Computational Materials Science (計算材料学特論)

http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms

Lecture materials for numerical analyses (by Kamiya)
数値解析に関する講義資料・pythonプログラム (神谷担当分)

Update News:

- **June 21, 16:25, 2026:** Lecture materials for June 23 has been uploaded: course_materials.zip
- **June 19, 10:49, 2026:** Final version: Lecture materials for June 19 has been updated: course_materials.zip
- **June 16, 15:38, 2026:** Final version: Lecture materials for June 16 has been updated: course_materials.zip
- **June 12, 17:17, 2026:** Final version: Lecture materials for June 12 has been updated: c

We would wait for five minuities (i.e., till 8:55).
In meantime
- **download the latest lecture materials (updated June 21st)**
- **hear the short audio guide.**
  English and Japanese versions available

FY2026

#03 June 23, 2026: Smoothing (平滑化), Linear least-squares method (
(方程式の解法)

Course materials (Lecture slides and python programs):

- course_materials.zip

5-8min audio guide:

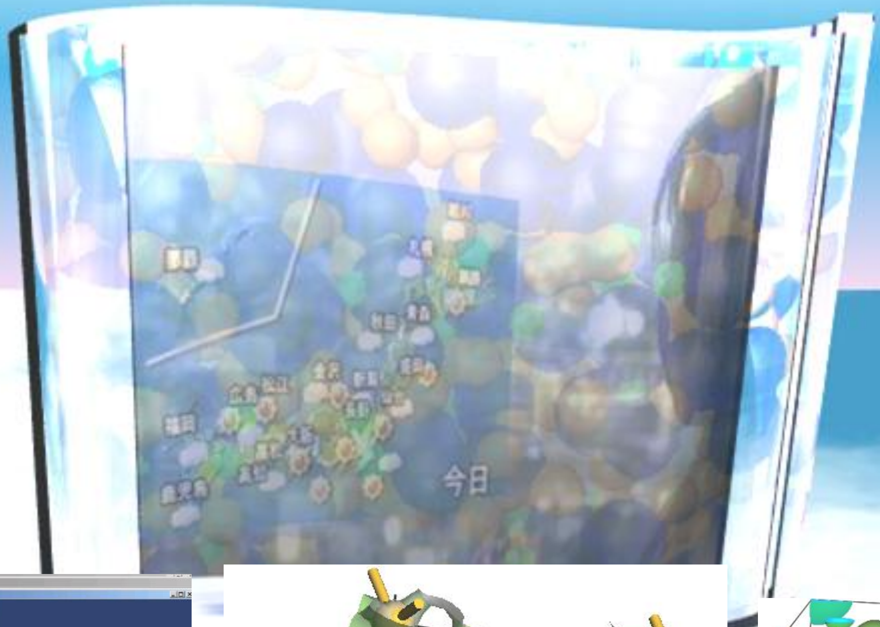
- 日本語: 0:00 / 5:56 (VOICEVOX 四国めたん&ずんだもん)
- English: 0:00 / 6:12

#03 June 19, 2026: Differential equation (微分方程式), Interpolation (補間), Smoothing (平滑化)

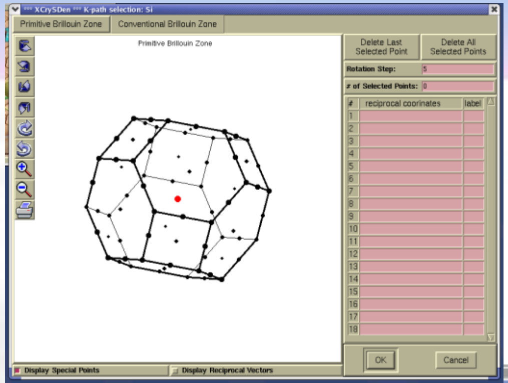
Course materials (Lecture slides and python programs):

