \times 10^{38}$

# Storing integers

- **Bits** can only have two values (1s and 0s)
- Represent integers using **base 2** system

Bit	7	6	5	4	3	2	1	0	
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$	
	0	0	0	0	0	0	0	0	= 0
	0	0	0	0	0	0	0	1	= 1
	0	0	0	0	0	0	1	0	= 2
	0	0	0	0	0	0	1	1	= 3
	0	0	0	0	0	1	0	0	= 4



## Storing integers (2)

- **Bits** can only have two values (1s and 0s)
- Represent integers using **base 2** system

Bit	7	6	5	4	3	2	1	0
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$
	0	0	1	1	0	1	0	1

= 53

$$\begin{aligned} 0x00110101 &= 0 \times 2^7 + 0 \times 2^6 + 1 \times 2^5 + 1 \times 2^4 + 0 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 \\ &= 0 + 0 + 32 + 16 + 0 + 4 + 0 + 1 \\ &= 53 \end{aligned}$$

# Storing integers (3)

- **Bits** can only have two values (1s and 0s)
- Represent integers using **base 2** system

Bit	7	6	5	4	3	2	1	0
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$
	0	1	1	0	1	1	0	0

= 108

$$\begin{aligned} 0x01101100 &= 0 \times 2^7 + 1 \times 2^6 + 1 \times 2^5 + 0 \times 2^4 + 1 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 0 \times 2^0 \\ &= 0 + 64 + 32 + 0 + 8 + 4 + 0 + 0 \\ &= 108 \end{aligned}$$

# Bytes and hex

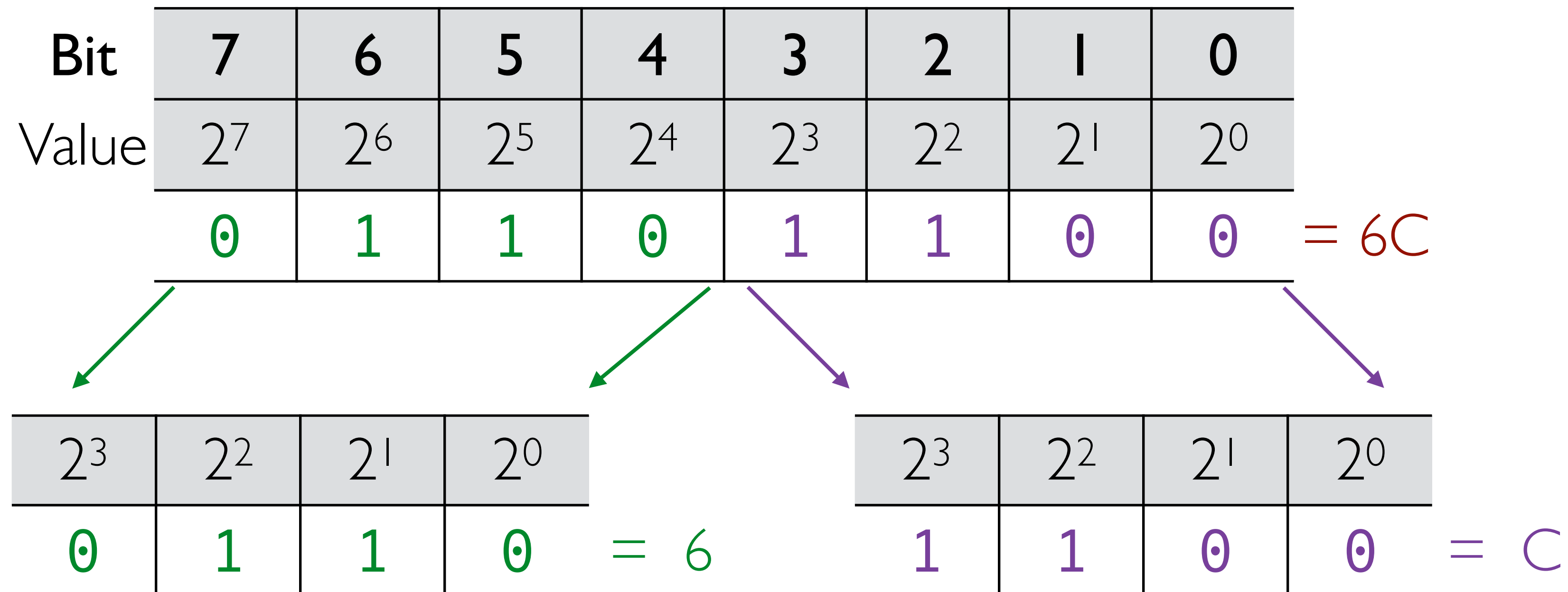
- Need: Print human-readable byte data
- But: Bits are difficult for humans to read
- Solution: Use **hexadecimal**
  - ◆ Base 16 system using characters 1-9 and A-F
  - ◆ Represent one byte with two hex digits

# Hexadecimal

- Base 16 numeric system
  - ◆ Represent numbers 0-9 with "0"-"9"
  - ◆ Represent numbers 10-15 with "A"-"F"
- Represent one byte with two hex digits
  - ◆ 0000 0000 becomes 0x00
  - ◆ 1111 1111 becomes 0xFF
  - ◆ 0000 1111 is 0x0F

# Decimal to hex

- Split byte into two half-bytes (nibbles)
- Find hex representation for each half



# Representations

- Decimal
  - ◆ Typical base 10 system
  - ◆ E.g., **108**
- Hexadecimal
  - ◆ Compact representation of bytes using base 16
  - ◆ E.g., **6C**
- Binary
  - ◆ How data is actually stored in computers
  - ◆ E.g., **01101100**

# What about negatives?

- Straightforward to encode *unsigned* numbers
- How to encode *signed* numbers?
  - ◆ Sign and magnitude
  - ◆ One's complement
  - ◆ Two's complement
- Need to choose a representation

# Sign and magnitude

- One bit stores sign (+ or -)
- Other bits store magnitude

Bit	7	6	5	4	3	2	1	0	
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$	
	0	0	1	1	0	1	0	1	= 53
	1	0	1	1	0	1	0	1	= -53

Sign bit



# One's complement

- Apply bitwise NOT operator
- Negative is "complement" of positive

Bit	7	6	5	4	3	2	1	0	
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$	
	0	0	1	1	0	1	0	1	= 53
Invert each bit →	1	1	0	0	1	0	1	0	= -53

# Two's complement

- Apply bitwise NOT operator and add 1
- One's complement plus one

Bit	7	6	5	4	3	2	1	0	
Value	$2^7$	$2^6$	$2^5$	$2^4$	$2^3$	$2^2$	$2^1$	$2^0$	
	0	0	1	1	0	1	0	1	= 53
Invert each bit	1	1	0	0	1	0	1	1	= -53

Add 1

# Signed representations

- Sign and magnitude
  - ◆ *Different* arithmetic for positive and negative
  - ◆  $+0$  and  $-0$  are both represented
- One's complement
  - ◆ *Similar* arithmetic for positive and negative
  - ◆  $+0$  and  $-0$  are both represented
- Two's complement
  - ◆ *Same* arithmetic for positive and negative
  - ◆ Single zero

