

# Computational Materials Science (計算材料学特論)

## Lecture materials updated

[http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE\\_programs.html?page=cms](http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms)

### COMPUTATIONAL MATERIALS SCIENCE 2025 Q2 2025年度Q2 計算材料学特論 (資料: 英語 + 日本語版)

Lecture materials for numerical analyses (by Kamiya)  
数値解析: 方程式の数値解法, 非線形最適化 (担当分)

We will wait for five minutes.

In the meantime, please make sure to download the lecture materials

#### Update News:

- June 27, 00:58 Lecture materials on June 27 have been updated ([20250627EquationOptimize.zip](#))

Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化)

Audio explanation generated by Google NotebookLM:

▶ 0:00 / 27:23

Google NotebookLMで生成した音声解説:

▶ 0:00 / 9:51

- June 20, 11:06 Final v

Smoothing (平滑化),

Also listen the AI-generated brief explanation of the lecture

Audio explanation generated by Google NotebookLM:

▶ 0:00 / 17:33

Google NotebookLMで生成した音声解説:

▶ 0:00 / 10:47

- June 17, 12:10 Final version of lecture materials on June 17 have been updated ([20250617Diffeq2.zip](#))

Differential equation (微分方程式), Molecular dynamics (分子動力学法), Interpolation (補間), Smoothing (平滑化)

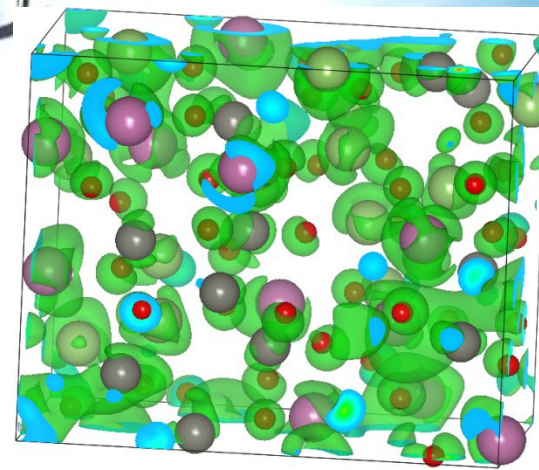
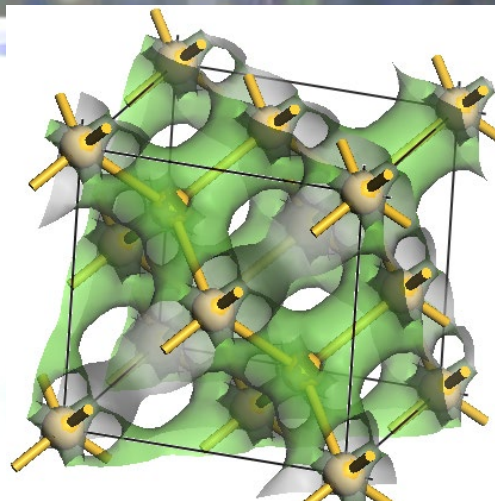
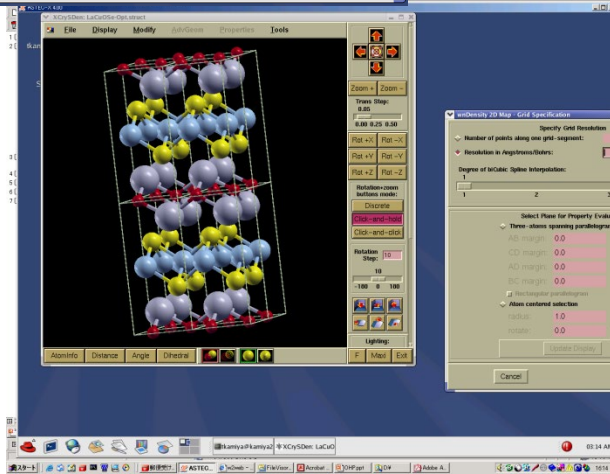
Audio explanation generated by Google NotebookLM:

▶ 0:00 / 15:33

Google NotebookLMで生成した音声解説:

▶ 0:00 / 9:10

神谷利夫



# New function: Google NotebookLM







[http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE\\_programs.html?page=cms](http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms)

## COMPUTATIONAL MATERIALS SCIENCE 2025 Q2 2025年度Q2 計算材料学特論 (資料: 英語 + 日本語版)

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)


### Google NotebookLM Chatbot


#### Update News:


- June 26, 06:01 Lecture materials on June 27 have been uploaded ([20250626EquationOptimize.zip](#))  
Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化)  
Audio explanation generated by Google NotebookLM:  0:00 / 23:34  
- June 20, 11:06 Final version of lecture materials on June 20 have been updated ([20250620InterporlateSmoothing2.zip](#))  
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)  
Google NotebookLMで生成した音声解説:  0:00 / 9:29  


# New function: Google NotebookLM


URL may change: Please access from the CMS web page

 Computational Materials Science 2025


 アナリティクス


 新機能！一般公開で共有する

 共有

 設定

PRO





ソース

チャット

Studio

## Computational Materials Science 2025

5 ソース

These academic materials, likely from a course on **Computational Materials Science**, provide a comprehensive overview of fundamental numerical methods. The first document introduces **computer basics** and various **sources of errors** in computation, such as round-off and truncation errors, emphasizing the importance of careful handling of floating-point numbers. It also covers **numeric representation** in different bases. The foundation, explaining **numerical differentiation** and **integration** techniques well as more advanced methods like Gauss-Legendre and Romberg integration to functions with anomalies. Finally, the materials briefly touch upon machine learning techniques for data analysis.

**NotebookLM only allows a single output language to be set for all notebooks, so the output language may vary between English and Japanese depending on the situation.**

入力を開始します...

5 個のソース



How do different numerical methods for differentiation and integration affect accuracy and error propagation in computational materials science?

What fundamental







ソース

チャット

Studio



How I can solve a differential equation with high precision?

To achieve high precision when solving a differential equation, you should consider the choice of numerical method, the step size used in the calculation, and careful handling of floating-point errors [1](#) [...](#).