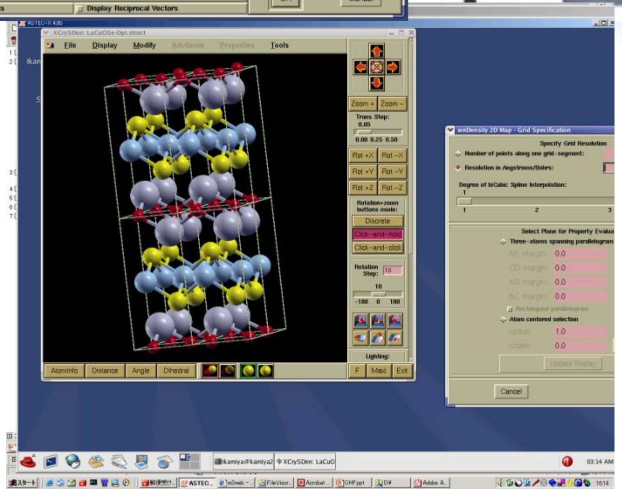
MAT.C505

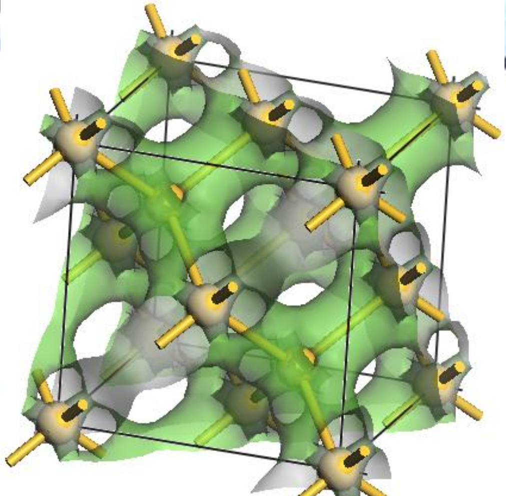
Computational Materials Science
計算材料学特論

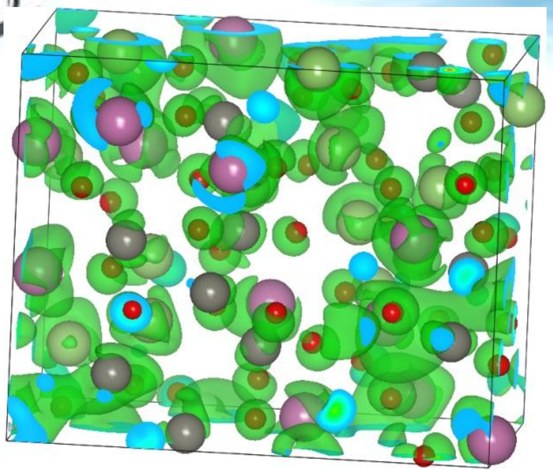


Toshio Kamiya
神谷利夫









Class Schedule

Lecture materials (Kamiya’s part): **http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/?page=cms**

授業　6月10日(水)～7月28日(火), 7月30日(木)　月曜の授業　7月23日(木)　期末試験･補講　7月29日(水), 7月31日(金)～8月6日(木)

#01 June 12 (Fri)　Kamiya (Fundamentals of computer, Sources of error (コンピュータの基礎、誤差), Numerical differentiation (数値微分))

#02 June 16 (Tue)　Kamiya (Numerical differentiation (数値微分), Numerical integration (数値積分), Differential equation (微分方程式))

#03 June 19 (Fri)　Kamiya (Differential equation (微分方程式), Molecular dynamics (分子動力学法), Interpolation (補間), Smoothing (平滑化))

#04 June 23 (Tue)　Kamiya (Smoothing (平滑化), Linear least-squares method (線形最小二乗法), Numerical solutions of equations (方程式の数値解法))

#05 June 26 (Fri)　Kamiya (Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化), Fourier transformation (フーリエ変換)

#06 June 30 (Tue)　Kamiya, Matrix (行列)

#07 July 3 (Fri)　Kamiya, Review (復習)

#08 July 7 (Tue)　Sasagawa (Review of quantum theory 1: 量子論おさらい1)

#09 July 10 (Fri)　Sasagawa (Review of quantum theory 2: 量子論おさらい2)

#10 July 14 (Tue)　Sasagawa (First principles calculations: basics 1 第一原理計算:基礎1)

#11 July 17 (Fri)　Sasagawa (First principles calculations: basics 2 第一原理計算:基礎2)

#12 July 2 (Fri)　Sasagawa (First principles calc.: applications 1 第一原理計算:応用1)

#13 July 24 (Fri)　Sasagawa (First principles calc.: applications 2 第一原理計算:応用2)

#14 July 28 (Fri)　Sasagawa (Classical and Quantum Computers 古典および量子コンピュータ)

Explanation of the answers
課題解答の解説

PROBLEM, June 23

- **Answer in English or Japanese**
- **Submit electronic file(s) via LMS until the midnight of June 24**

  (If LMS doesn’t work, send the files to kamiya.t.aa@m.titech.ac.jp.
  In this case, file name must include your STUDENT ID and FULL NAME)
- Common formats (.pdf, .txt., .docx, .xlsx, .pptx) are acceptable, but NO APPLE-ONLY files

PROBLEM:

Smoothen the data DOS(E) in dos.xlsx
by simple moving average method and polynomial fit method.