# Signed representations

- Sign and magnitude
  - ◆ *Different* arithmetic for positive and negative
  - ◆  $+0$  and  $-0$  are both represented
- One's complement
  - ◆ *Similar* arithmetic for positive and negative
  - ◆  $+0$  and  $-0$  are both represented

- Two's complement
  - ◆ *Same* arithmetic for positive and negative
  - ◆ Single zero

Typical implementation

# Integer overflow

- Can only store so many values
- Larger magnitudes "overflow"

8-bit integer

Decimal	Binary
127	0111 1111
126	0111 1110
...	. . .
2	0000 0010
1	0000 0001
0	0000 0000

127+1

Decimal	Binary
-1	1111 1111
-2	1111 1110
...	. . .
-126	1000 0010
-127	1000 0001
-128	1000 0000

= -128

# Common integer representations

- 32-bit integer
  - ◆ Unsigned max:  $2^{32}-1 = 4,294,967,296$
  - ◆ Signed range:  $-2,147,483,648$  to  $+2,147,483,647$
- 64-bit integer
  - ◆ Unsigned max:  $2^{64}-1$
  - ◆ Signed range:  $-2^{63}$  to  $+2^{63}-1$

# What about real numbers?

- Difficult to represent versus integers
- Infinite range of possible values
  - ◆ Not all values can be stored precisely
  - ◆ Need to trade off between range and precision
- What about "special" values?
  - ◆ E.g.,  $+\infty$ ,  $-\infty$ , and NaN

# Motivation: Scientific notation

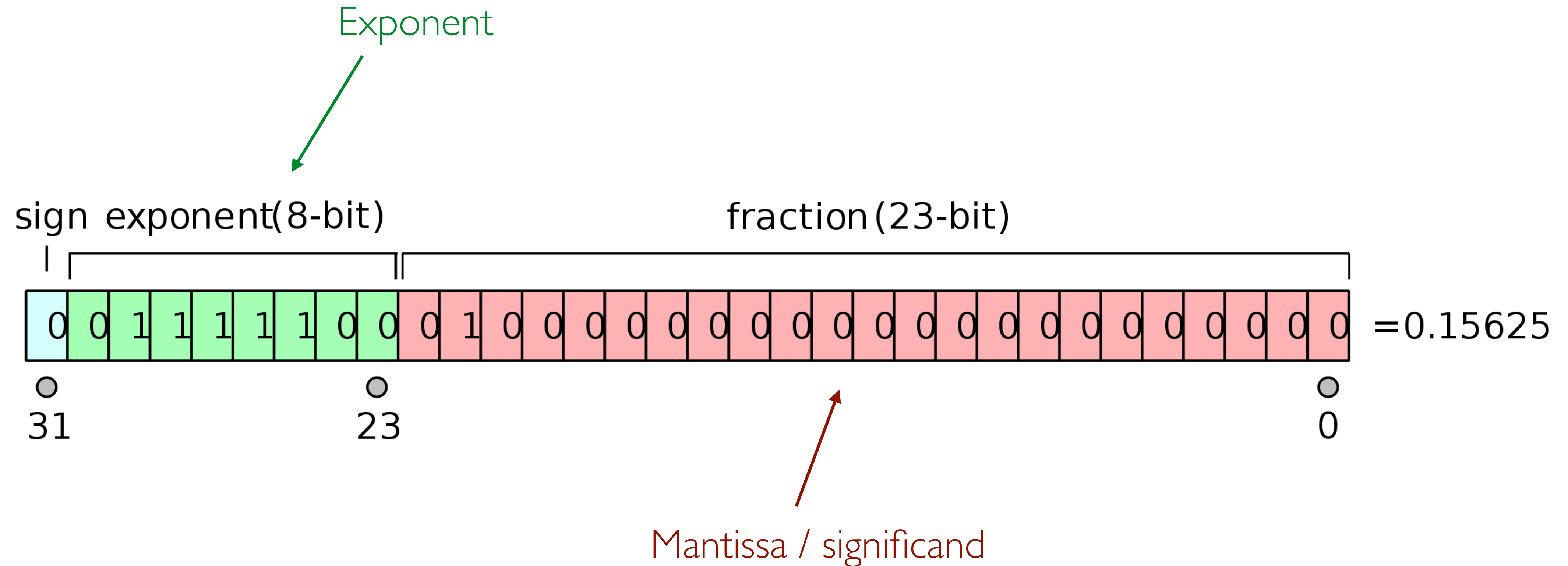
- Similar to floating point representation
- Represent numbers as  $m \times 10^n$ , where
  - ◆  $n$  is an integer called the *exponent*
  - ◆  $m$  is a real number (typically between 1 and 10)
  - ◆  $m$  is called the *significand* or *mantissa*
- E.g.,  $1,234 = 1.234 \times 10^3$



# IEEE 754: Floating point

- Standard for representing real numbers
- Storage similar to scientific notation
  1. Sign bit
  2. Exponent
  3. Mantissa/significand
- Special sequences for  $+\infty$ ,  $-\infty$ , and NaN