Here are key approaches based on the sources:

- **Choose Higher-Order Numerical Methods** Higher-order methods generally offer better accuracy for a given step size compared to simpler methods [3](#) [...](#).
  - **Euler Formula (オイラー法)**: This is the simplest method, but its accuracy is "not good," and it is "asymmetric" with respect to time, which can lead to larger errors [2](#).
  - **Heun Formula (ホイン法)**: This method improves upon the Euler formula by averaging approximations, leading to better accuracy. It uses an estimate of the next step from the Euler formula to refine the calculation [2](#) [6](#).
  - **Runge-Kutta Formulas (ルンゲークッタ公式)**: These are highly recommended for achieving higher precision. The sources specifically mention 3-stage 3-order and 4-stage 4-order Runge-Kutta formulas [3](#) [...](#). Plots comparing various methods demonstrate that **Runge-Kutta methods, particularly the 3rd and 4th order, exhibit significantly higher accuracy** and better convergence over time than Euler and Heun methods [4](#) [5](#).
  - **Methods for Second-Order Differential Equations**: For second-order differential equations, which can be broken down into two simultaneous first-order equations, methods like Verlet, velocity Verlet, and Leap Frog are discussed [9](#) [...](#).

# Class Schedule

Lecture materials (Kamiya's part): [http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE\\_programs.html?page=cms](http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms)

- #01 June 10 (Tue) Kamiya (Fundamentals of computer, Sources of errors (コンピュータの基礎、誤差))
- #02 June 13 (Fri) Kamiya (Numerical differentiation/integration (数値微分/積分))
- #03 June 17 (Tue) 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 20 (Fri) 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 24 (Tue) Canceled
- #06 June 27 (Fri) **Kamiya (Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化))**
- #07 July 1 (Tue) Kamiya (Fourier transformation (フーリエ変換), Matrix (行列), Applications (応用))
- #08 July 4 (Fri) Sasagawa (Review of quantum theory 1: 量子論おさらい1)
- #09 July 8 (Tue) Sasagawa (Review of quantum theory 2: 量子論おさらい2)
- #10 July 11 (Fri) Sasagawa (First principles calculations: basics 1 第一原理計算: 基礎1)
- #11 July 15 (Tue) Sasagawa (First principles calculations: basics 2 第一原理計算: 基礎2)
- #12 July 18 (Fri) Sasagawa (First principles calc.: applications 1 第一原理計算: 応用1)
- #13 July 22 (Tue) Sasagawa (First principles calc.: applications 2 第一原理計算: 応用2)
- #14 July 25 (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 20

## **PROBLEM:**

**Smoothen the data DOS(E) in dos.xlsx  
by simple 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 describe them.**

