Tools Seminar

Week 6 - Scientific Computing

Hongzheng Chen

Mar 22, 2020

1

Introduction

Scientific Computation

Mostly involve applied mathematics and computational mathematics

- Quantitative finance (stock)
- Physical simulation (fluid, illumination, cloth $\rightarrow$ CG)
- Computational biology (gene)
- Molecular dynamics (protein)
- Ocean circulation
- Weather/Climate prediction

Scientific Computation

Mostly involve applied mathematics and computational mathematics

- Astronomy (1st black hole photo → digital image processing)

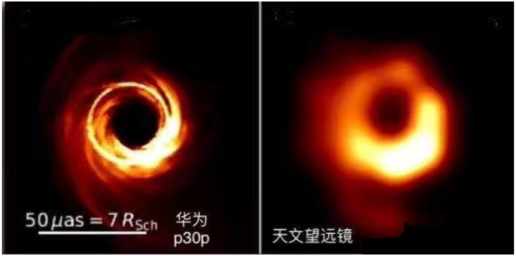


Fig source: Weibo

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} [(f(\mathbf{x}) - \mathbf{y})^{\mathrm{T}} \mathbf{R}^{-1} (f(\mathbf{x}) - \mathbf{y}) + (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \Lambda^{-1} (\mathbf{x} - \boldsymbol{\mu})] \;,$$

where $\hat{\mathbf{x}}$ is the photo needed to be reconstructed.

Scientific Computation

Mostly involve applied mathematics and computational mathematics

- Epidemics (COVID-19 $\to$ SEIR model)

$$\text{Susceptible}(S) \xrightarrow{\beta} \text{Exposed}(E) \xrightarrow{\sigma} \text{Infectious}(I) \xrightarrow{\gamma} \text{Recovered}(R)$$

$$\begin{cases} \frac{\mathrm{d}S}{\mathrm{d}t} = \mu N - \nu S - \frac{\beta SI}{N} \\ \frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\beta SI}{N} - \upsilon E - \sigma E \\ \frac{\mathrm{d}I}{\mathrm{d}t} = \sigma E - \gamma I - \nu I \\ \frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I - \nu R \end{cases}$$

Scientific Computation

Mostly involve applied mathematics and computational mathematics

- Epidemics (COVID-19 $\rightarrow$ SEIR model)

$$\text{Susceptible}(S) \xrightarrow{\beta} \text{Exposed}(E) \xrightarrow{\sigma} \text{Infectious}(I) \xrightarrow{\gamma} \text{Recovered}(R)$$

$$\begin{cases} \frac{\mathrm{d}S}{\mathrm{d}t} = \mu N - \nu S - \frac{\beta S I}{N} \\ \frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\beta S I}{N} - \upsilon E - \sigma E \\ \frac{\mathrm{d}I}{\mathrm{d}t} = \sigma E - \gamma I - \nu I \\ \frac{\mathrm{d}R}{\mathrm{d}t} = \gamma I - \nu R \end{cases}$$

* Supercomputing enables more complex applications to be done

Features of Scientific Computation

Gap between sci. comp. & real computer:

Real Computer		**Sci. Comp.**
discrete	$\Longleftrightarrow$	continuous
integer	$\Longleftrightarrow$	**real numbers**

Features of Scientific Computation

Gap between sci. comp. & real computer:

Real Computer		**Sci. Comp.**
discrete	$\Longleftrightarrow$	continuous
integer	$\Longleftrightarrow$	**real numbers**

IEEE 754 binary floating point standard

$$(-1)^s \times m \times 2^{e-127}$$

Be careful of the **roundoff error**!
Try $5.2 - 5$ in Python

Features of Scientific Computation

Most of them are **matrix computation**! (GEMM)
e.g. gradient descent, convolution, Gauss-Seidel, ...

$$c_{ij} = \sum_k a_{ik} b_{kj}$$

```
for (int i = 0; i < M; i++)
    for (int j = 0; j < N; j++)
        for (int k = 0; k < K; k++)
            C[i][j] += A[i][k] * B[k][j];
```

Features of Scientific Computation

Most of them are **matrix computation**! (GEMM)
e.g. gradient descent, convolution, Gauss-Seidel, ...

$$c_{ij} = \sum_k a_{ik} b_{kj}$$

```
for (int i = 0; i < M; i++)
    for (int j = 0; j < N; j++)
        for (int k = 0; k < K; k++)
            C[i][j] += A[i][k] * B[k][j];
```

Time complexity: $O(n^3)$, is it true?