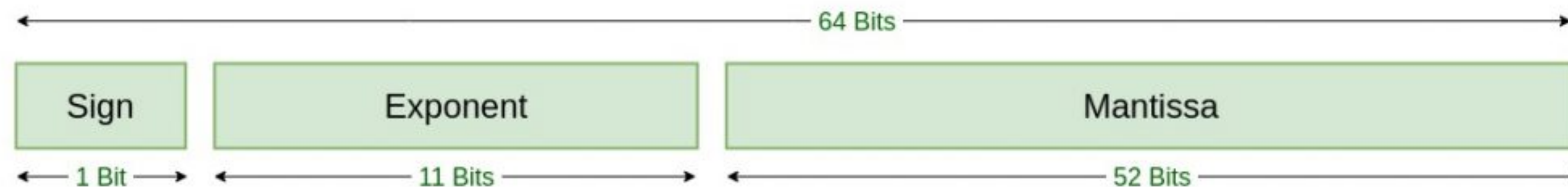
# "Single" precision: 32-bit float



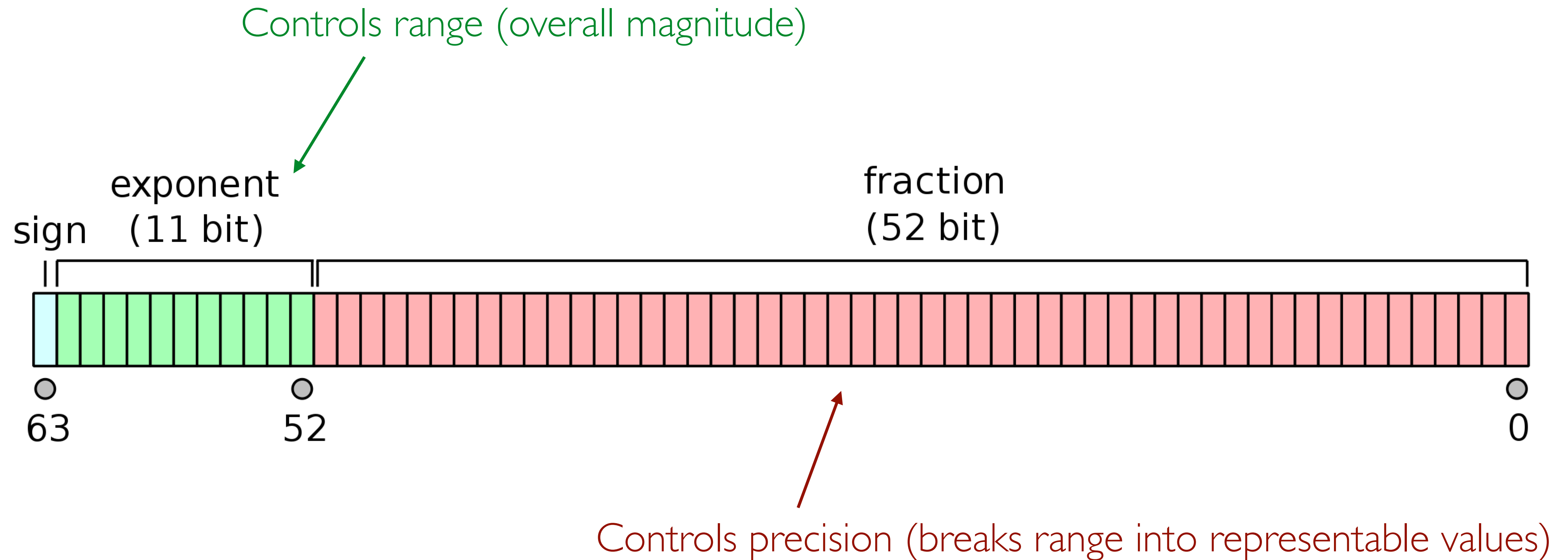
[https://en.wikipedia.org/wiki/IEEE\\_754-1985#/media/File:IEEE\\_754\\_Single\\_Floating\\_Point\\_Format.svg](https://en.wikipedia.org/wiki/IEEE_754-1985#/media/File:IEEE_754_Single_Floating_Point_Format.svg)

# Floating point representation

- Exponent controls range
  - ◆ Scales overall magnitude of the number
  - ◆ Allows for very large and very small numbers
- Mantissa controls precision
  - ◆ Breaks overall range into finite number of points
  - ◆ These are the points that can be represented



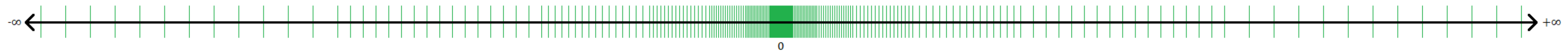
# "Double" precision: 64-bit float



[https://en.wikipedia.org/wiki/IEEE\\_754-1985#/media/File:IEEE\\_754\\_Double\\_Floating\\_Point\\_Format.svg](https://en.wikipedia.org/wiki/IEEE_754-1985#/media/File:IEEE_754_Double_Floating_Point_Format.svg)

# Trade-off between range and precision

- Floating point can store either:
  - ◆ Very large numbers, OR
  - ◆ Very small numbers
- Cannot precisely store both at once
  - ◆ Larger numbers are separated by wider "gaps"
  - ◆ For sufficiently large  $x$ , floating point says  $x + 1 = x$
- *Caution: consider scale of your computations*



# Precision in floating point arithmetic

- Many values cannot be precisely represented
- Small floating point errors can compound or underflow/overflow over many computations
- Use caution with floating point arithmetic:
  - ◆ Never check for perfect equality — always some error
  - ◆ Transform unstable operations (e.g., product vs. sum of logs)
  - ◆ Use algorithms with greater **numeric stability**

# "Special" values

- Positive and negative infinity
  - ◆ Exponent is all 1s
  - ◆ Mantissa is all 0s
- Not-a-number (NaNs)
  - ◆ Exponent is all 1s
  - ◆ Any part of mantissa is non-0s
- "Subnormal" numbers
  - ◆ Exponent is all 0s
  - ◆ Ensure small differences  $x - y \neq 0$  when  $x \neq y$

# Common float representations

- 32-bit float ("single"-precision)
  - ◆ 8-bit exponent and 23-bit mantissa
  - ◆ ~7 digits of decimal precision
- 64-bit float ("double"-precision)
  - ◆ 11-bit exponent and 52-bit mantissa
  - ◆ ~16 digits of decimal precision



# MATRICES AND ARRAYS

# Numeric computing

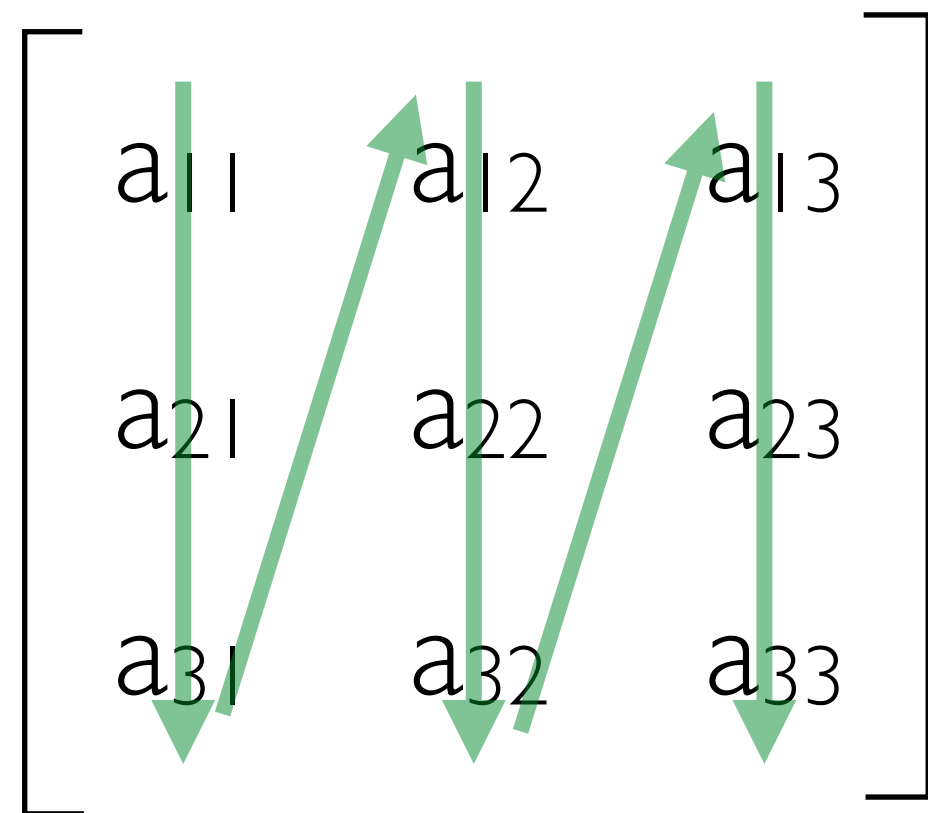
- Need to represent matrices and  $N$ -D arrays
  - ◆ Linear algebra
  - ◆ Machine learning
- Representation must be efficient
  - ◆  $O(1)$  access of numeric elements
  - ◆ Compact storage
  - ◆ Fast traversal
  - ◆ Data size is typically fixed

