Mathematical computing 2023

Teaching Staff of the Course

MATLAB:

Responsible teacher

Prof. Ilkka Tittonen

Assistant

Tom Rindell and Saku Laesvuori

MATHEMATICA:

Responsible teacher

Dr. Pasi Ylä-Oijala

Assistant

Pyry Kiviharju

Practicalities of the course

Lectures and exercises take place in Hall U9 in Undergraduate Centre

- Lectures on Wednesdays at 12:15 – 14:00
- First lecture September 6th, 2023
- Exercises on Fridays at 12:15 – 14:00

The course is done by solving the weekly exercises

- A new topic is introduced every Wednesday and the same topic may be continued on Friday’s exercise class. Solutions of homework problems will be discussed on Friday’s class as well
- The return deadline of exercise solutions is always on Thursday at 21:00

Code of Conduct: Collaboration and group work in learning is encouraged, but

- Copying the homework solutions from others is forbidden
- Everyone prepares their solutions independently

Passing the course

The grading of this course is based on weekly home exercises

- 20 pts/week => total 240 pts
- Minimum criteria for passing is 50% of the max points (120/240) and 30% of the points from both parts (MATLAB and MATHEMATICA)
- **DISCLAIMER:** The final grading is adjusted if necessary
- There is no exam

Contents and Learning goals

- The main learning goal of this course is the **development of one's skills in computational modelling and problem solving in physics and engineering**. BSc level studies in Math, physics and engineering is assumed and some experience in programming. Active participation in this course greatly develops one's **fluency in using Matlab and Mathematica** software which both are general programming tools backed up with extensive mathematical capability.
- **Learning is facilitated by weekly homework problems** which illustrate mathematical and algorithmic approaches in solving tasks which are frequently encountered in studies and research work, but which cannot be solved using only pen and paper. The instruction of the course elaborates the theoretical backgrounds of homework tasks but addresses also mathematical and programming concepts which are relevant for solutions.
- Course topics include e.g. data analysis, linear algebra, applications of mathematical transforms, differential and integral equations. Contents may vary slightly every year to avoid unnecessary repetition and to foster development.
- After the course one should feel comfortable when facing and solving problems encountered in science and engineering disciplines. Typical examples are data analysis, modelling and visualization tasks or programming challenges involving implementation of sophisticated mathematical operations.

Matlab topics

- Week 1: Basic Matlab commands, plotting of data
- Week 2: Data importing, file operations, data analysis
- Week 3: Optimization
- Week 4: Fourier transform and frequency domain analysis
- Week 5: Finite-difference methods
- Week 6: Intro to machine learning

- Week 7: Exam weak, no teaching

Selected studies from previous years:

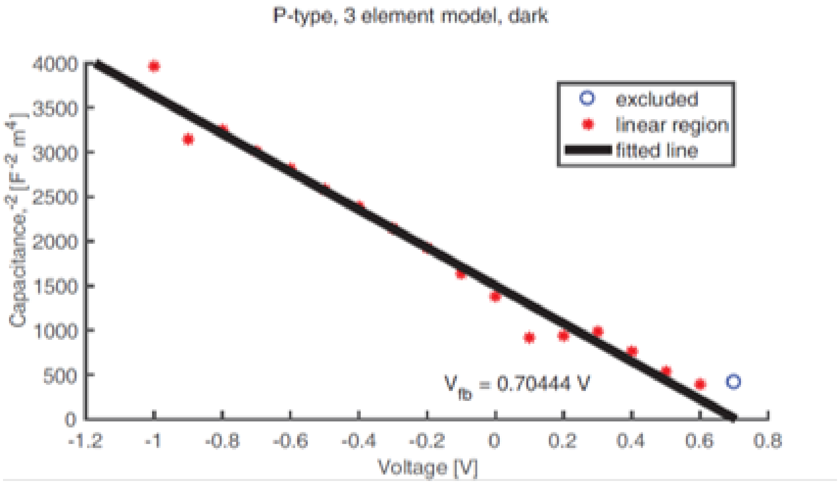
File operations

Acquisition → Processing → Visualization → Including a model → Analysis

cv_500wcm2_KoH_p_02_-1-0.txt

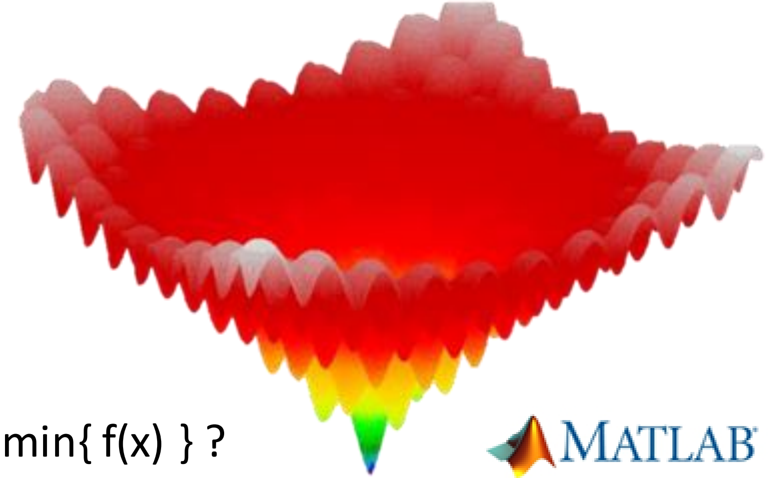
```
ZAHNER CV file
Date : 12.04.19
System : KoH_p_02
Temp : 0.1+-0.0C
Time : 15:30:56-15:50:59
Slew rate : 50mV/s

UinV     IinA      tins
0    1.2072065e-6     0
0    9.0704926e-7     1e-1
0    6.2164512e-7     3e-1
0    3.6077194e-7     5e-1
0    1.1786887e-7     7e-1
-4.9495375e-3   -2.1863909e-6   9e-1
-1.5008275e-2   -3.6769333e-6   1.1
-2.5067013e-2   -4.6210088e-6   1.3
-3.4966087e-2   -5.5549177e-6   1.5
-4.5024825e-2   -6.3723613e-6   1.7
-5.5083563e-2   -7.278342e-6    1.9
-6.4982637e-2   -8.176868e-6    2.1
-7.5041375e-2   -9.024631e-6    2.3
-8.494045e-2    -9.8839814e-6   2.5
-9.4999187e-2   -1.0810732e-5   2.7
-1.0505793e-1   -1.1729691e-5   2.9
-1.14957e-1 -1.2672574e-5   3.1
```

```
clear;
set(0,'Defaulttextinterpreter','tex');
cellArea = 1e4*pi*(2e-3)^2; %cm2

[filename, folder] = uigetfile({'*.txt;*.csv'},'MultiSe
fullFileName = fullfile(folder, filename);

if ischar(filename)
    data = ZahnerData2(fullFileName);
else
    for ii = 1:length(filename)
        data(ii) = ZahnerData2(fullFileName(ii));
    end
end



figure(3);
clf
hold on
for ii = 1:length(data)

plot(data(ii).voltage,data(ii).current*1e3/cellArea,'li


end
hold off
title(data(1).headerData(2,2),'interpreter','none');
xlabel('voltage vs. RHE (V)');
ylabel('current density, [mA cm^(-2)]');
```