**Submit the excel file.**

**See [dos\\_smoothing\\_answer.xlsx](#)**

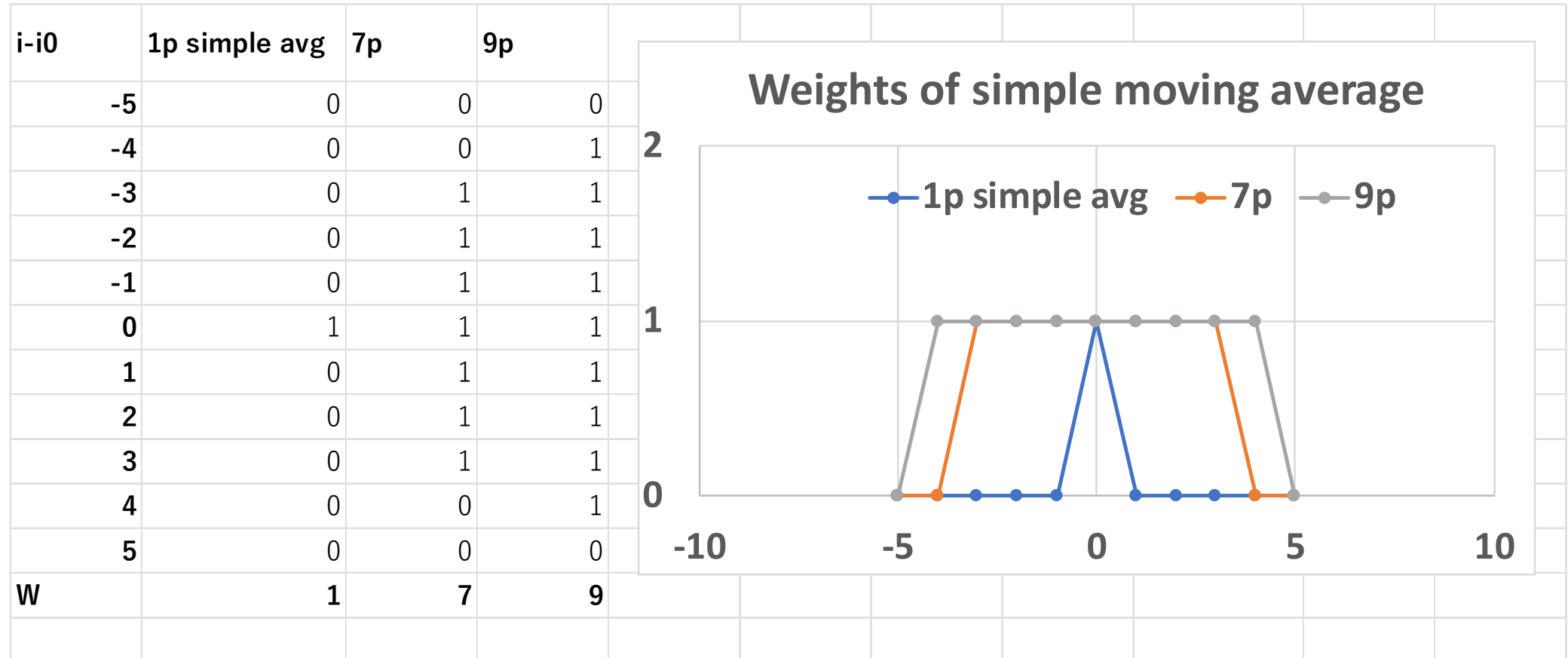


# Smoothing

## Simple moving average (2m+1 points)

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

## Weight



# Smoothing

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

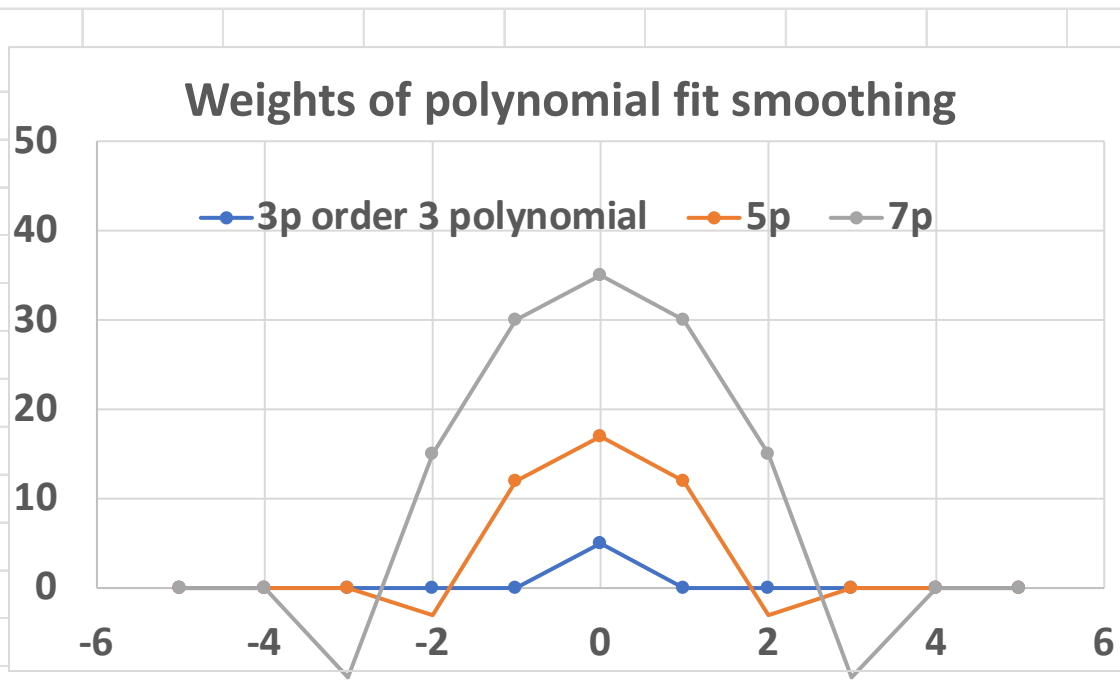
$$w_{23}(j) = 3m(m+1) - 1 - 5j^2 \quad j = -m, \dots, -1, 0, 1, \dots, m$$

$$W_{23} = (4m^2 - 1)(2m + 3)/3$$

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

$w_{23}(j)$

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:

`mmult(range1, range2):`

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

`transpose(range1)`

Transpose the matrix (vector) given in the range1

See “**7p(transpose+mmult)**” column in dos\_smoothing\_answer.xlsx

# PROBLEM, June 27

- Submit electronic file(s) via LMS in 2 days  
(If LMS doesn't work, send the files to [kamiya.t.aa@m.titech.ac.jp](mailto:kamiya.t.aa@m.titech.ac.jp).  
In this case, file name must include your STUDENT ID and FULL NAME)

## PROBLEM:

Solve  $5\cos(x) - x = 0$ .

- Plot the functions  $y = 5\cos(x)$  and  $y = x$  in the range  $x = 0 - 3$ , find an initial  $x$  for Newton-Raphson method.
- Solve  $5\cos(x) - x = 0$  by Newton-Raphson method at least with four significant digits.
- Mandatory:** Tell your opinions or suggestions for improvements regarding how the lectures are conducted, particularly in relation to the use of AI tools like NotebookLM.
- Optional:** Propose if you have any other numerical analysis you want to learn in Computational Materials Science
- Optional:** Propose if you have any python program (should be simple) you want to learn