# Considerations for matrices

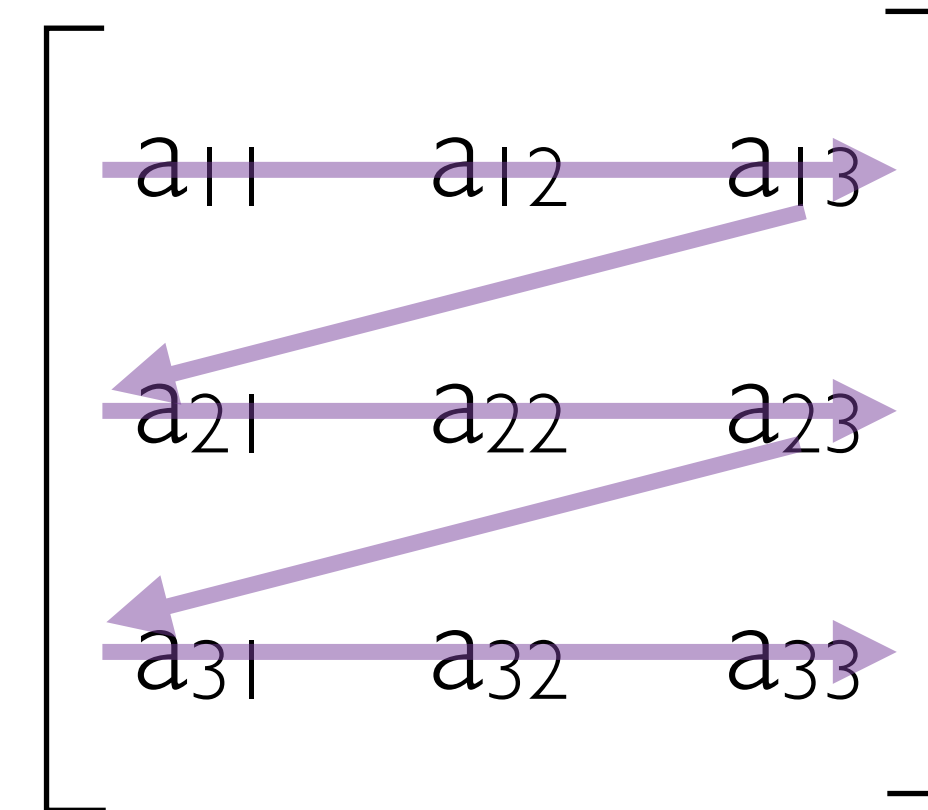
- Patterns of access
  - ◆ *Locality in memory* improves performance
  - ◆ Prefer to store **rows** or **columns** as major dimension?
- Patterns of data
  - ◆ Does the matrix have a **structure**? (e.g., *diagonal*)
  - ◆ How **dense/sparse** is the matrix?
    - Sparse matrices (mostly 0 elements) common in some applications
    - Storing only non-zero elements could save a lot of space

