EL2310 – Scientific Programming

Lecture 1: Introduction

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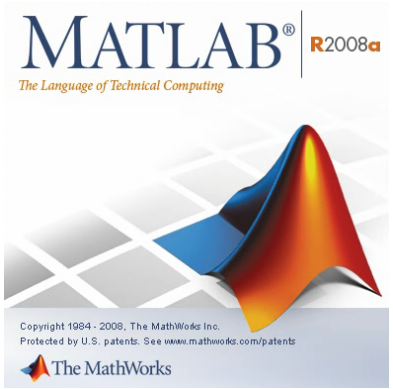
Overview

Welcome

- Lecturer: Yasemin Bekiroglu (yaseminb@kth.se)
- Course overview
  - 17 lectures (2 x 45 min. each)
  - presentations
  - 3 project assignments
- 7.5 credits
- Grade: Pass / Fail

Content

- Part I - MATLAB
- Part II - C
- Part III - C++



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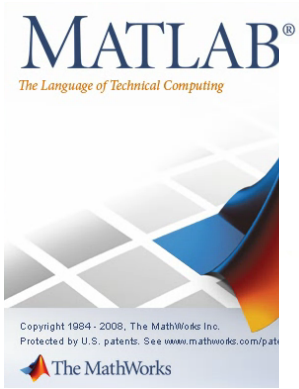

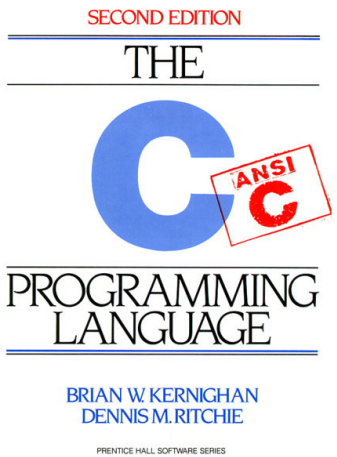

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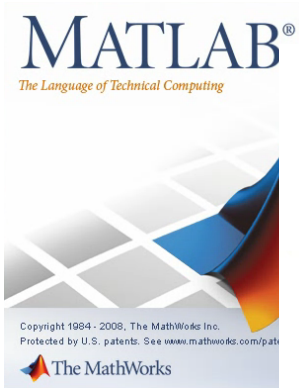
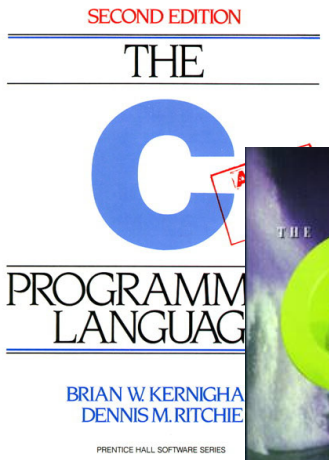
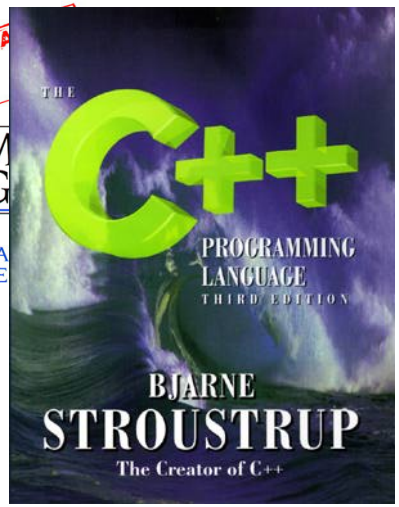






What is your motivation and background?

- What programming languages have you heard of/used?
- What are likely usage scenarios for scientific programming in your future?

Harness the power!

- Today a Sony PS4 has a peak performance of 1.84 TFLOPS (1 TFLOP = 10^{12} FLOPS). 1 GFLOP (1 GFLOP = 10^{9} FLOPS) costs 0.22 USD today and costed 8.3 trillion USD in 1961 in inflation adjusted 2012 dollars (see the WIKIPEDIA articles on Moore's law and FLOPS).
- We are on course for a supercomputer with a performance of 10^{18} FLOPS.
- Your cellphone has more power than a supercomputer a few decades ago.
- Computing is a facilitator in modern science and business.