**How to solve equations?**

**More sophisticated algorithms**



# Newton-Raphson method

**Solve  $f(x) = 0$**

Start from initial guess:  $x_0$

$x_0 + dx$  is supposed to be a solution

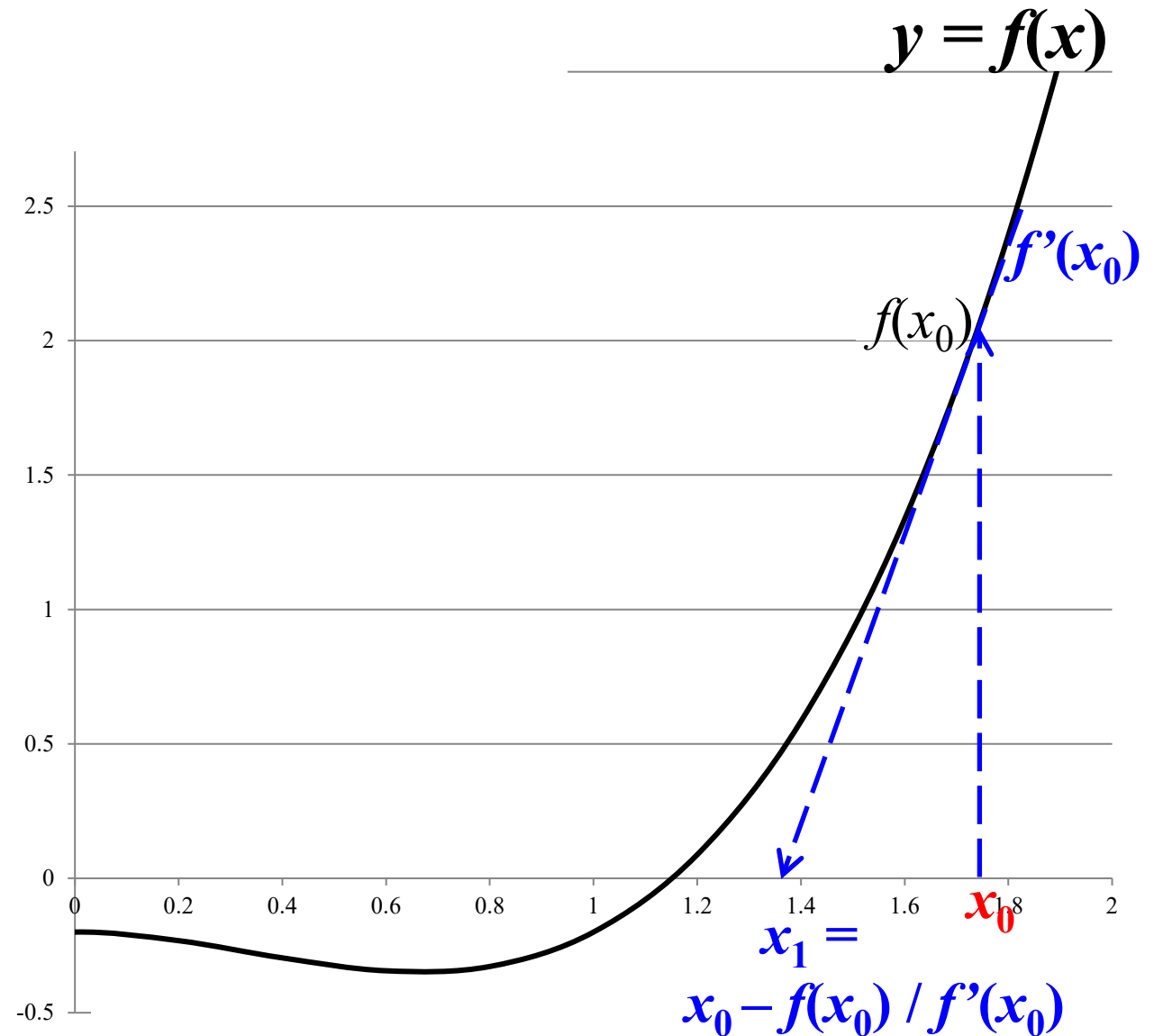
$$f(x_0 + dx) = f(x_0) + dx f'(x_0) \sim 0$$

$$\Rightarrow x_1 = x_0 + dx = x_0 - f(x_0) / f'(x_0)$$

Stabilize convergence:

$$x_{k+1} = x_k - f(x_k) / f'(x_k) / (1 + \lambda)$$

$\lambda$ : Damping Factor

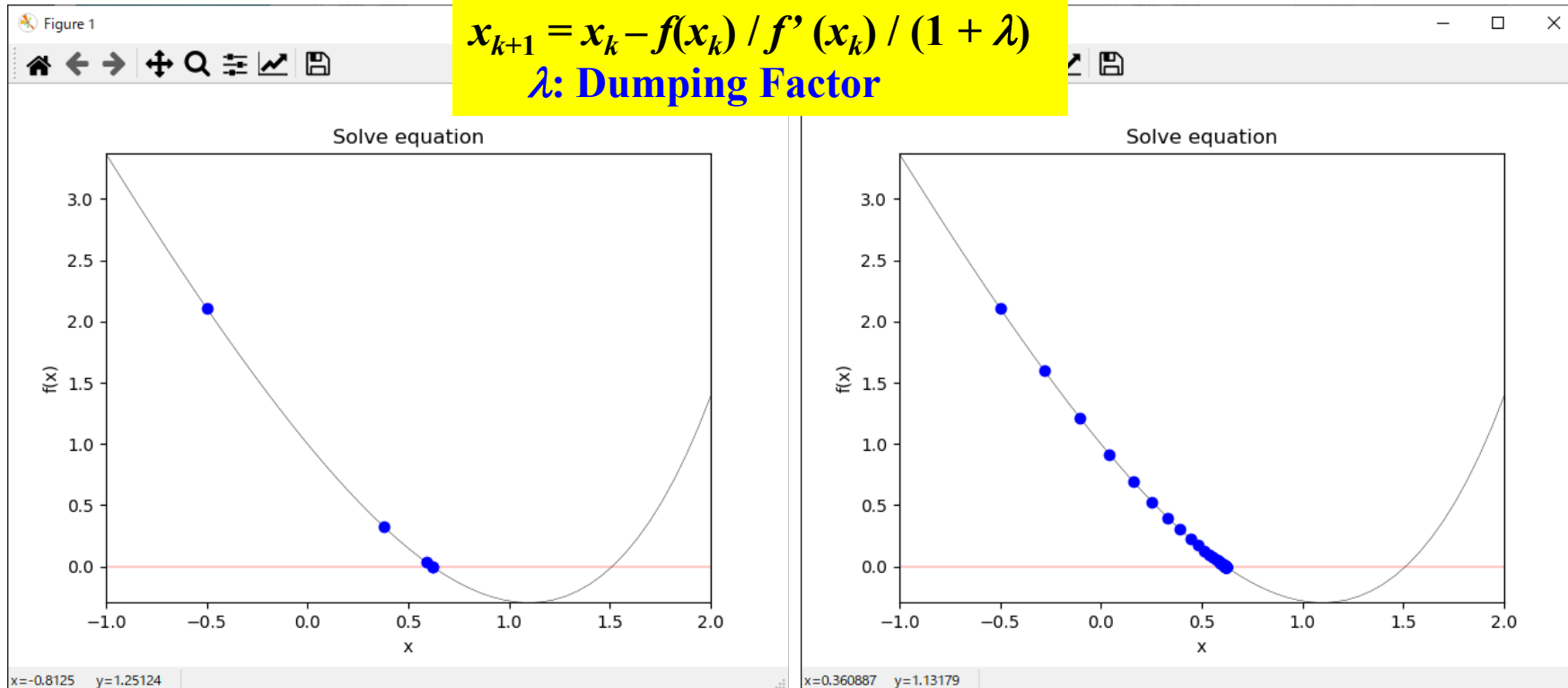


# Program: equation-newton-Raphson.py

Usage: python equation-newton-raphson.py x0 dump t<sub>sleep</sub>

$$f(x) = \exp(x) - 3.0x$$

python equation-newton-raphson.py -0.5 0      python equation-newton-raphson.py -0.5 3