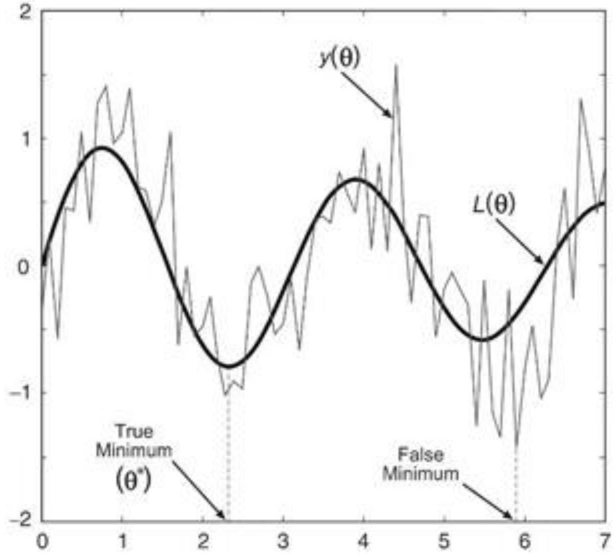


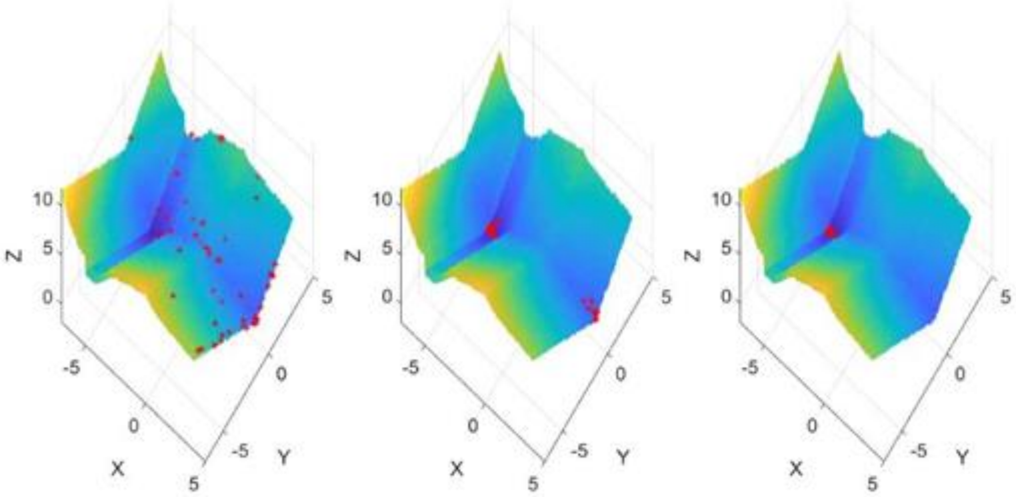
Flat band voltage ~0.7V

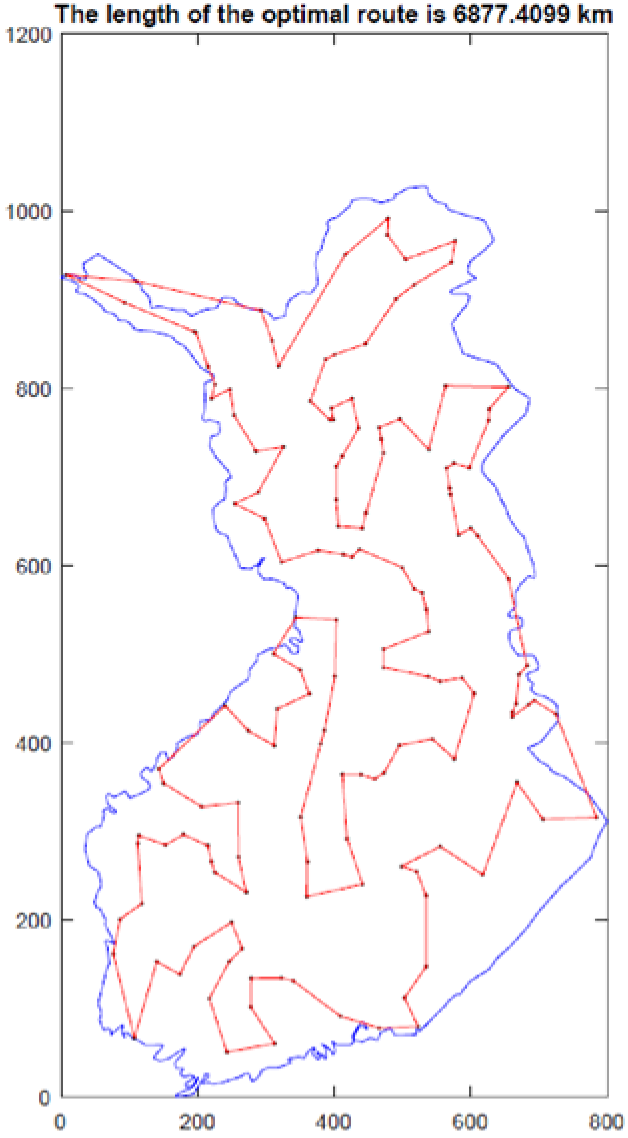
Optimization



min{ f(x) } ?