Motivation for the Course

- Programming is a key competence for todays engineers
- Some courses depend on you being able to program
  - Programming will be a **tool** not subject of study.
- Starts with MATLAB:
  - Scientific computing
  - Tailored for Master students

Motivation for the Course

- We will investigate several tools for solving scientific/engineering problems
- The key question is to determine the appropriate tool in order to efficiently solve a task.

Why MATLAB?

- MATLAB is a tool for interactive numerical computations
- Focus on rapid prototyping with complex computations
- Extensive code-base for:
  - control
  - signal processing
  - optimization
  - image processing
- We can easily visualize and analyze data
- Used in many engineering companies, and extensively at KTH

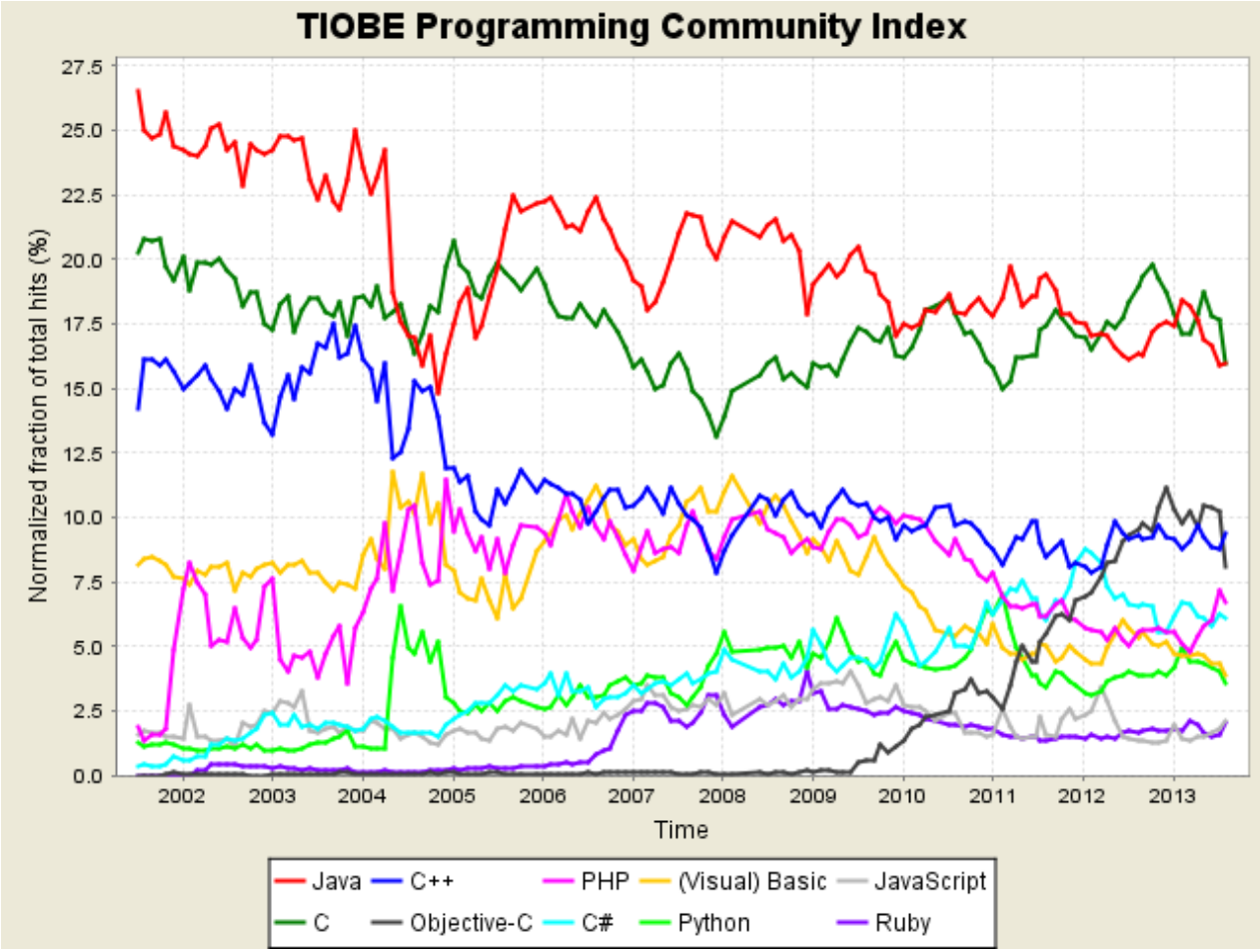
Why C?