# Newton-Raphson method

Solve  $f(x) = 0$

Start from initial guess:  $x_0$

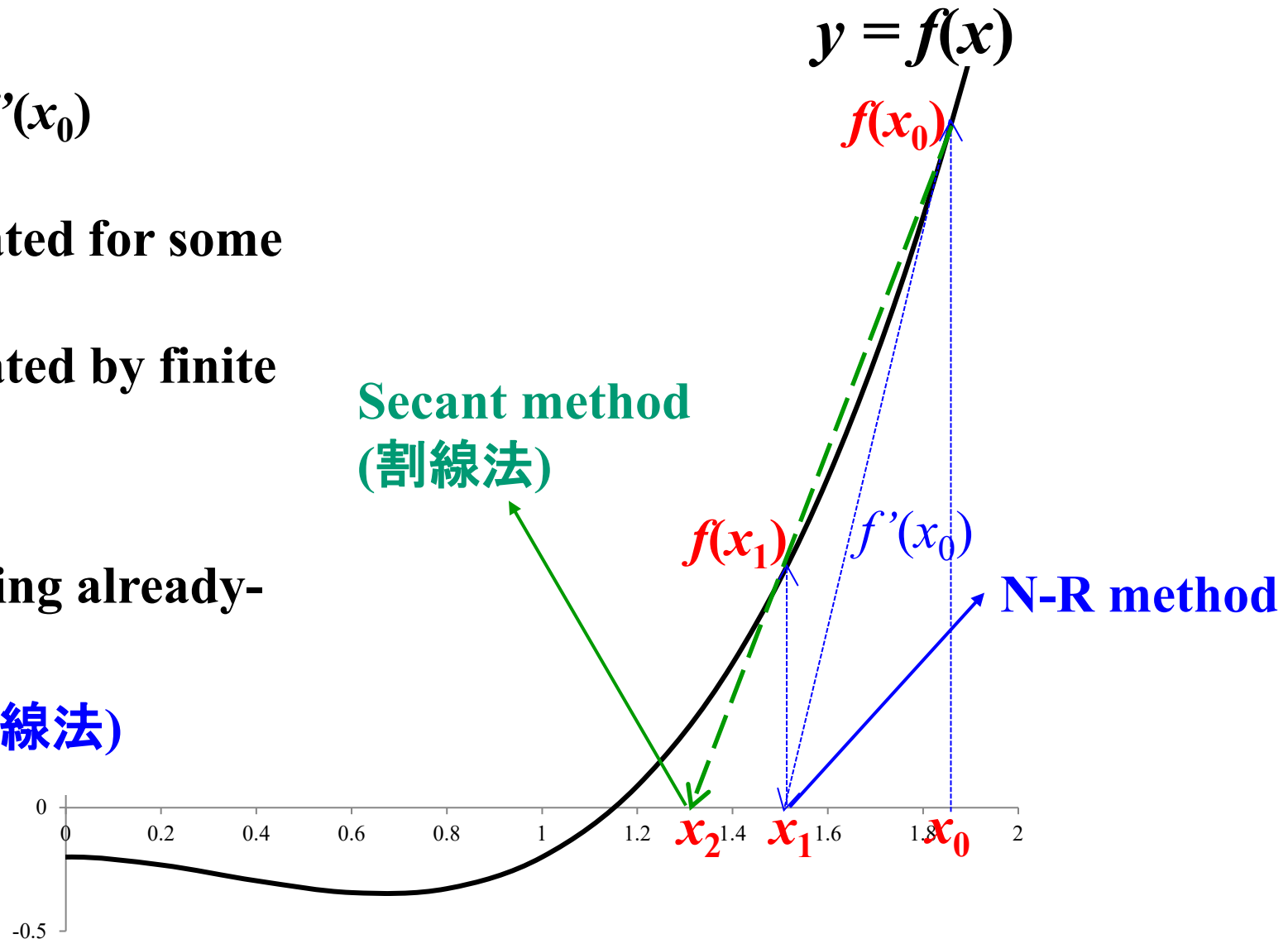
repeat:  $x_1 = x_0 + dx = x_0 - f(x_0) / f'(x_0)$

- $f'(x_0)$  can be analytical calculated for some cases
- $f'(x_0)$  is more often approximated by finite difference