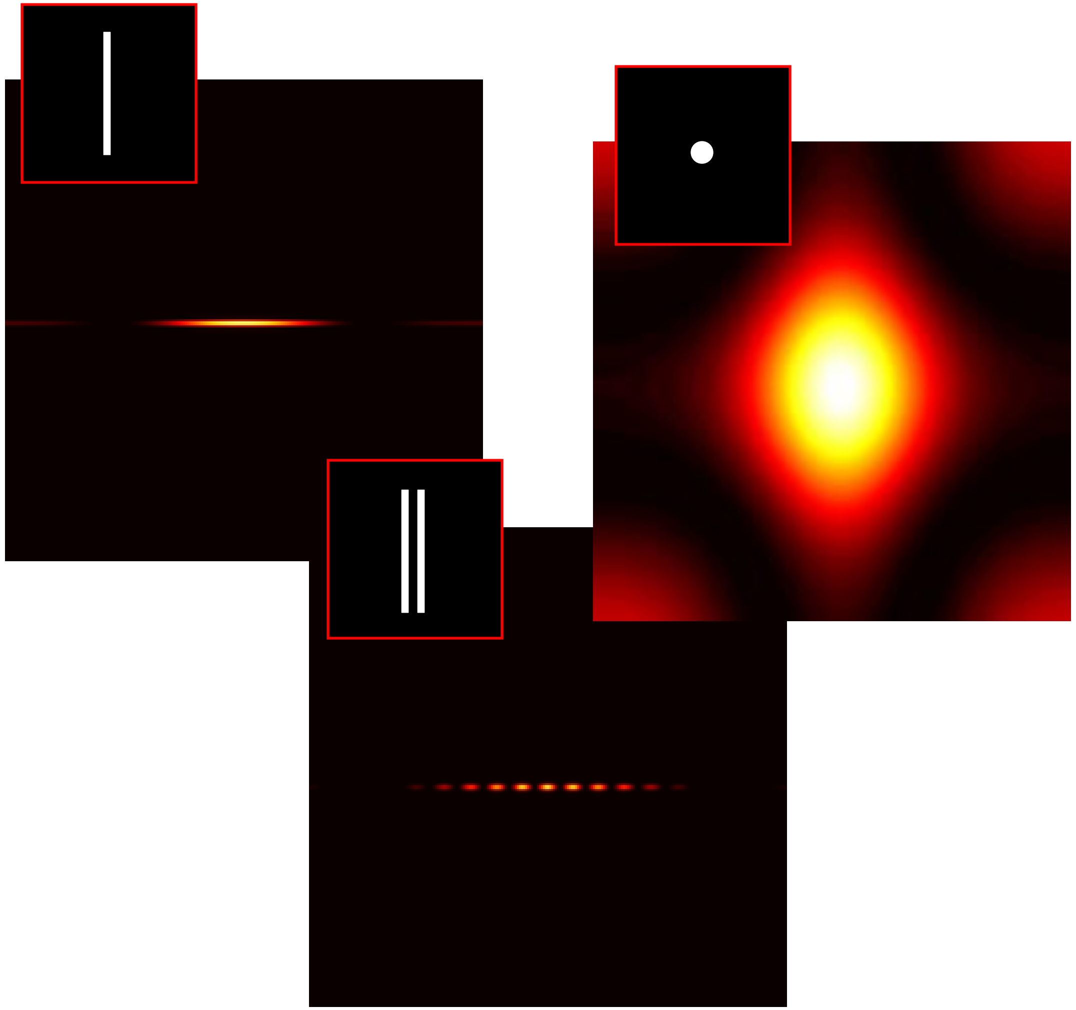




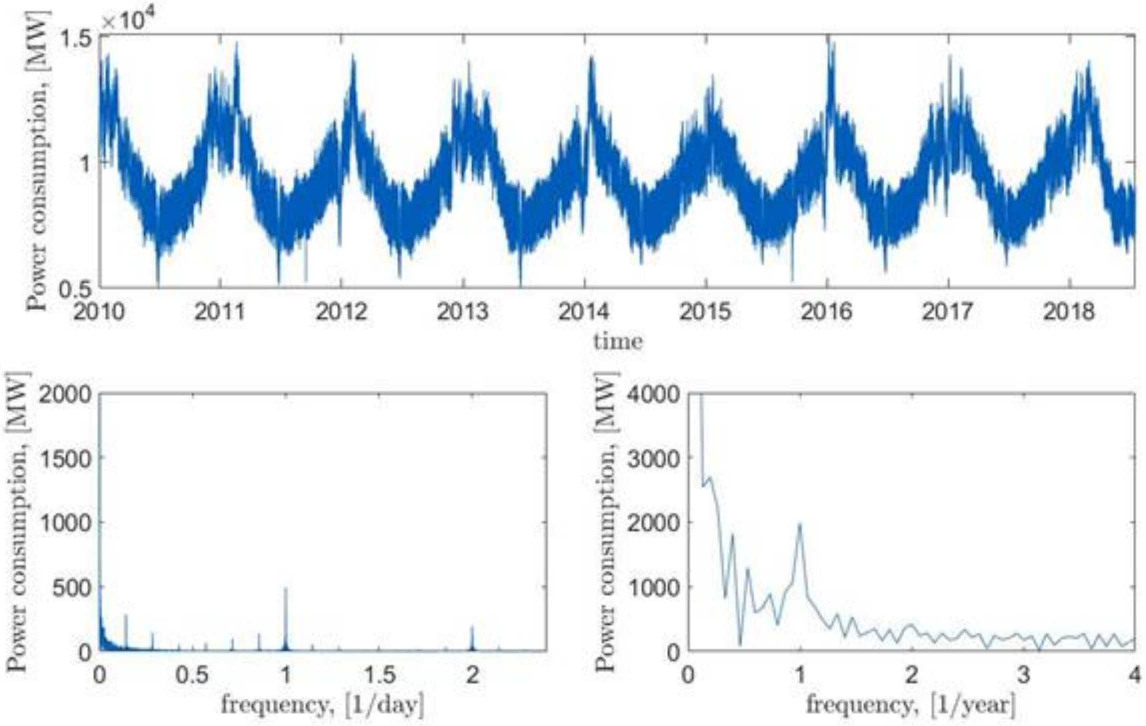


Fourier analysis

Wave diffraction