# Storing dense matrices

- Store data as an **array** + **dimensions**
- Column-major vs. row-major order



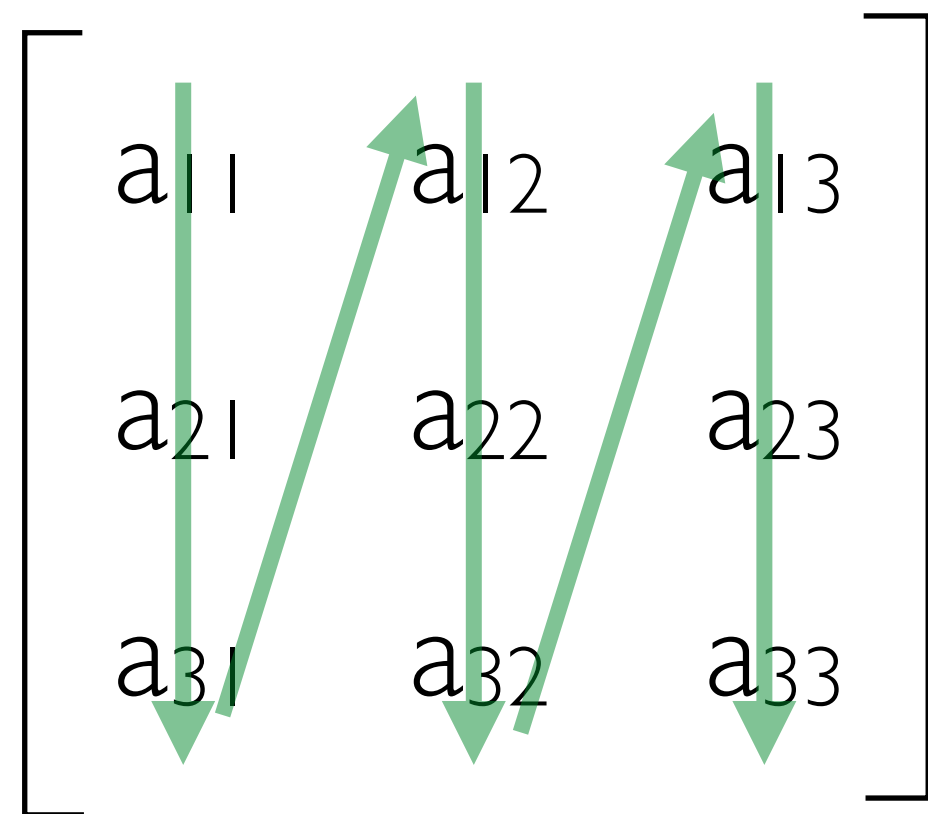
Column-major order



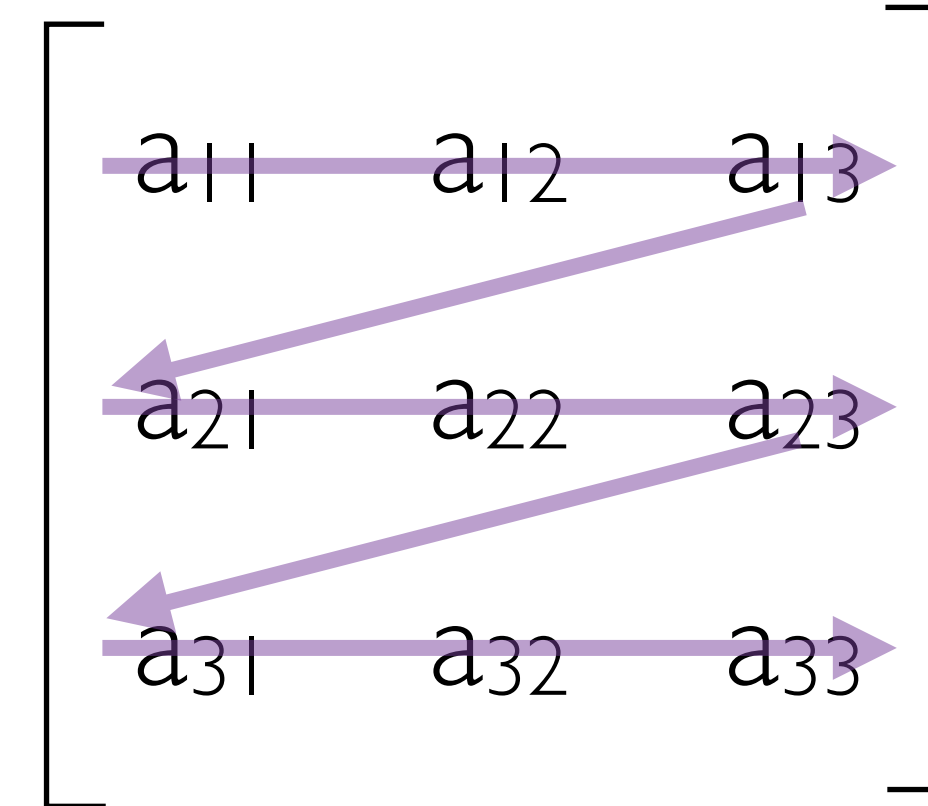
Row-major order

# Storing dense matrices (2)

- Why arrays?
  - ◆ Most efficient for numeric computing
  - ◆ Arrays provide  $O(1)$  access
  - ◆ Arrays provide *locality in memory*