- Most often used “low-level” language
- Allows “closer” interaction with hardware
- Used for system programming: OS, embedded systems
- Examples: Linux Kernel, MATLAB
- Many languages borrow from C:
  C#, Go, Java, JavaScript, Perl, PHP
- Free compilers available for most architectures/hardware

Why C++?

- Used extensively in industry and academia
- Intermediate-level programming language
- Many benefits of C with enhancements and new programming patterns
- Real-time applications mostly use C/C++
- The language of robotics (ROS, PCL)!
- Constantly developed and standardized: C++11
- Free compilers available for most architectures

Programming Language Popularity



Programming Language Popularity

Position Aug 2013	Position Aug 2012	Delta in Position	Programming Language	Ratings Aug 2013	Delta Aug 2012	Status
1	2	↑	Java	15.978%	-0.37%	A
2	1	↓	C	15.974%	-2.96%	A
3	4	↑	C++	9.371%	+0.04%	A
4	3	↓	Objective-C	8.082%	-1.46%	A
5	6	↑	PHP	6.694%	+1.17%	A
6	5	↓	C#	6.117%	-0.47%	A
7	7	=	(Visual) Basic	3.873%	-1.46%	A
8	8	=	Python	3.603%	-0.27%	A
9	11	↑↑	JavaScript	2.093%	+0.73%	A
10	10	=	Ruby	2.067%	+0.38%	A
11	9	↓↓	Perl	2.041%	-0.23%	A
12	15	↑↑↑	Transact-SQL	1.393%	+0.54%	A
13	14	↑	Visual Basic .NET	1.320%	+0.44%	A
14	12	↓↓	Delphi/Object Pascal	0.918%	-0.09%	A–
15	20	↑↑↑↑↑	MATLAB	0.841%	+0.31%	A–

MATLAB vs. C/C++

MATLAB:

- Interpreted (executed by interpreter program)
- \+ Fast developing time
- \- Slow run-time in certain cases
- \+ Portable
- Better for scientific code

C/C++:

- Compiled (and executed directly by CPU)
- \- Slower developing time
- \+ Possible to write fast programs
- \= Standard libraries are portable
- Better for system programming

Goals

- Have an understanding for basic concepts in programming
- Be able to read, process and display data in MATLAB
- Solve problems and implement algorithms in MATLAB
- Know how to use MATLAB in other courses

Goals

- Be able to read and process data in programs written in C and C++
- Solve problems and implement algorithms in C and C++
- Be able to read and understand existing code
- Understanding the importance of writing readable code
- Know which tools to use to solve various scientific problems

Course Organization

- 3 parts - one for each language, i.e. MATLAB, C and C++
- Lectures (homeworks)
- Presentations
- Projects
- Help sessions

Presentations

- Walk-through of simple problems
- Each student will have to take part in a presentation
- Goals:
  - Become familiar with the computing environment
  - Prepare for the projects
  - Come up with questions before project deadline
- Co-operation is encouraged
- Ask questions during help sessions, lecture break

Projects

- Larger scientific problems to solve
- So, you will learn something more than just programming
- The projects should be solved individually
- Graded: pass/fail
- One project exam session for each project
- Project needs to be submitted before a deadline
- To pass the course, pass all three projects

Help Sessions

- One help session before each project deadline
- See schedule for dates
- Do you have laptops?
- Additional Q/A sessions during lecture breaks

Course Homepage

- `http://www.csc.kth.se/~yaseminb/el2310.html`
- General course information
- Schedule
- Slides from the lectures
- Course materials

Bilda

- Online learning tool `http://bilda.kth.se`
- News and announcements
- Assignment submission
- Questions (do NOT use e-mail)
- Forums and discussions
- Feedback

Literature & Materials

- No course book in the normal sense
- Plenty of good information available online
  - Manuals / Guides / Tutorials
  - Blogs
  - Discussion forums (StackOverflow)
  - Videos (YouTube) / Webinars
  - Use a search engine
- Some will be listed on the course website
- Share valuable resources with each other on **Bilda**.

Focus on Self-studying

- The lectures and labs can show you the basics, but you need to learn to seek programming knowledge and study on your own
- MATLAB is available on "KTH-CD"
  - `http://progdist.ug.kth.se`
- Tools for C/C++ are available with all Linux distributions
  - See course website
- **Strongly** recommended that you use Linux.