Features of Scientific Computation

Most of them are **matrix computation**! (GEMM)
e.g. gradient descent, convolution, Gauss-Seidel, ...

$$c_{ij} = \sum_k a_{ik} b_{kj}$$

```
for (int i = 0; i < M; i++)
    for (int j = 0; j < N; j++)
        for (int k = 0; k < K; k++)
            C[i][j] += A[i][k] * B[k][j];
```

Time complexity: $O(n^3)$, is it true?
Optimistically regard the memory as plain, but ...

Memory Hierarchy

Recommend to read CSAPP!

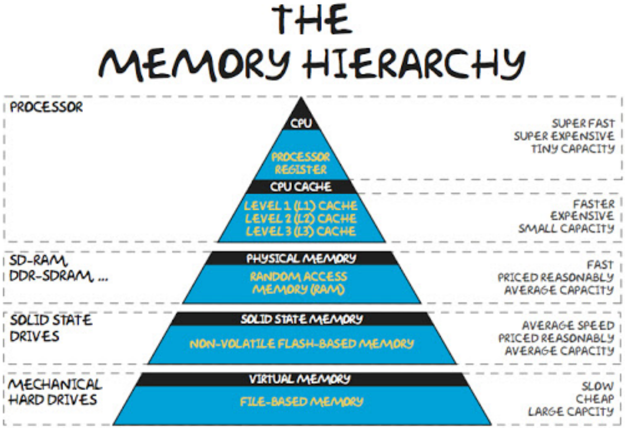
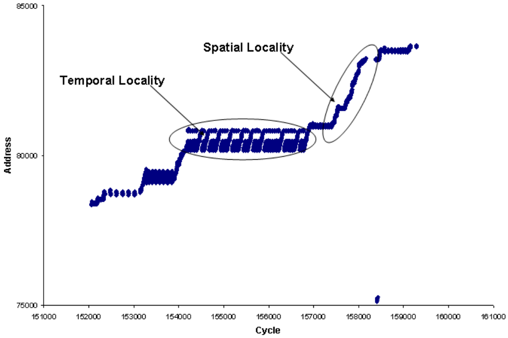


Fig source: http://computerscience.chemeketa.edu/cs160Reader/ComputerArchitecture/MemoryHeirarchy.html

Temporal & Spatial Locality

Recommend to read CSAPP!




```
int sum = 0;
for (int i = 0; i < 10; ++i)
    sum = sum + a[i];
```

Fig source:
https://stackoverflow.com/a/49325155

Back to GEMM

You should know how to store a 2D array in computer memory

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

- Row-major: `{{1,2},{3,4}}` (C/C++)
- Column-major: `{{1,3},{2,4}}` (Matlab)

Back to GEMM

```
for (int i = 0; i < M; i++)
    for (int j = 0; j < N; j++)
        for (int k = 0; k < K; k++)
            C[i][j] += A[i][k] * B[k][j];
```

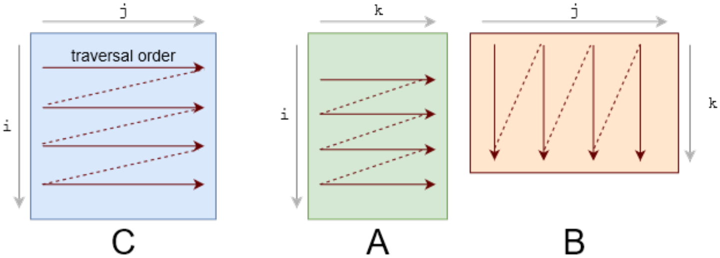


Fig source: Sahnimanas

Back to GEMM

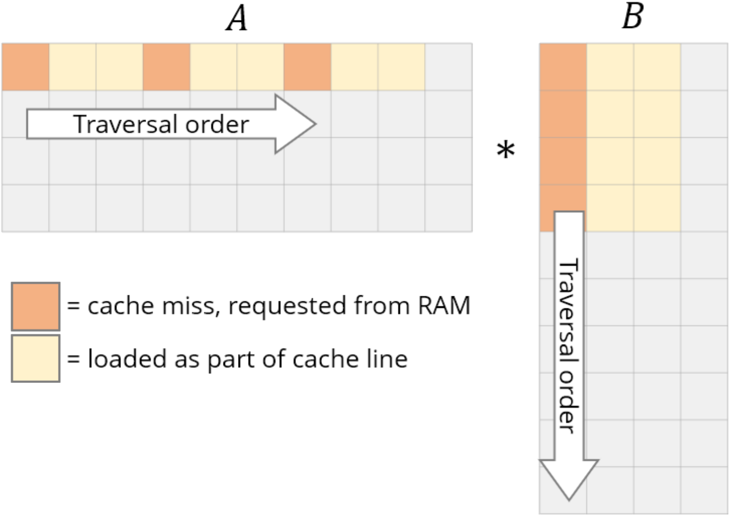


Fig source: Sahnimanas

Back to GEMM

```
for (int i = 0; i < M; i++)
    for (int k = 0; k < K; k++) // reordering
        for (int j = 0; j < N; j++)
            C[i][j] += A[i][k] * B[k][j];
```