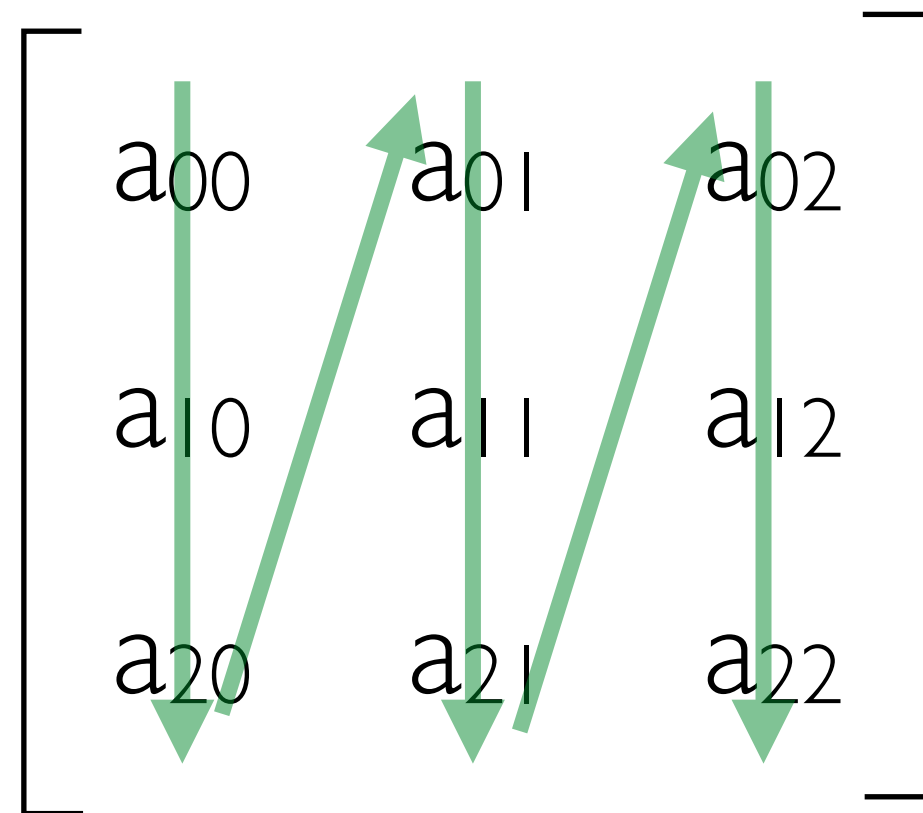
Column-major order



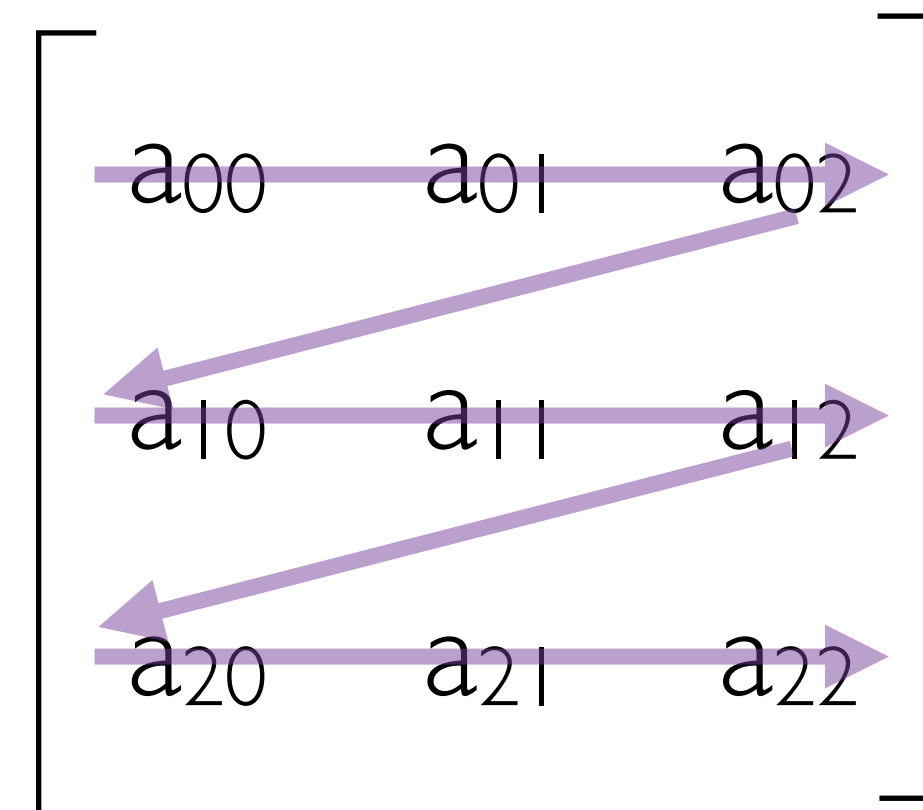
Row-major order

# Accessing dense matrix elements

Column-major order



Row-major order

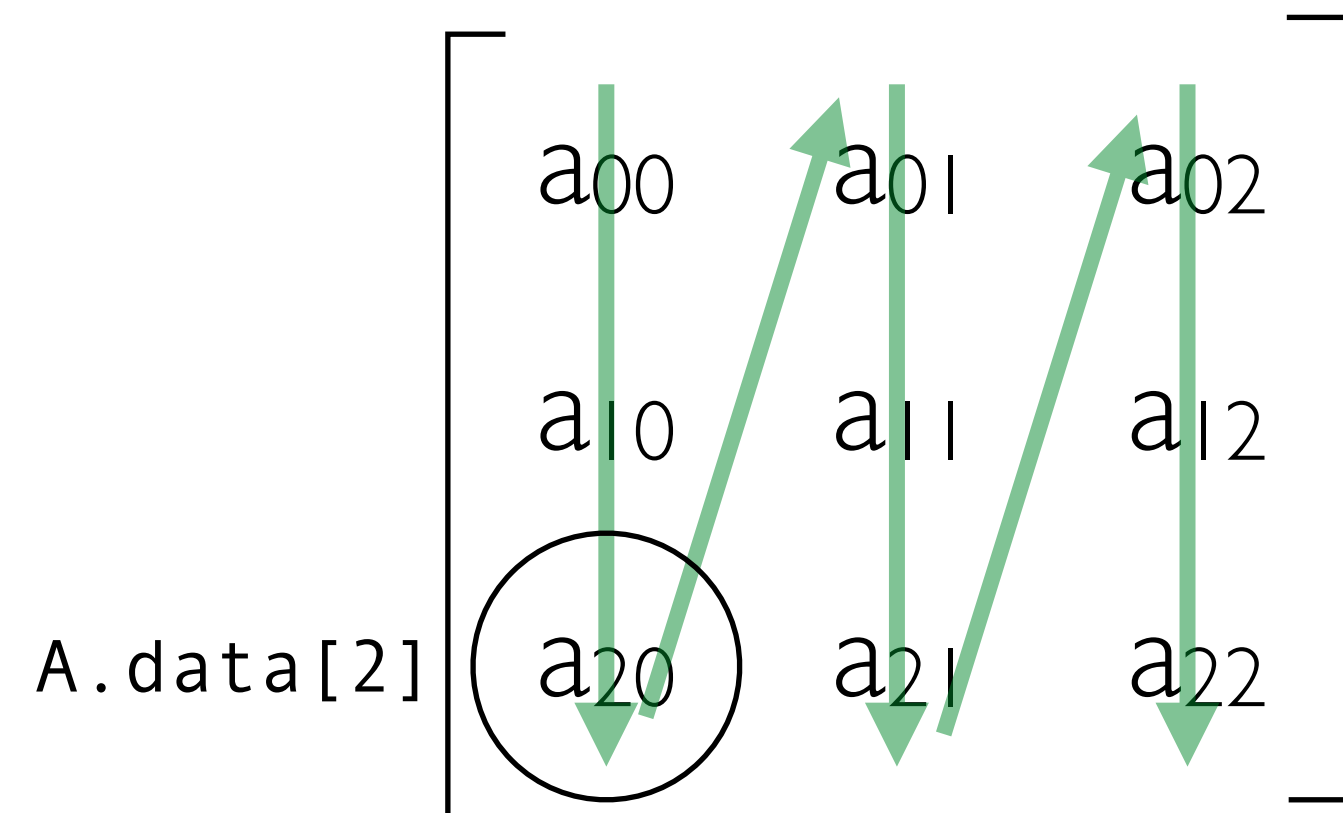


$$A[i,j] = A.data[j * nrow + i]$$

$$A[i,j] = A.data[i * ncol + j]$$

# Accessing dense matrix elements (2)

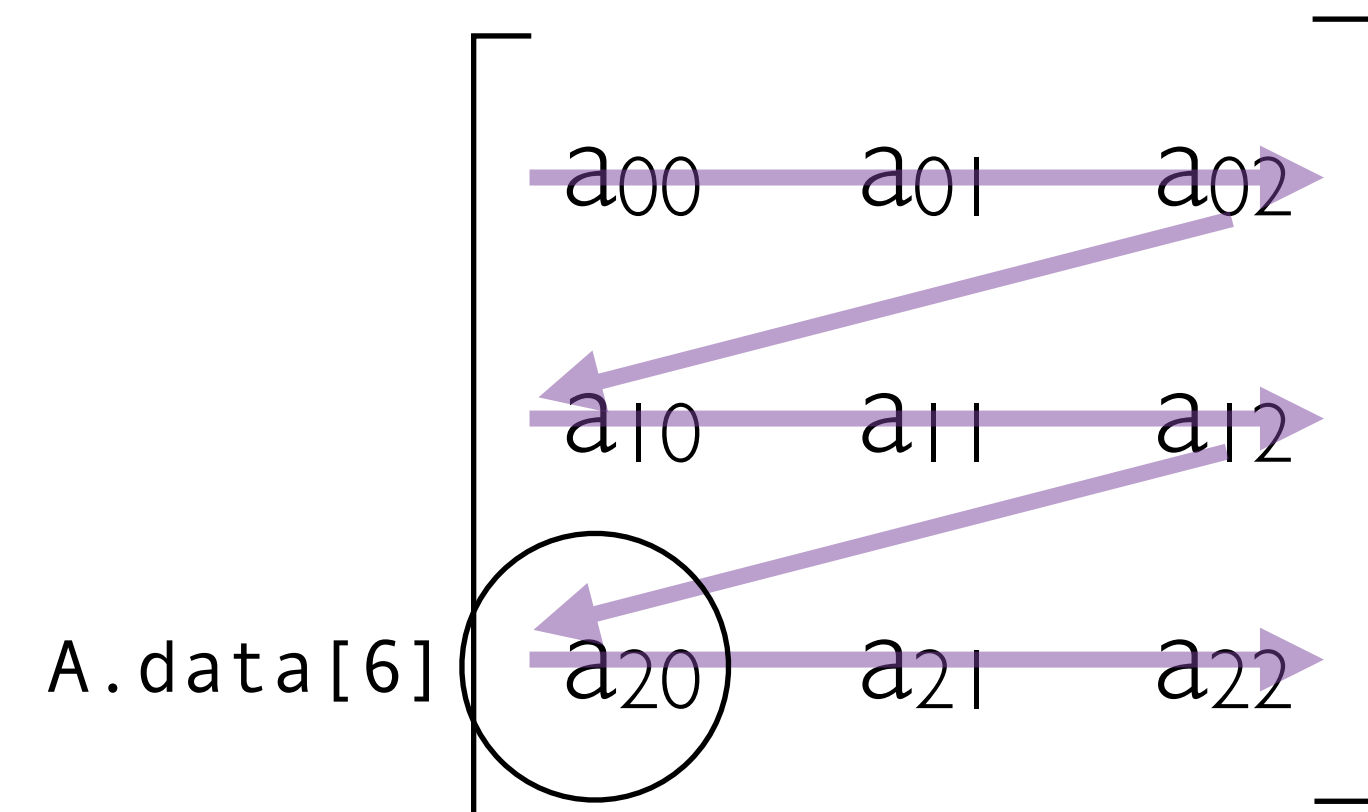
Column-major order



$$A[i, j] = A.data[j * nrow + i]$$

$$\begin{aligned} A[2, 0] &= A.data[0 * 3 + 2] \\ &= A.data[2] \end{aligned}$$

Row-major order



$$A[i, j] = A.data[i * ncol + j]$$

$$\begin{aligned} A[2, 0] &= A.data[2 * 3 + 0] \\ &= A.data[6] \end{aligned}$$

# Considerations for sparse matrices

- Most data elements are 0
  - ◆ E.g., a *document-term matrix* for text modeling
  - ◆ Storing all elements is **not** space efficient
  - ◆ More compact to store *only nonzero elements*
- Sparse compression
  - ◆ How easy to construct/modify?
  - ◆ How easy to access/compute on?