Add them and plot the raw DOS(E) and the smoothed data in an Excel file.

You can choose smoothing parameters as you like, but explicitly descrive them.
Submit the excel file.

Optional: Any questions and impressions of the lecture style are welcome
Request of other numerical methods for the last day, July 3rd

PROBLEM, June 23

PROBLEM:

Smoothen the data DOS(E) in dos.xlsx
by simple moving average method and polynomial fit method.

Add them and plot the raw DOS(E) and the smoothed data in an Excel file.

You can choose smoothing parameters as you like, but explicitly descrive them.
Submit the excel file.

See dos_smoothing_answer.xlsx

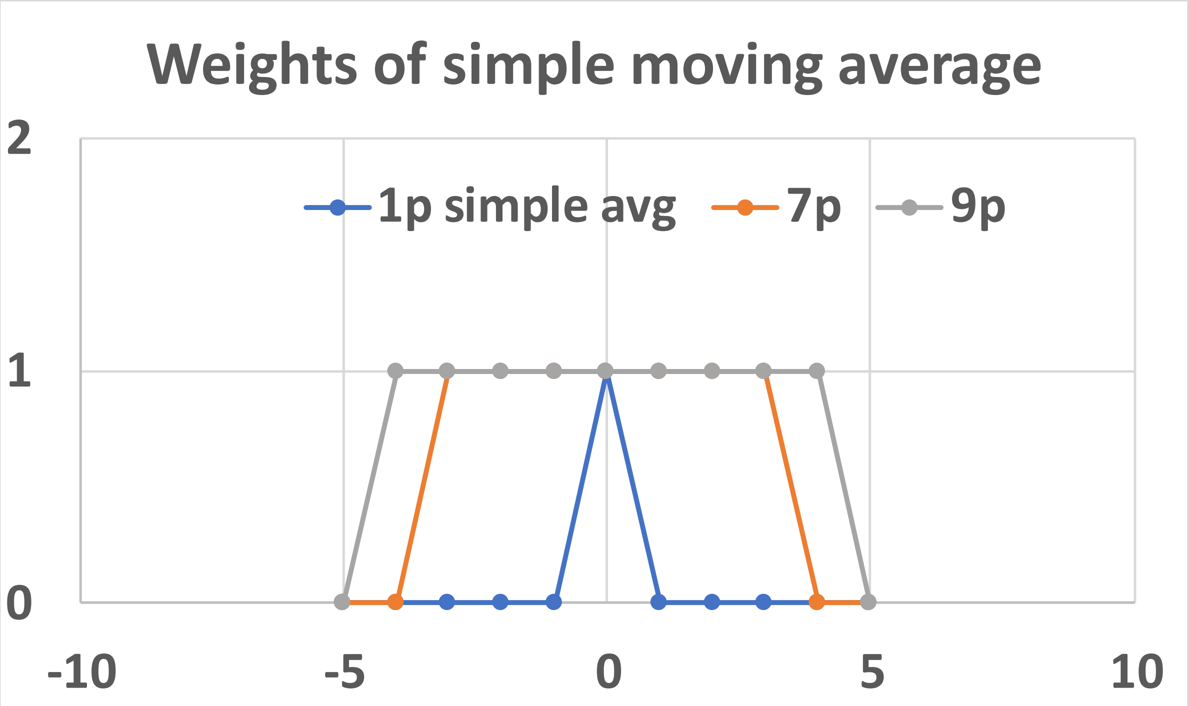
Smoothing

Simple moving average (2m+1 points)

$$y_{i,smoothed} = \frac{1}{2m+1}\sum_{j=i-m}^{i+m} y_j = \sum_{j=i-m}^{i+m} w_j y_j$$

Weight w_j/W

i-i0	1p simple avg	7p	9p
-5	0	0	0
-4	0	0	1
-3	0	1	1
-2	0	1	1
-1	0	1	1
0	1	1	1
1	0	1	1
2	0	1	1
3	0	1	1
4	0	0	1
5	0	0	0
W	1	7	9