$$\frac{f(x_0+h) - f(x_0-h)}{2h}$$

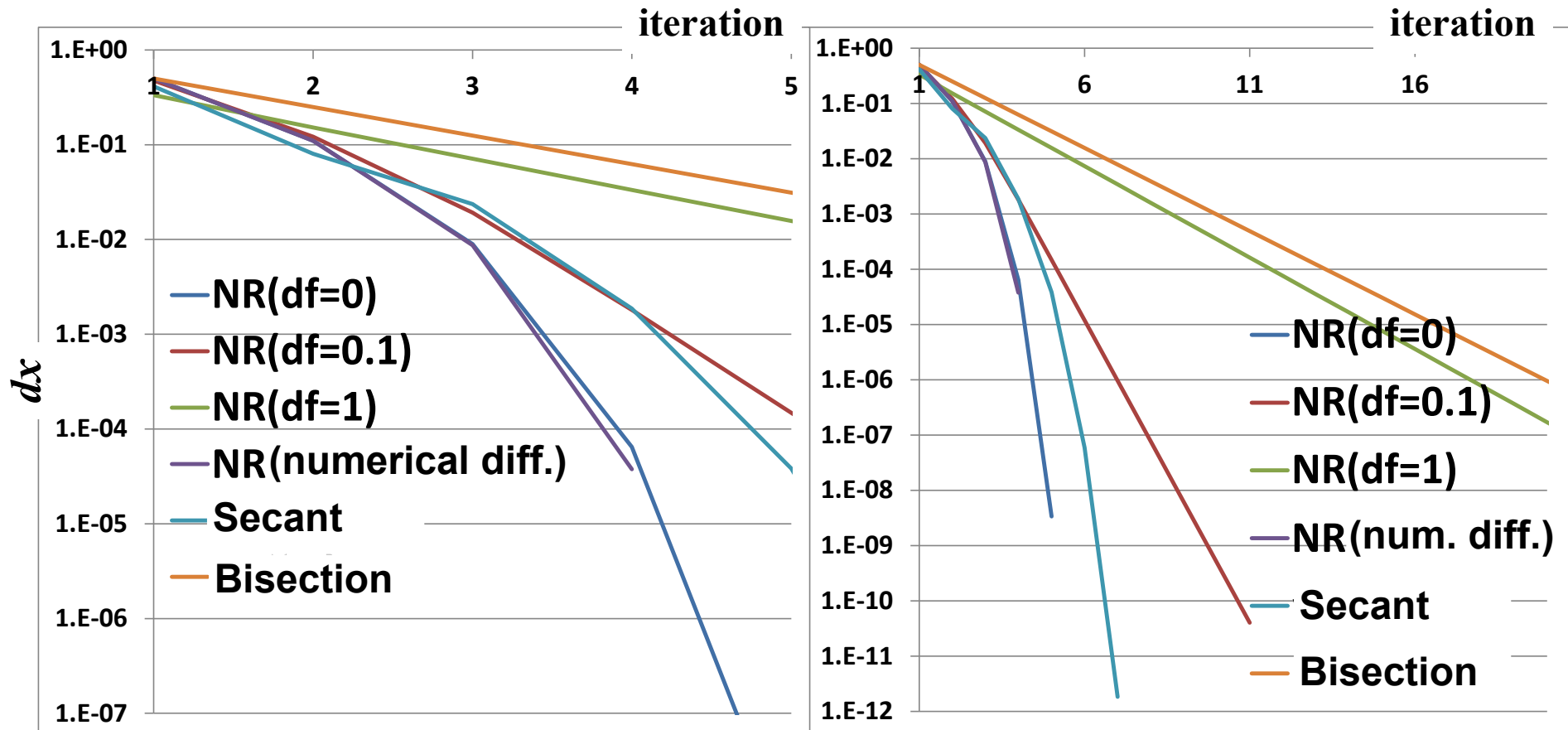
- $f'(x_0)$  can be approximated using already-calculated values

$$\frac{f(x_1) - f(x_0)}{x_1 - x_0} \quad \text{Secant method (割線法)}$$



# Effect of dumping factor: Convergence process

$f(x) = \exp(x) - 3x = 0$  (initial  $x = 0$ )      Exact 0.619061



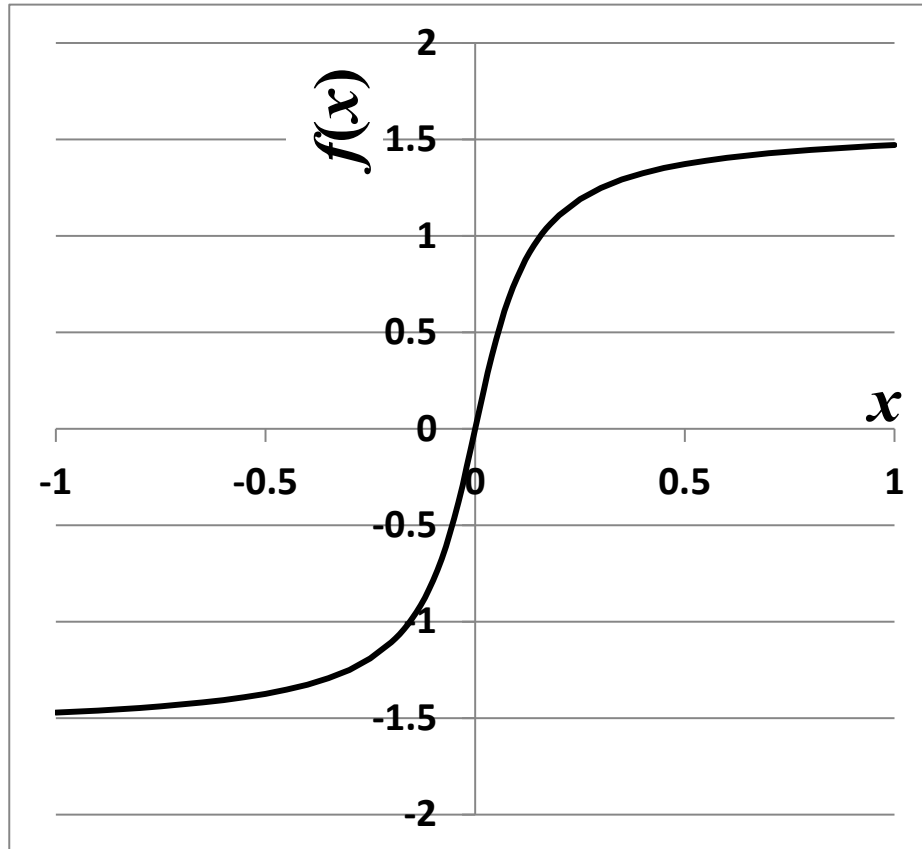
$$x_{k+1} = x_k - f(x_k) / (f'(x_k) + \lambda)$$
  