# Sparse matrix representations

- Ease of construction
  - ◆ Dictionary of keys (DOK)
  - ◆ List of lists (LIL)
  - ◆ Coordinate list (COO)
- Ease of computation
  - ◆ Compressed sparse row (CSR)
  - ◆ Compressed sparse column (CSC)

# Sparse matrix representations (2)

- Dictionary of keys
  - ◆ Keys are tuples of coordinates
  - ◆  $(\text{row}, \text{column}) \rightarrow \text{value}$
- List of lists
  - ◆ Store a list of nonzero elements in each row/column
  - ◆  $[(\text{row}, \text{value}), (\text{row}, \text{value}), \text{etc.}]$
- Coordinate list
  - ◆ Store array of coordinate for each element
  - ◆  $(\text{row}, \text{column}, \text{value})$

# Sparse matrix representations (3)

- Compressed sparse row (CSR)
  - ◆ Compress rows
  - ◆ Fast access to whole **rows**
  - ◆ Difficult to construct **columns**
- Compressed sparse column (CSC)
  - ◆ Compress columns
  - ◆ Difficult to construct **rows**
  - ◆ Fast access to whole **columns**

# Compressed sparse row (CSR)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ◆ Data array of non-zero elements (length *nnz*)
  - ◆ Index array of column indices (length *nnz*)
  - ◆ Pointer array of row slices in *index array* (length  $m+1$ )

$$\begin{bmatrix} 0 & 11 & 0 & 22 \\ 33 & 0 & 0 & 44 \\ 0 & 55 & 0 & 0 \end{bmatrix}$$

```
data = [11, 22, 33, 44, 55] # data values
ind  = [ 1,  3,  0,  3,  1] # col indices
ptr  = [ 0,  2,  4,  5]    # row slices
```

*nnz*

# Working with CSR

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ♦ Data array of non-zero elements (length  $nnz$ )
  - ♦ Index array of column indices (length  $nnz$ )
  - ♦ Pointer array of row slices in *index array* (length  $m+1$ )

Row 0

0	11	0	22
33	0	0	44
0	55	0	0

```
data = [11, 22, 33, 44, 55]
ind  = [ 1,  3,  0,  3,  1]
ptr  = [ 0,  2,  4,  5]
```

```
row0_data = data[ptr[0]:ptr[0+1]]
           = [11, 22] # values
row0_ind  = ind[ptr[0]:ptr[0+1]]
           = [ 1,  3] # col indices
```

# Working with CSR (2)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ♦ Data array of non-zero elements (length *nnz*)
  - ♦ Index array of column indices (length *nnz*)
  - ♦ Pointer array of row slices in *index array* (length  $m+1$ )

Row 1

0	11	0	22
33	0	0	44
0	55	0	0

```
data = [11, 22, 33, 44, 55]
ind  = [ 1,  3,  0,  3,  1]
ptr  = [ 0,  2,  4,  5]
```

```
row1_data = data[ptr[1]:ptr[1+1]]
           = [33, 44] # values
row1_ind  = ind[ptr[1]:ptr[1+1]]
           = [ 0,  3] # col indices
```

# Working with CSR (3)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ♦ Data array of non-zero elements (length  $nnz$ )
  - ♦ Index array of column indices (length  $nnz$ )
  - ♦ Pointer array of row slices in *index array* (length  $m+1$ )

Row 2

0	11	0	22
33	0	0	44
0	55	0	0

```
data = [11, 22, 33, 44, 55]
ind  = [ 1,  3,  0,  3,  1]
ptr  = [ 0,  2,  4,  5]
```

```
row2_data = data[ptr[2]:ptr[2+1]]
           = [55] # values
row2_ind  = ind[ptr[2]:ptr[2+1]]
           = [ 1] # col indices
```

# Compressed sparse column (CSC)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ◆ Data array of non-zero elements (length *nnz*)
  - ◆ Index array of row indices (length *nnz*)
  - ◆ Pointer array of column slices in *index array* (length  $n+1$ )

$$\begin{bmatrix} 0 & 11 & 0 & 22 \\ 33 & 0 & 0 & 44 \\ 0 & 55 & 0 & 0 \end{bmatrix}$$

```
data = [33, 11, 55, 22, 44] # data values
ind  = [ 1,  0,  2,  0,  1] # row indices
ptr  = [ 0,  1,  3,  3,  5] # col slices
```

*nnz*



# Working with CSC (2)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ◆ Data array of non-zero elements (length *nnz*)
  - ◆ Index array of row indices (length *nnz*)
  - ◆ Pointer array of column slices in *index array* (length  $n+1$ )

0	11	0	22
33	0	0	44
0	55	0	0

Column 0

```
data = [33, 11, 55, 22, 44]
ind  = [ 1,  0,  2,  0,  1]
ptr  = [ 0,  1,  3,  3,  5]
```

```
col0_data = data[ptr[0]:ptr[0+1]]
           = [33] # values
col0_ind  = ind[ptr[0]:ptr[0+1]]
           = [ 1] # row indices
```

# Working with CSC (3)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ♦ Data array of non-zero elements (length *nnz*)
  - ♦ Index array of row indices (length *nnz*)
  - ♦ Pointer array of column slices in *index array* (length  $n+1$ )

$$\begin{bmatrix} 0 & 11 & 0 & 22 \\ 33 & 0 & 0 & 44 \\ 0 & 55 & 0 & 0 \end{bmatrix}$$

Column 1

```
data = [33, 11, 55, 22, 44]
ind  = [ 1,  0,  2,  0,  1]
ptr  = [ 0,  1,  3,  3,  5]
```

```
col1_data = data[ptr[0]:ptr[0+1]]
           = [11, 22] # values
col1_ind  = ind[ptr[0]:ptr[0+1]]
           = [ 0,  2] # row indices
```

# Working with CSC (4)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ◆ Data array of non-zero elements (length *nnz*)
  - ◆ Index array of row indices (length *nnz*)
  - ◆ Pointer array of column slices in *index array* (length  $n+1$ )

0	11	0	22
33	0	0	44
0	55	0	0

Column 2

```
data = [33, 11, 55, 22, 44]
ind  = [ 1,  0,  2,  0,  1]
ptr  = [ 0,  1,  3,  3,  5]

col2_data = data[ptr[0]:ptr[0+1]]
          = [] # values
col2_ind  = ind[ptr[0]:ptr[0+1]]
          = [] # row indices
```