Programming Environment

- Matlab has a built-in IDE (Integrated Development Environment)
- We will not use an IDE for C/C++
- For C/C++, the tools are *gcc* (compiler) and an editor (e.g. vim/emacs)
- An IDE “hides” things you should know!

System

- For C/C++ we cannot support all systems
- Free open-source programs (i.e. Linux)
- Environments
  - Own system
  - Virtual Machine through `http://www.virtualbox.org/`
  - CSC Computers
- Your assignments will be checked in Virtual Machine

Registration

If you are registered you should be able to,

- Log in to Bilda `http://bilda.kth.se`
- Have access to the CSC computers.

If not let me know.

Value of Feedback

- The quality of the course depends on your feedback!
- Not only at the end of the course (evaluation), but during the course
- Use **Bilda** as mode of interaction **NOT** email
- This course cannot be tailored for everyone, since your backgrounds vary dramatically

End of Part 0

Acknowledgements

- The course has been developed and improved previously by several people, including Patric Jensfelt, Carl Henrik Ek, Kai Hübner, Andrzej Pronobis and Florian Pokorny.
- The lectures on MATLAB are partially based on material from
  - Mikael Johansson, EE/KTH (course 2E1215)
  - Fredrik Gustavsson, Linköping (course TSRT04)

Part I - Introduction to MATLAB

- MATLAB background
- Basics
- Interactive calculations
- Matrices and vectors

MATLAB Background

- MATLAB = MATrix LABoratory
- Commercialized 1984 by Mathworks
- Heavily extended since then
- A standard tool today
- Array programming language: arrays are fundamental types
- Makes numerical computations easy

Alternatives

- There are alternatives such as
  - *NumPy/IPython - Numerical interactive computations in Python*
  - Octave (free and language mostly compatible with MATLAB)
  - Scilab
  - Matrix-X
- Additional Symbolic complements (using traditional mathematical notation)
  - Maple
  - Mathematica

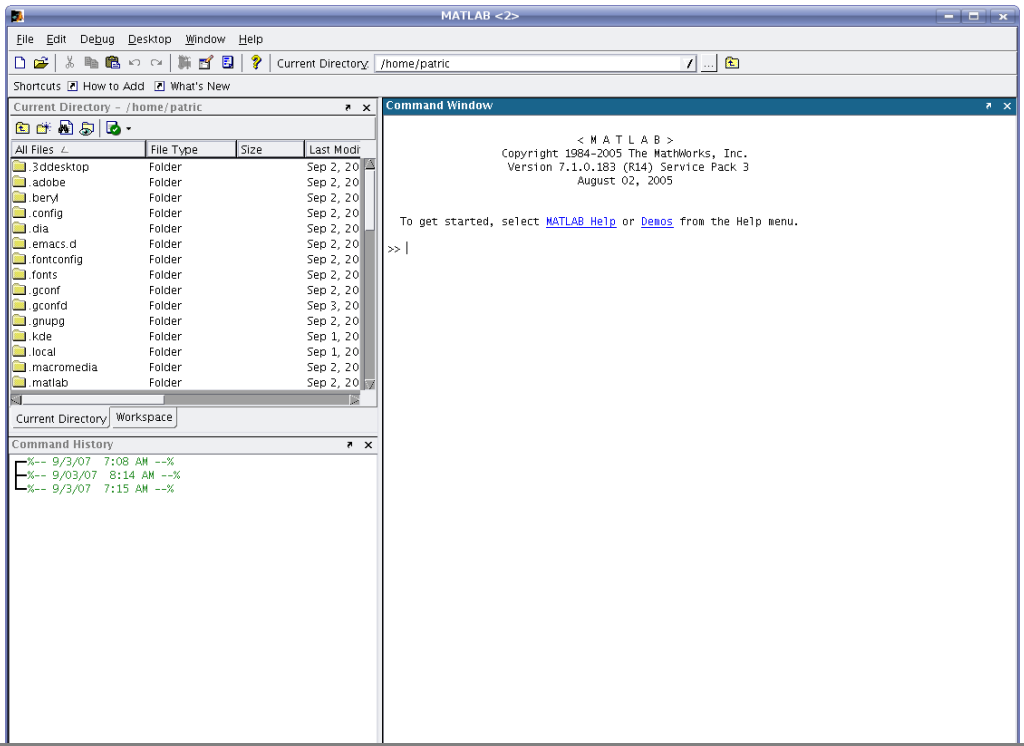
Alternatives

- Matlab/C/C++ can be combined
- You can write highly optimized code in C/C++ and connect it to MATLAB using compiled MEX files.
- Python and other interpreted languages also allow you to do this.