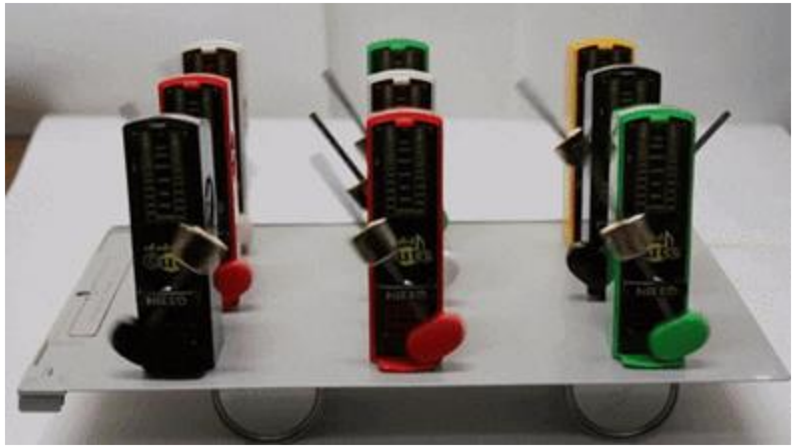
Power consumption in Finland



Dynamic systems

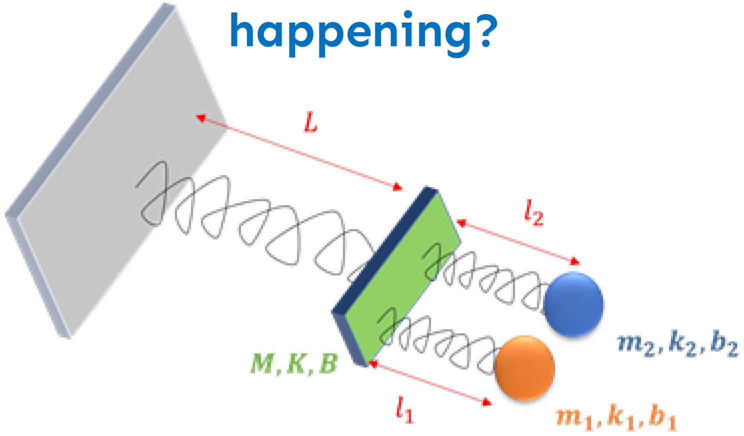