 $\lambda$ : Dumping Factor

NR: Newton-Raphson method  
df: Dumping Factor

# Case Newton method succeeds

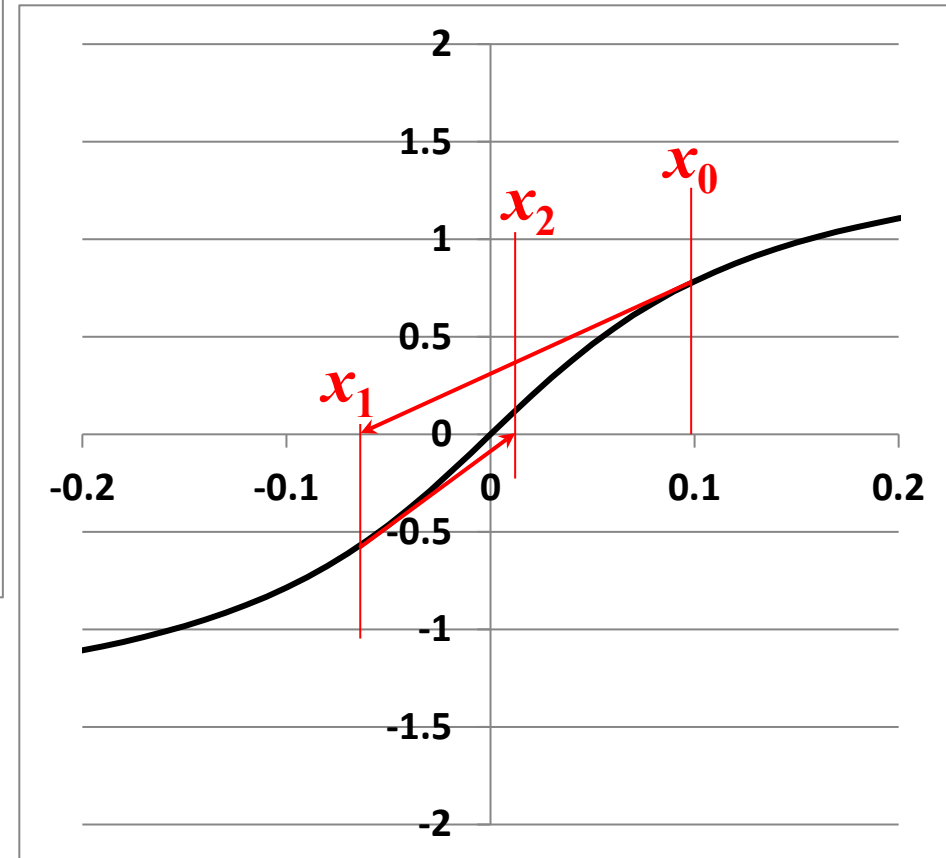
$$f(x) = \tan^{-1}(10x)$$

initial  $x = 0.1$



**A case to reach convergence**

i	x	f(x)	df/dx	dx
0	0.1	0.7854	5	-0.1571
1	-0.05708	-0.5187	7.54257	0.06877
2	0.011686	0.11633	9.86527	-0.0118
3	-0.00011	-0.0011	9.99999	0.00011
4	1.15E-10	1.2E-09	10	-1E-10

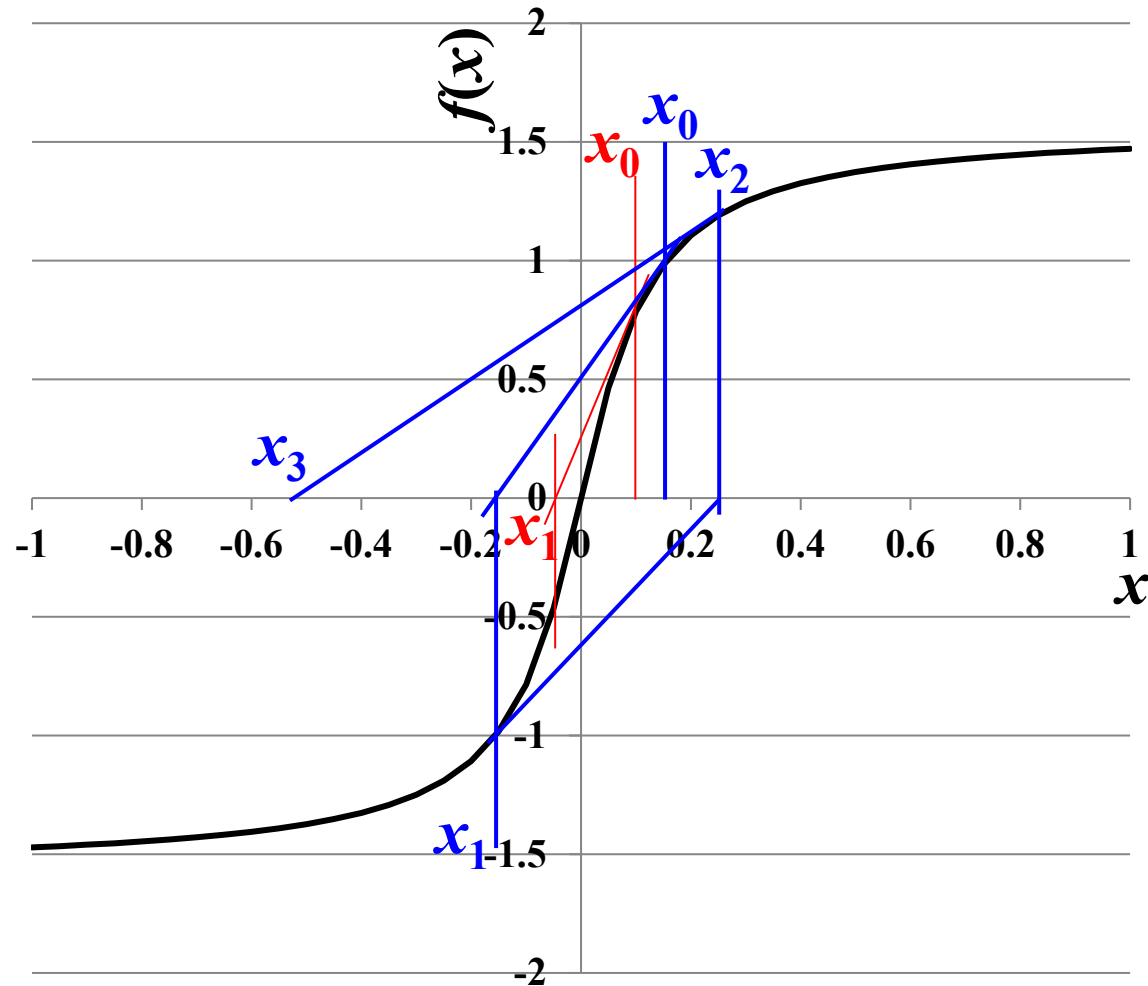




# Case Newton method fails

$$f(x) = \tan^{-1}(10x)$$

initial  $x = 0.15$



**Diverged ( $\lambda = 0$ )**

i	x	f(x)	df/dx	dx
0	0.15	0.98279	3.07692	-0.3194
1	-0.16941	-1.0375	2.58404	0.40152
2	0.232112	1.164	1.56553	-0.7435
3	-0.51141	-1.3777	0.36827	3.74095
4	3.229546	1.53984	0.00958	-160.76
5	-157.529	-1.5702	4E-06	389644
6	389486.7	1.5708	1.1E-12	-1E+12