Running MATLAB

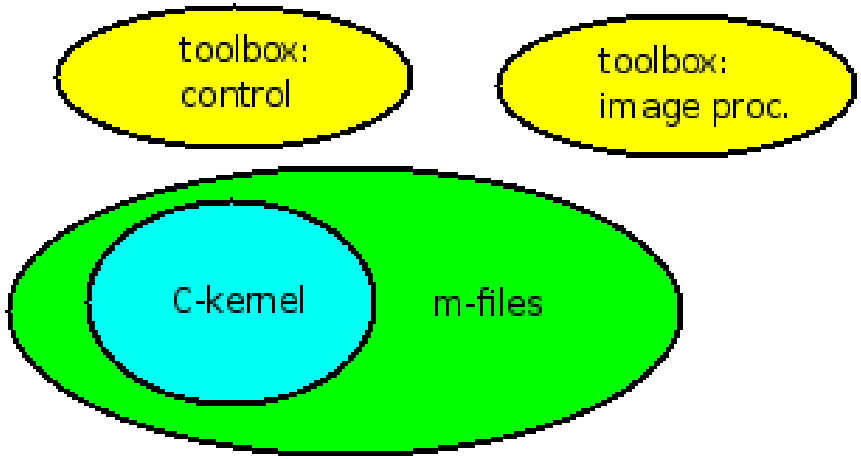
- Available for Windows, Unix/Linux, Mac
- Great introductory video from MathWorks
- You can start with:

  `www.csc.kth.se/~yaseminb/el2310-lab-matlab.pdf`



MATLAB Construction

- Core functionality based on compiled C-routines
- Most functionality given as .m-files
- Grouped into toolboxes
- .m-files
  - contain source code
  - can be copied and altered
  - are platform independent (same on PC, Unix/Linux, Mac)



Command Window vs .m-files

- Code can be entered directly into the command window
  - Using MATLAB in an interactive fashion
- Code can also be stored in .m files
  - Write your program in an .m file
  - Whole program is executed using a single command

Interactive Calculations

- You do not need to declare variables in MATLAB
- It is interactive

```
>> 1+2*3

ans =

     7

>> sin(pi)

ans =

   1.2246e-16

>>
```

Interactive Calculations

- Let's have a look at the IDE

Documentation

- Help with syntax and function definitions

  `>> help <function>`

  Ex: “help sin”
- To look for a function with unknown name

  `>> lookfor <keyword>`
- Advanced hyperlinked help browser

  `>> doc`

  `>> doc <function>`

  Can also be accessed through the “Help” menu item

Variables

- Look at what variables are defined with

  ```
  >> who
  >> whos
  ```

- Clear variables with

  ```
  >> clear [variable(s)]
  ```

- Suppress output with ending ";" (semicolon)

```
>> sin(pi);
>> A = [1 2; 3 4];
>> B = 4;
>> who

Your variables are:

A    B    ans
```

```
>> whos
  Name      Size                    Bytes  Class

  A         2x2                        32  double array
  B         1x1                         8  double array
  ans       1x1                         8  double array

Grand total is 6 elements using 48 bytes

>> clear
>> who
>> whos
```

Loading and Saving Variables

- You can save all variables in memory with
  `>> save <filename>`
- To save some variables do
  `>> save <filename> var1 var2 ... varN`
- You can load them back into memory with
  `>> load <filename>`

Saving Command Window Text

- You can use the function `diary` to record what you are doing
- Allows you to go back and check what commands were issued
- Start the diary with
  `>> diary [filename]` or `>> diary('filename')`
  without the filename argument the diary file will be called "diary"
- To suspend/restart a diary, call:
  `>> diary on` `>> diary off`
- If you call `diary` without an argument you toggle diary on/off

Vectors

- Matrix and vector operations are at the very core of MATLAB
- For speed try to formulate a problem in terms of matrix operations
- Vector $v = [\ 1 \quad 2 \quad 3 \quad 4\ ]$ is defined by

```
>> v=[1 2 3 4];
```

- Vector $w = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$ is defined by

```
>> w=[1; 2; 3; 4];
```

Vectors Cont'd

- Can create a vector with "colon-notation"

```
>> v = start_value:step:end_value
```

- Ex: To create a vector with number 1 3 5 7 you do

```
>> v = 1:2:7
```

- Notice that step can be negative to create for example 7 5 3 1

```
>> v = 7:-2:1
```

Indexing Vectors

- To access a certain value in a vector do
  `>> v(i)`
  where `i` is the index of the value

- Note: All indices start at 1 in MATLAB.