Predicting the future?

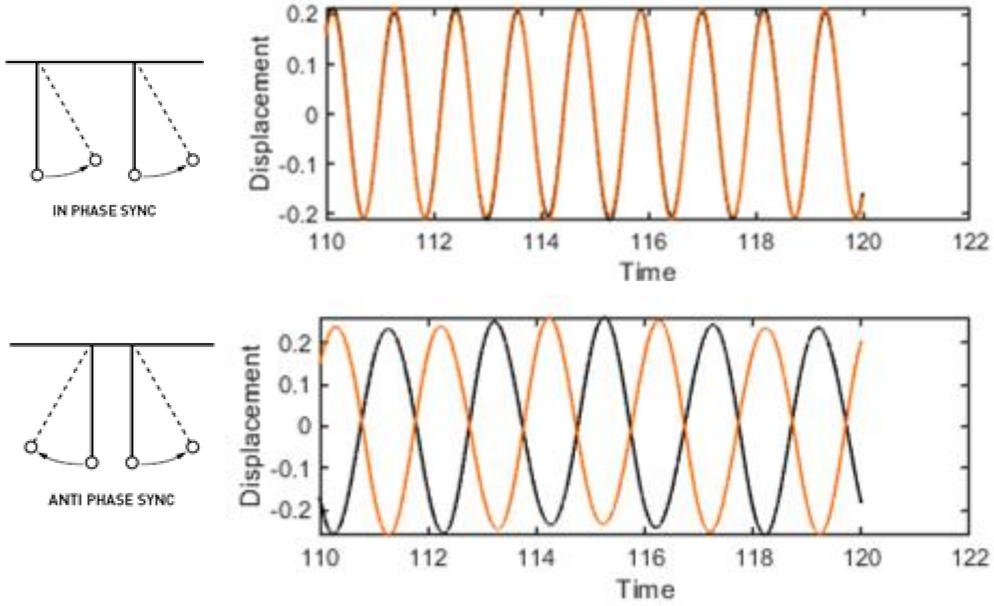
Huygens
1665



Youtube
2018

What's
happening?