Smoothing

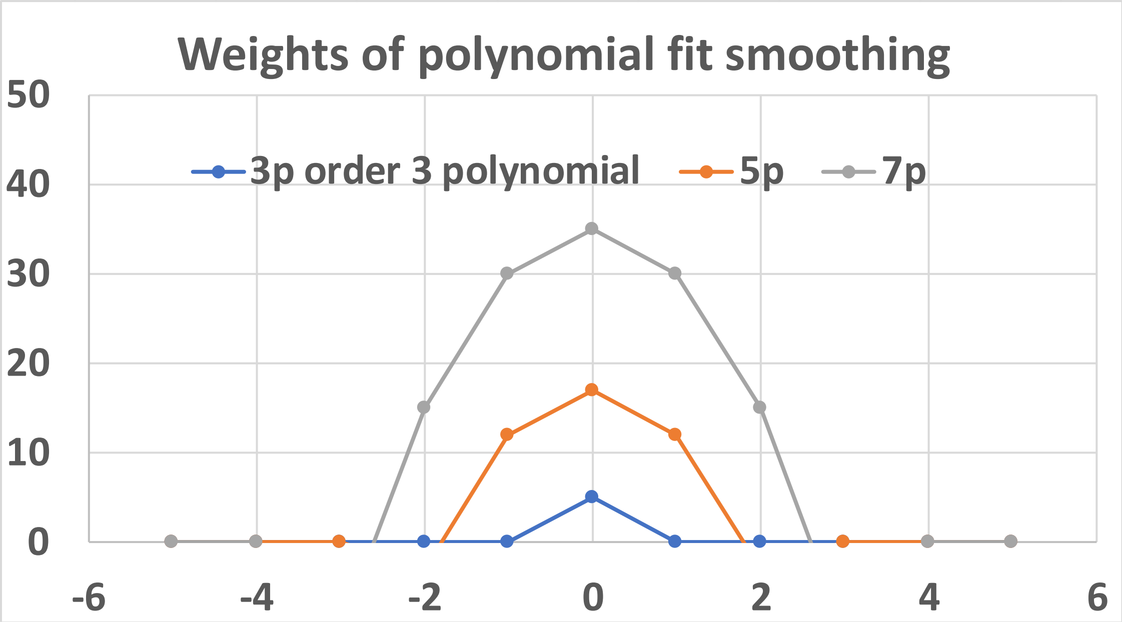
Order 2 and 3 polynomial fit using (2*m*+1) points

$$w_{23}(j) = 3m(m+1) - 1 - 5j^2 \quad j = \text{-m}, \cdots, \text{-1}, 0, 1, \cdots, \text{m}$$
$$W_{23} = (4m^2 - 1)(2m+3)/3$$

$$y_{i,smoothed} = \frac{1}{W_{23}} \sum_{j=i-m}^{i+m} w_{23}(j) y_j$$

Weight $w_{23}(j)/W$

i-i0	3p order 3 polynomial	5p	7p
-5	0	0	0
-4	0	0	0
-3	0	0	-10
-2	0	-3	15
-1	0	12	30
0	5	17	35
1	0	12	30
2	0	-3	15
3	0	0	-10
4	0	0	0
5	0	0	0
W	5	35	105



A smart answer by student

Use Excel matrix functions:

See “**7p(transpose+mmult)**” **column in dos_smoothing_answer.xlsx**

mmult(range1, range2):

Multiply matrixes (vectors) given in the ranges range1 and range2

transpose(range1)

Transpose the matrix (vector) given in the range1

Use Excel product sum:

See “**7p(sum)**” **column in dos_smoothing_answer.xlsx**

=SUM(**$B2:$B12*M$3:M$13**)/SUM(M$3:M$13)

Use Excel product sum function:

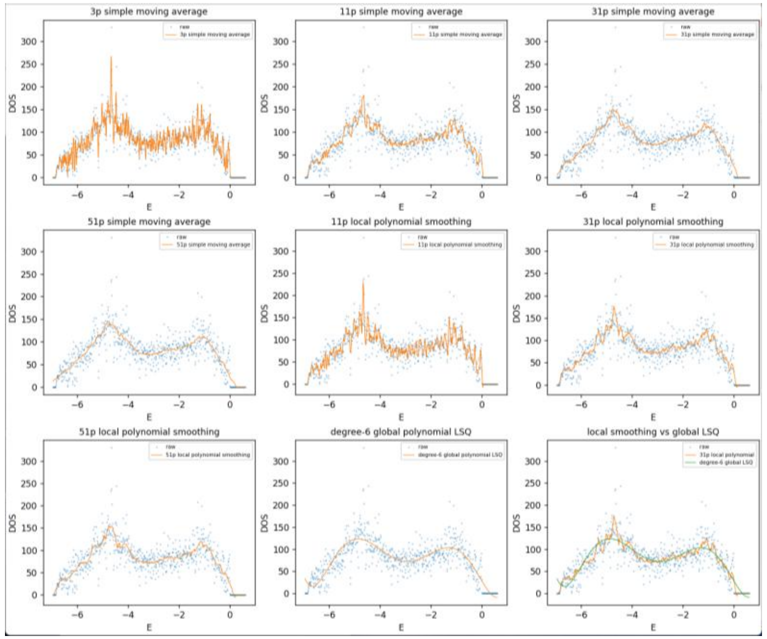
See “**7p(sumproduct)**” **column in dos_smoothing_answer.xlsx**