# Working with CSC (5)

- Consider  $m \times n$  matrix
- Store only ***nnz*** non-zero elements
  - ◆ Data array of non-zero elements (length *nnz*)
  - ◆ Index array of row indices (length *nnz*)
  - ◆ Pointer array of column slices in *index array* (length  $n+1$ )

$$\begin{bmatrix} 0 & 11 & 0 & 22 \\ 33 & 0 & 0 & 44 \\ 0 & 55 & 0 & 0 \end{bmatrix}$$

Column 3

```
data = [33, 11, 55, 22, 44]
ind  = [ 1,  0,  2,  0,  1]
ptr  = [ 0,  1,  3,  3,  5]

col3_data = data[ptr[0]:ptr[0+1]]
          = [22, 44] # values
col3_ind  = ind[ptr[0]:ptr[0+1]]
          = [ 0,  1] # row indices
```

# N-dimensional arrays

- Principles generalize to dense N-D arrays
  - ◆ Store data as a single array (as in data structure)
  - ◆ Store array shape (size in each dimension)
  - ◆ Calculate location of elements on-the-fly (cheap)
- Sparse N-D arrays more challenging
  - ◆ Simple to store in COO format, but poor performance
  - ◆ Which dimension to compress?

# INTRO TO NUMPY

# Numerical Python

- NumPy provides efficient matrices and arrays
  - ◆ *ndarray* implements N-dimensional arrays
  - ◆ Attribute **shape** gives the dimensions
  - ◆ Attribute **dtype** gives data type (*int32*, *float64*, etc.)
- Sparse matrices also supported
  - ◆ **csr\_matrix** for compressed sparse row matrices
  - ◆ **csc\_matrix** for compressed sparse column matrices

# Matrices in NumPy

- Default to *row-major* order
  - ◆ Can be changed with **order** attribute
  - ◆ Row-major is "C" or C-style
  - ◆ Column-major is "F" or Fortran-style
- Specify **shape** and **dtype**
  - ◆ Matrices/arrays can be *reshaped* on demand
  - ◆ All elements are same data type



# Integer array

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.int32)
```

```
In : A
```

```
Out:
```

```
array([[1, 2],  
       [3, 4]], dtype=int32)
```

# Float array

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float32)
```

```
In : A
```

```
Out:
```

```
array([[1., 2.],  
       [3., 4.]], dtype=float32)
```

# Scalar addition

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float64)
```

```
In : 100 + A
```

```
Out:
```

```
array([[101., 102.],  
       [103., 104.]], dtype=float32)
```

# Scalar multiplication

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float64)
```

```
In : 100 * A
```

```
Out:
```

```
array([[100., 200.],  
       [300., 400.]], dtype=float32)
```

# Unary operations

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float64)
```

```
In : np.log(A + 1)
```

```
Out:
```

```
array([[0.6931472, 1.0986123],  
       [1.3862944, 1.609438 ]], dtype=float32)
```

# Elementwise matrix addition

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float64)
```

```
In : A + A
```

```
Out:
```

```
array([[2., 4.],  
       [6., 8.]], dtype=float32)
```

# Matrix multiplication

```
In : import numpy as np
```

```
In : A = np.array([[1, 2], [3, 4]], dtype=np.float64)
```

```
In : A.dot(A)
```

```
Out:
```

```
array([[ 7., 10.],  
       [15., 22.]], dtype=float32)
```

# Slicing a matrix

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B[:, :]
```

```
Out:
```

```
array([[ 0.,  1.,  2.,  3.],  
       [ 4.,  5.,  6.,  7.],  
       [ 8.,  9., 10., 11.],  
       [12., 13., 14., 15.]])
```



## Slicing a matrix (2)

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B[0, :]
```

```
Out:
```

```
array([ 0.,  1.,  2.,  3.])
```

## Slicing a matrix (3)

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B[:,0]
```

```
Out:
```

```
array([ 0.,  4.,  8., 16.])
```

## Slicing a matrix (4)

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B[:3, :3]
```

```
Out:
```

```
array([[ 0.,  1.,  2.],  
       [ 4.,  5.,  6.],  
       [ 8.,  9., 10.]])
```

# "Broadcasting" in NumPy

- Operations expect matrices with same shape
- **Broadcasting** relaxes this constraint
- Dimensions are *compatible* if:
  - ◆ They are equal, or
  - ◆ One of them is 1
- "Broadcast" smaller matrix over larger one

# "Broadcasting" in NumPy

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \end{bmatrix} - \begin{bmatrix} 6 & 7 & 8 & 9 \end{bmatrix}$$

→

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \end{bmatrix} - \begin{bmatrix} 6 & 7 & 8 & 9 \\ 6 & 7 & 8 & 9 \\ 6 & 7 & 8 & 9 \\ 6 & 7 & 8 & 9 \end{bmatrix}$$

## "Broadcasting" in NumPy (2)

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \end{bmatrix} - \begin{bmatrix} 1.5 \\ 5.5 \\ 9.5 \\ 13.5 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \\ 12 & 13 & 14 & 15 \end{bmatrix} - \begin{bmatrix} 1.5 & 1.5 & 1.5 & 1.5 \\ 5.5 & 5.5 & 5.5 & 5.5 \\ 9.5 & 9.5 & 9.5 & 9.5 \\ 13.5 & 13.5 & 13.5 & 13.5 \end{bmatrix}$$

# Summarization and "broadcasting"

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B
```

```
Out:
```

```
array([[ 0.,  1.,  2.,  3.],
       [ 4.,  5.,  6.,  7.],
       [ 8.,  9., 10., 11.],
       [12., 13., 14., 15.]])
```

```
In : B - B.mean(0) # [6., 7., 8., 9.]
```

```
Out:
```

```
array([[ -6.,  -6.,  -6.,  -6.],
       [ -2.,  -2.,  -2.,  -2.],
       [  2.,   2.,   2.,   2.],
       [  6.,   6.,   6.,   6.]])
```

# Summarization and "broadcasting"

```
In : B = np.array(np.arange(16), dtype=np.float64)
```

```
In : B.shape = (4, 4)
```

```
In : B
```

```
Out:
```

```
array([[ 0.,  1.,  2.,  3.],  
       [ 4.,  5.,  6.,  7.],  
       [ 8.,  9., 10., 11.],  
       [12., 13., 14., 15.]])
```

```
In : B - B.mean(1).reshape((4,1)) # [1.5, 5.5, 9.5, 13.5]
```

```
Out:
```

```
array([[ -1.5,  -0.5,   0.5,   1.5],  
       [ -1.5,  -0.5,   0.5,   1.5],  
       [ -1.5,  -0.5,   0.5,   1.5],  
       [ -1.5,  -0.5,   0.5,   1.5]])
```



# Advanced NumPy

- Random number generation
- Linear algebra
  - ◆ Matrix inversion
  - ◆ Singular value decomposition
  - ◆ Linear equation solver
- Sparse matrices
- Memory-mapped arrays