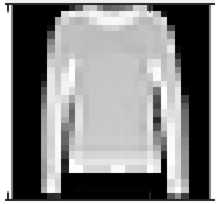
Machine learning

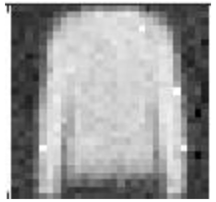
Knowledge from data

Clustering / classification

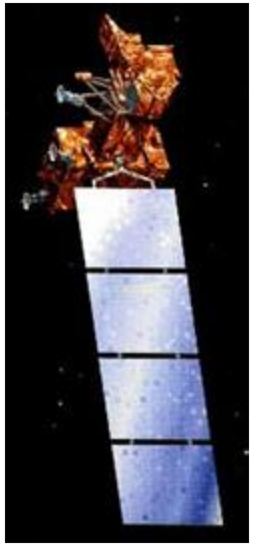
Autoencoder

748 → compression → 100 → decompression → 748



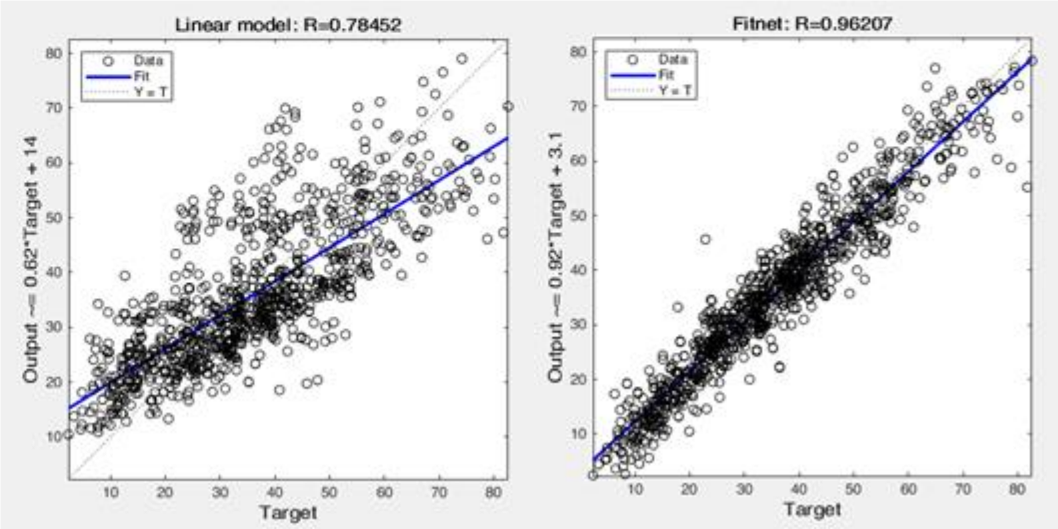


classification



1	red soil
2	cotton crop
3	grey soil
4	damp grey soil
5	soil with vegetation stubble
6	mixture class
7	very damp grey soil

regression



Mathematica overview

- The second part of the course focuses on the mathematical calculation, problem solving, and visualization using Mathematica and Wolfram Language (WL).
- WL is a high-level “knowledge-based” programming language including roughly 6000 functions.
- **The power of Mathematica is that it combines analytical (symbolic) and numerical computations, with a huge number of efficient built-in functions and sophisticated visualization tools.**
- Mathematica has a very useful help tool, with lots of examples and applications, but sometimes finding a correct function can be tedious and time-consuming

Mathematica topics

- Week 8: Notebook documentation and basics of Wolfram language
- Week 9: Calculus (differentiation, integration, etc.)
- Week 10: Visualization and graphics
- Week 11: Differential equations (ODE and PDE)
- Week 12: Data analysis, manipulation and optimization
- Week 13: Engineering applications