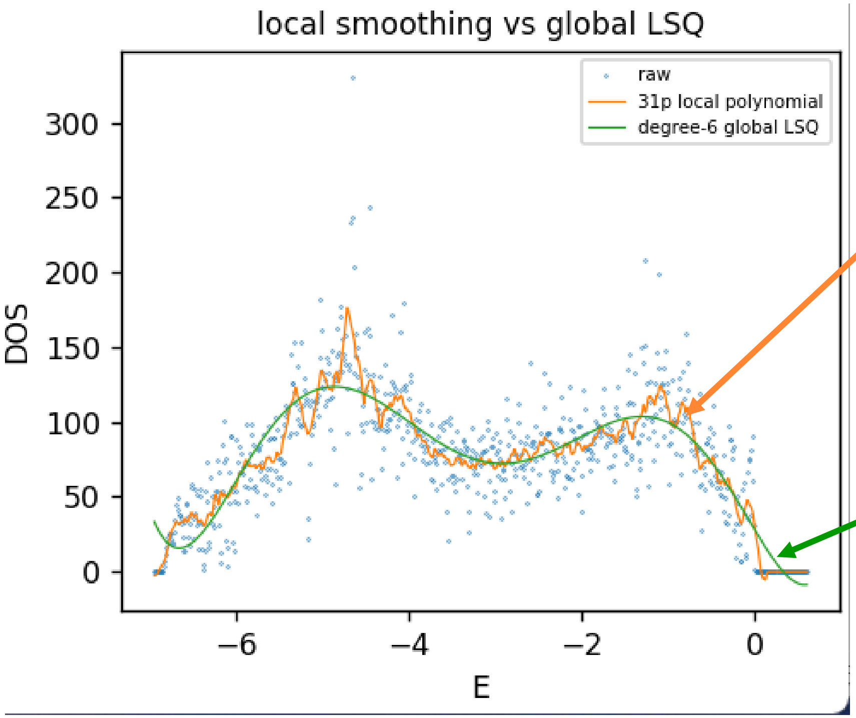
SUMPRODUCT(range1, range2):

Calculate the dot product of two vectors given in range1 and range2

Compare local polynomial smoothing and global polynomial LSQ fitting

> Python smoothing-answer.py





Local polynomial smoothing:

- Polynomial coefficients do not have physical meaning
- Different polynomials are used for different data points.
- Reduces noise while retaining some fine structures.

Global polynomial lsq:

- One polynomial is fitted to all data points.
- Gives a smooth global trend.
- Very smooth, but can lose fine structures.

移動窓多項式平滑化	**moving-window** polynomial smoothing	Different polynomials are used for different data point
局所多項式平滑化	**local** polynomial smoothing	
Savitzky–Golay平滑化	Savitzky–Golay smoothing/filter	One of moving poly smoothing
全域多項式最小二乗近似	**global** polynomial least-squares fitting	One polynomial is fitted to all data points

PROBLEM, June 26

- **Answer in English or Japanese**
- **Submit electronic file(s) via LMS by midnight on June 28**

  (If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
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- Common formats (.pdf, .txt., .docx, .xlsx, .pptx) are acceptable, but NO APPLE-ONLY files

PROBLEM:

Solve 5cos(x) – x = 0.

(i) Plot the functions y = 5cos(x) and y = x in the range x = 0 – 3, find an initial x for Newton-Raphson method.

(ii) Solve 5cos(x) – x = 0 by Newton-Raphshon method at least with four significant digits.

Additional mandatory item: Choose one of the following

(i) Write any quetion, comment, opinion, or impression about the lectures

(ii) Propose if you have any numerical analysis method / simple python program that you would like to learn