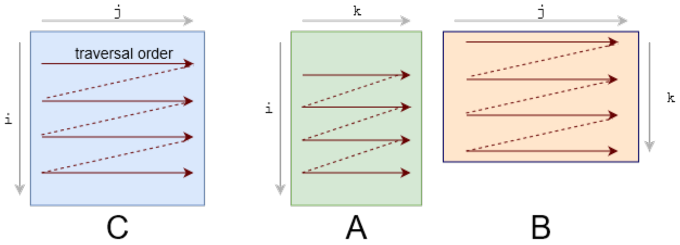


Fig source: Sahnimanas

Data organization greatly affects performance, more than 10x speedup!!!

Scientific Computation Requirements

- Calculus
- Linear Algebra
- Differential Equations (pde / ode)
- Convex Optimization
- Numerical Computing
- Computer System & Architecture
- Parallel Computing
- ...

Scientific Computation Requirements

- Calculus
- Linear Algebra
- Differential Equations (pde / ode)
- Convex Optimization
- Numerical Computing
- Computer System & Architecture
- Parallel Computing
- $\cdots$

Thankfully, we have lots of tools to support sci. comp.

2

Package Management

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1
6. Successfully compiled but the package not found, go back to 2

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1
6. Successfully compiled but the package not found, go back to 2
7. Run the package but get runtime error, go back to 1

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1
6. Successfully compiled but the package not found, go back to 2
7. Run the package but get runtime error, go back to 1
8. ...

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1
6. Successfully compiled but the package not found, go back to 2
7. Run the package but get runtime error, go back to 1
8. ...

Why we need package management?

Installing third-party library for C/C++ is very awkward (boost, OpenGL, ...)

1. Download source code with magic version from some unknown webpages
2. Put the code in some system folder that is hard to find
3. Compile the library
4. If gcc/make version not correct, go back to 1
5. If dependency files not found, go back to 1
6. Successfully compiled but the package not found, go back to 2
7. Run the package but get runtime error, go back to 1
8. ...

Thus, we need tools to help us **build, manage, upgrade, remove** different kinds of packages

Package Management

Fortunately, Python has powerful package management tools!

- Windows: Anaconda (conda)
  - The complete data science platform
  - If you want to use your own GPU for deep learning in the future, you should install
  - Remember to change the mirror to Tsinghua, or downloading will be very slow
- Linux: pip (The Python Package Installer)
  - Be careful of your Python version (2 or 3)
  - `sudo apt install python-pip`
  - `sudo apt install python3-venv python3-pip`
  - `pip3 -V`

Package Management

- `pip install ...`
- `pip install --upgrade ...`
- `pip uninstall ...`
- `pip list`

Environment Management

If you need to regularly change Python version, please create a virtual environment!

`pip3 install virtualenv`

- `which python3`
- `virtualenv -p /usr/bin/python3 mypy3`
- `source mypy3/bin/activate`
  - Then you can directly call Python 3 by `python`
- `deactivate`

conda has inherent environment management tool:

- `conda create -n your_env_name python=your_py_version`
- `activate env_name`
- `deactivate`

Environment Management

pipreqs: Automatically generate python dependencies

- `pip3 install pipreqs`
- `pipreqs /<your_project_path>/`
- `pip3 install -r requirements.txt`

Jupyter Notebook

Jupyter notebook: A extremely powerful web-based interactive interface

- `pip3 install notebook`
- `jupyter notebook`
  - You should first `cd` to the folder you want to open
- Code, data, figure, notes (Markdown)
- Also valid on Github and VS Code
- Next-generation notebook: Jupyter Lab

3

SciPy

SciPy

SciPy: a Python-based ecosystem of open-source software for mathematics, science, and engineering

- NumPy: Base N-dimensional array package
- SciPy library: Fundamental library for scientific computing (FFT, signal, opt, ...)
- Matplotlib: Comprehensive 2-D plotting
- IPython: Enhanced interactive console
- SymPy: Symbolic mathematics
- pandas: Data structures & analysis