Mathematica examples

Symbolic and numerical calculus

$$\partial_x \texttt{Sin[x y] / (x^2 + y^2)} = \frac{y\,\mathrm{Cos}[x\,y]}{x^2 + y^2}$$

$$\int \texttt{(x^2 + Sin[x])}\, dx = \frac{x^3}{3} - \mathrm{Cos}[x]$$

$$\int_{-1}^{1}\int_{0}^{1-x^2}\int_{0}^{2-z} \nabla_{\{x,y,z\}} \cdot \left\{x\,y,\ y^2 + e^{x\,z^2},\ \mathrm{Sin}[x\,y]\right\} dy\,dz\,dx = \frac{184}{35}$$

$$\sum_{i=1}^{\infty}\sum_{j=1}^{i} \frac{1}{j^2\,(i+1)^2} = \frac{\pi^4}{120}$$

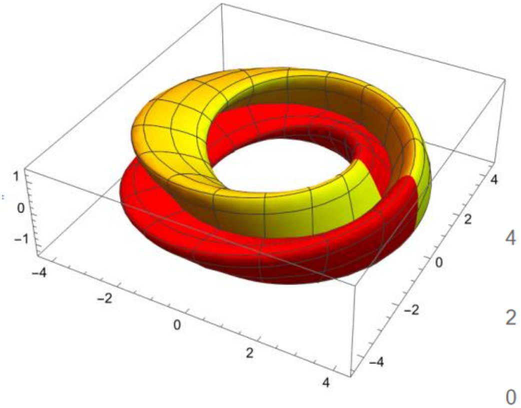
(Differential) equation solution

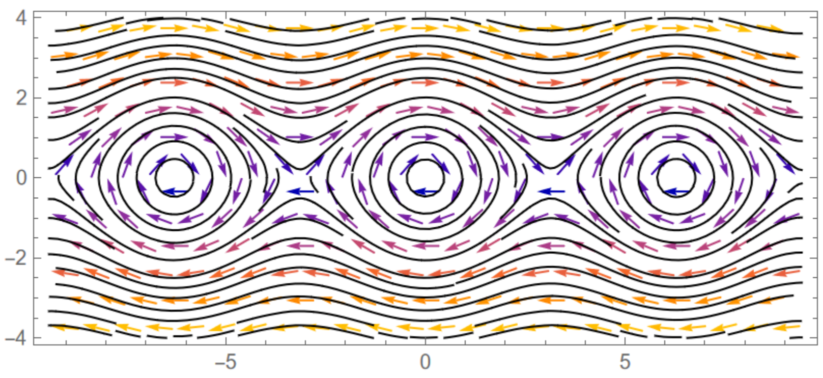
$$\texttt{DSolve[y'[x] + y[x] == a Sin[x], y[x], x]} \quad y[x] \to e^{-x}\,c_1 + \frac{1}{2}\,a\,(-\mathrm{Cos}[x] + \mathrm{Sin}[x])$$

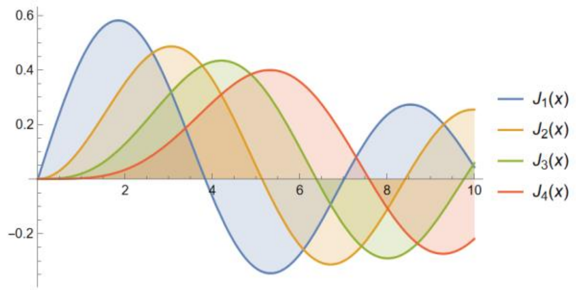
```
eqn = I ħ D[ψ[x, t], t] == -ħ^2 / (2 m) D[ψ[x, t], {x, 2}];
bcs = {ψ[0, t] == 0, ψ[d, t] == 0};

DSolve[Join[{eqn}, bcs], ψ[x, t], {x, t}]
```

$$\psi[x, t] \to \sum_{K[1]=1}^{\infty} e^{-\frac{i\,\pi^2\,t\,\hbar\,K[1]^2}{2\,d^2\,m}}\, c_{K[1]}\, \mathrm{Sin}\left[\frac{\pi\,x\,K[1]}{d}\right]$$

Graphics and visualization







and many more …

```
With[
 {c = EntityValue[EntityClass["Country", "Europe"],
    EntityProperty["Country", "CapitalLocation"]]},
 GeoListPlot[c[[Last@FindShortestTour[c]]],
  Joined → True]]
```