Matrices

- Matrices (2D arrays) are defined similarly
- Matrix $A = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 5 & 6 \end{bmatrix}$ is defined by

```
>> A = [1 2 3; 3 5 6];
```

- Note: MATLAB is case sensitive

Dimensions

- You can check the size of a matrix with `>> size(A)` which will return the number of rows and columns
- You can ask specifically for the number of rows or columns
- To get number of rows

  ```
  >> size(A,1)
  ```

  and number of columns

  ```
  >> size(A,2)
  ```

Matrix Operations

- You can use all common operators with the matrices such as

  ```
  >> C = A + B;
  ```

  or

  ```
  >> C = A * B;
  ```

  assuming that the involved matrices have the right dimensions.
- You can mix scalars and matrices such as

  ```
  >> C = A + 2;
  ```

  in which case the scalar adapts to fit the situation (here it will expand to a matrix of the same size as A with all elements equal to 2).
- Even functions like sin and cos can be applied to matrices in which case they operate on each element.

Matrix Transpose

- To transpose a matrix do

```
>> B = A'
```

- Note that the transpose will conjugate complex entries
- To avoid this use

```
>> B = A.'
```

Indexing Matrices

- Index individual elements with

  `>> A(i,j)`

  where `i` is the row and `j` is the column

```
>> A=[1 4 7;2 5 8; 3 6 9]

A =

     1     4     7
     2     5     8
     3     6     9

>> A(2,3)

ans =

     8
```

Indexing Matrices Cont'd

- Index sub-matrices

```
>> A([1 3],[2 3])
```

```
>> A=[1 4 7;2 5 8; 3 6 9]

A =

     1     4     7
     2     5     8
     3     6     9

>> A([1 3],[2 3])

ans =

     4     7
     6     9
```

Indexing Matrices Cont'd

- Sometimes convenient with single index notation
- Matrix elements ordered column by column

$$A = \begin{bmatrix} a_1 & a_4 & a_7 \\ a_2 & a_5 & a_8 \\ a_3 & a_6 & a_9 \end{bmatrix}$$

that is, $A(n) = a_n$ with the above ordering

```
>> A=[1 4 7;2 5 8; 3 6 9]

A =

     1     4     7
     2     5     8
     3     6     9

>> A(5)

ans =

     5
```

Indexing Matrices Cont'd

- Convert from subscripts (i, j) to linear indices
- Works for multiple (i, j) pairs stored in two arrays

```
>> A=[1 4 7;2 5 8; 3 6 9]

A =

     1     4     7
     2     5     8
     3     6     9

>> subindex = sub2ind(size(A), [1 2 3], [3 2 1])

subindex =

     7     5     3

>> A(subindex)

ans =

     7     5     3
```

Wrap Up

Today:

- Introduction to the Course
- Introduction to MATLAB
- Next time (Wed 13-15, Room V34): Matlab as a Tool

Tasks for next time:

- Log into Bilda, check out course page
- Get and install MATLAB
  `http://progdist.ug.kth.se`
- Bring your laptop next time
- Take a look at the exercises

The First Presentation: PCA

- Explain what Principal Component Analysis (PCA) does, how it works and for what type of problems it is used.
- Implement it, compare your implementation with Matlab's built-in pca function on a dataset with different classes that has a large dimensionality. You can create your own data with multiple classes with random samples or use an already available dataset (from Matlab or another source).

The First Presentation: PCA

- Visualize the data in the new space and observe if data samples from the same classes are close to each other.
- How should we choose the number of eigen vectors to represent data without losing information?
- How can we implement a PCA-based face recognition method? (http://vision.ucsd.edu/content/yale-face-database)

The Second Presentation: Kmeans

- Explain what kmeans clustering algorithm does, how it works and for what type of problems it is used.
- Implement it and apply it on the IRIS dataset (load fisheriris)
- Compare your implementation with Matlab's built-in function. Do you get the same results?
- What are the factors that affect the performance of the algorithm?
- Apply your function to another dataset and evaluate the performance: e.g., kmeansdata.mat from Matlab