* Anaconda must contain scipy package

For Linux, install by `pip3 install scipy`

Numpy

Numpy: `pip3 install numpy`

- A powerful N-dimensional array object
- Sophisticated (broadcasting) functions
- Tools for integrating C/C++ and Fortran code (core part of numpy is written in C)
  - Integrated with Intel Math Kernel Library (MKL), thus is super fast!
- Useful linear algebra, Fourier transform, and random number capabilities
- Indexing, slicing, and iterating functions the same way as in Python

Tutorial:
https://docs.scipy.org/doc/numpy/user/quickstart.html

The Basics

`import numpy as np`

- `np.array([[1,2,3],[4,5,6]])`
- `a.shape`, `a.size`, `a.ndim`
  - Be careful of the shape of `np.array([1,2,3])`
  - Differentiate between `(3,)` and `(3,1)`
- `a.dtype`
  - Python is strong-typed
  - `a.astype(np.float64)`
- `a.reshape((3,2))`
  - Input a tuple! Not transpose! Return a new array!
  - Distinguish with `a.T`
  - `a.resize` is inplace

Array Creation

- `np.zeros((3,4))`
- `np.ones((3,4))`
- `np.arange(1,10,1)` $[a, b)$
- `np.linspace(0,1,10)`
- `np.random.random((3,4))`

Stacking

- `np.column_stack((a,b))`, `np.hstack`
- `np.row_stack((a,b))`, `np.vstack`

Basic Operations

Arithmetic operations are **element-wise** if both are arrays of same size!

- `+,-,*,/,**`
- `<,>,==`

Broadcasting

Broadcasting rules: Examine if two dimensions are compatible

- they are equal, or
- one of them is 1

```
Image  (3d array): 256 x 256 x 3
Scale  (1d array):             3
Result (3d array): 256 x 256 x 3

A      (2d array): 5 x 4
B      (1d array):     1
Result (2d array): 5 x 4

A      (4d array): 8 x 1 x 6 x 1
B      (3d array):     7 x 1 x 5
Result (4d array): 8 x 7 x 6 x 5
```

- `+,-,*,/,**    <,>,==`
- `np.sin`, `np.exp`, `np.sqrt`

Matrix Product

Notice: $*$ for numpy array is the element-wise or **Hadamard product**, denoted as

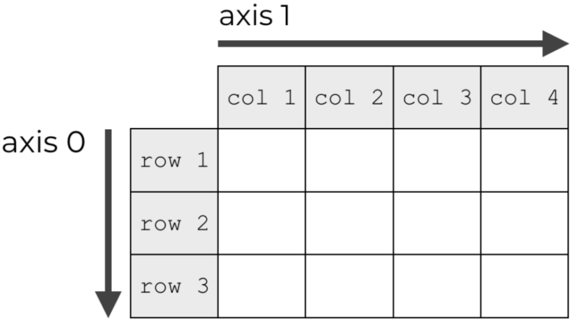
$$(A \circ B)_{ij} = (A)_{ij}(B)_{ij}$$

The true **matrix product** can be called as shown below

```
>>> a @ b                         # matrix product
>>> a.dot(b)                      # another matrix product
>>> c = np.matrix([[1,2],[3,4]])
>>> c * d                         # also matrix product
```

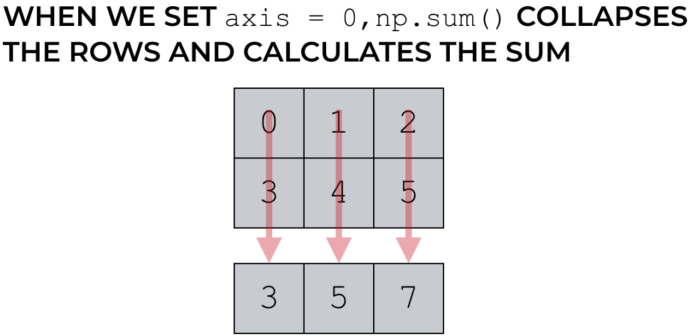
Clustering Functions

Axis: Extremely important! Ref:
https://www.sharpsightlabs.com/blog/numpy-axes-explained/



Clustering Functions

Axis: Extremely important! Ref: https://www.sharpsightlabs.com/blog/numpy-axes-explained/



`np.sum(a,axis=0)`, `np.mean`, `np.min`, `np.max`, `F.softmax` (pytorch)

Indexing & Slicing

Basic indexing & Slicing:

- `a[:]`, `a[:6:2]`, `a[::-1]`
- `b[ : , 1:3]`, `b[ : , 2]`

Fancy indexing: Use array of indices

- `a[b]`
- `a[a>2]`
- Even assignment is allowed, like `a[a>2] = 0`

Linear Algebra

- `np.eye`
- `a.transpose`
- `np.linalg.inv(a)`
- `np.linalg.trace(a)`
- `np.linalg.solve(a,y)`
- `np.linalg.eig(a)`

More About Product Summation

`np.einsum(equation, *operands)` (Einstein summation convention)

Transpose	$c_{ij} = a_{ji}$	$c_{ij} = a_{ji}$	`ij->ji`
Dot product	$c = \sum_i a_i b_i$		
Outer product	$c_{ij} = a_i b_j$		
Summation	$c_i = \sum_j a_{ij}$		
Trace	$c = \sum_i a_{ii}$		
Hadamard product	$c_{ij} = a_{ij} b_{ij}$		
Matrix-vector product	$c_i = \sum_j A_{ij} b_j$	$c_i = a_{ij} b_j$	`ij,j->i`
Matrix-matrix product	$c_{ik} = \sum_j a_{ij} b_{jk}$		
Tensor product	$c_{kl} = \sum_i \sum_j a_{ijk} b_{ijl}$		

More About Product Summation

`np.einsum(equation, *operands)` (Einstein summation convention)

Transpose	$c_{ij} = a_{ji}$	$c_{ij} = a_{ji}$	`ij->ji`
Dot product	$c = \sum_i a_i b_i$	$c = a_i b_i$	`i,i->` or `i,i`
Outer product	$c_{ij} = a_i b_j$	$c_{ij} = a_i b_j$	`i,j->ij`
Summation	$c_i = \sum_j a_{ij}$	$c_i = a_{ij}$	`ij->i`
Trace	$c = \sum_i a_{ii}$	$c = a_{ii}$	`ii`
Hadamard product	$c_{ij} = a_{ij} b_{ij}$	$c_{ij} = a_{ij} b_{ij}$	`ij,ij->ij`
Matrix-vector product	$c_i = \sum_j A_{ij} b_j$	$c_i = a_{ij} b_j$	`ij,j->i`
Matrix-matrix product	$c_{ik} = \sum_j a_{ij} b_{jk}$	$c_{ik} = a_{ij} b_{jk}$	`ij,jk->ik`
Tensor product	$c_{kl} = \sum_i \sum_j a_{ijk} b_{ijl}$	$c_{kl} = a_{ijk} b_{ijl}$	`ijk,ijl->kl`

Easy to write, and very efficient!
Ref:

- https://stackoverflow.com/a/33641428
- https://zhuanlan.zhihu.com/p/71639781

Some hints for efficient implementation

- Do NOT use naive Python loop!
- Think of matrix/tensor representation instead of scalar
- Use inherent matrix operators

4

Math Softwares

Math Softwares for Scientific Computing

3M in Mathematics

- Matlab: Numeric computation, C-like grammar, efficient for engineering
- Mathematica: Symbolic computation, Wolfram Language, fantastic visualization effect, rich documentation (highly recommended!)
- Maple: Symbolic computation, few people use now (DONT USE!)

* Many computation tasks can be done by Python/Julia now, and the importance of Matlab is sharpen.

Installation

- Matlab R2019b (student version)
  - Use the campus Internet to download
- Mathematica 12.0
  - $50 for student version
  - Online version: https://www.wolframcloud.com/

Basic Usage

Similar to Python's interactive window, but with much more powerful functional support

- Type in display mode
  - Ctrl+2: square root
  - Ctrl+4: superscript
  - Ctrl+/: fraction
- `Solve[equ,var]`
  - == represents equal, = means assignment
  - Symbolic, high-order, parameter, equation systems
  - `NSolve` for numerical results
  - `Reduce` for constrained solutions
- `D[f]`, `Integral[f,var]`, `Integral[f,{var,x_min,y_min}]`
  - High-order, multiple variables
  - Display the steps

Basic Usage

- `Sum[exp,var]`
- `Simplify[exp]`
- `Plot[f,{x,x_min,x_max}]`
  - `ContourPlot`, `ListLinePlot`, `ParametricPlot`
- You can even copy the formulas as LaTeX
- The most powerful thing: Enormous database!
- Explore more in
  - https://www.wolfram.com/mathematica/
  - https://www.zhihu.com/question/27834147

*** Make the best of the manual!**

5

Summary

Summary

- Introduction
- Package management: pip, Anaconda
- Useful tools: virtualenv, pipreqs, jupyter notebook
- Numpy: fancy indexing, broadcasting, linear algebra
- Math software: Matlab, Mathematica

* We won't cover Python's OOP & stl in the seminar, but please be familiar with it