$$x_{k+1} = x_k - f(x_k) / (f'(x_k) + \lambda)$$

$\lambda$ : Damping Factor

**Stabilize convergence  
by choosing  $\lambda(\lambda = 1)$**

i	x	f(x)	df/dx	dx
0	0.15	0.98279	3.07692	-0.2411
1	-0.09106	-0.7387	5.46675	0.11422
2	0.023161	0.2276	9.49088	-0.0217
3	0.001466	0.01466	9.99785	-0.0013
4	0.000133	0.00133	9.99998	-0.0001
5	1.21E-05	0.00012	10	-1E-05
6	1.1E-06	1.1E-05	10	-1E-06
7	1E-07	1E-06	10	-9E-08
8	9.09E-09	9.1E-08	10	-8E-09
9	8.27E-10	8.3E-09	10	-8E-10

# Program: Electron density in metal

## Issues for integrating $N(e)f(e)$

- Wide integration range  $E = 0 \sim E_F + \alpha k_B T$  – several eV (accuracy at the order of  $\exp(-\alpha)$ )
  - Important range for accuracy is the range of  $\alpha k_B T \sim 0.1$  eV around  $E_F$
  - For numerical integration,  $E$  mesh  $\Delta E$  should be very small around  $E_F$  (if  $0.01\alpha k_B T$ ,  $\Delta E \sim 1$  meV)  
=> Not good to use the same  $\Delta E$  for the whole integration range  $E = 0 \sim E_F + \alpha k_B T$
- => ▪ **Divide integration range** (Analytical integration may be employed for  $0 \sim E_F - \alpha k_B T$ )
- **Better to employ accuracy-guaranteed library for integration**  
`python integrate.quad()` can accept accuracy as `epsrel` variable

## Program: N-integration-metal.py

Ex.: `python N-integration-metal.py 300 5.0`

At 300 K,  $E_F = 5.0$  eV

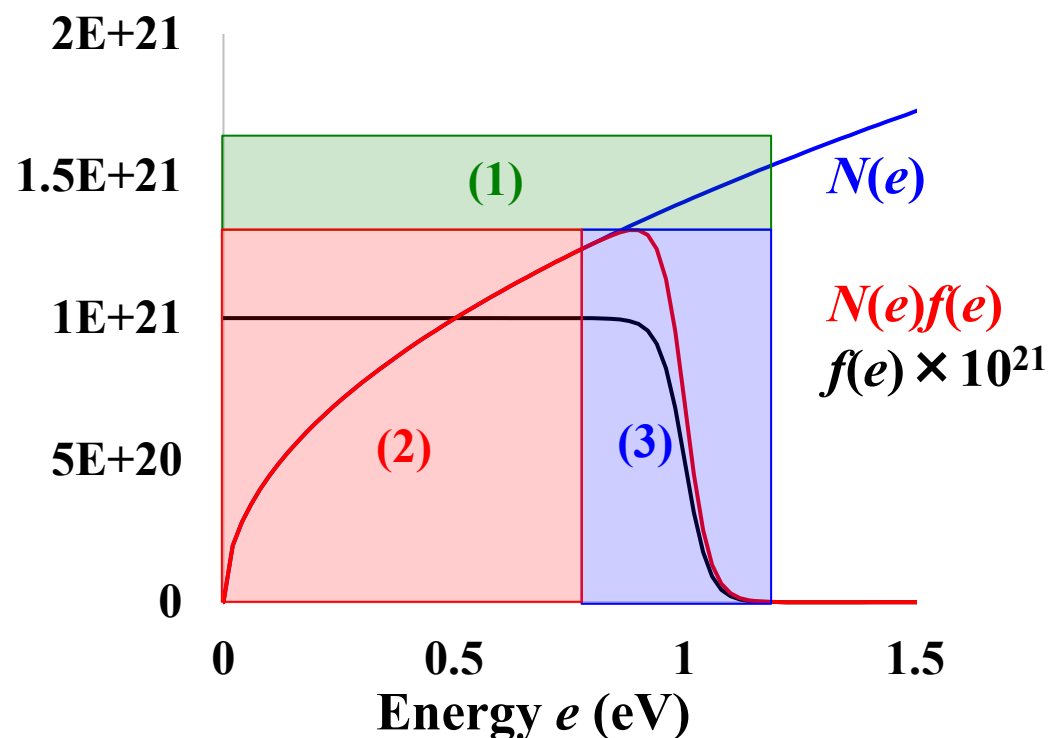
Time is measured for 300 cycles calculation

8 digit accuracy (`epsrel = 1e-8`),  $\alpha = 6$ :

range	time (300 cycles)
(1) $0 \sim E_F + \alpha k_B T$	0.109 s
(2) $0 \sim E_F - \alpha k_B T$	0.063 s
(3) $E_F - \alpha k_B T \sim E_F + \alpha k_B T$	0.016 s

(2) + (3) is faster by ~30 % than (1).

Employing analytical integration for (2)  
is faster by a factor of 10



# Program: $T$ dependence of $E_F$ for metal

$E_F(T)$  is determined by  $N_e = \int N(e)f(e, E_F)de$  for the given electron number  $N_e$

$N(e)f(e, E_F)$  is integrated in the range  $E = 0 - \infty$  (actually up to  $E_F + \alpha k_B T$ )

The initial value of  $E_F(T)$  can be taken as the analytical form of  $E_F(0)$  at 0 K.

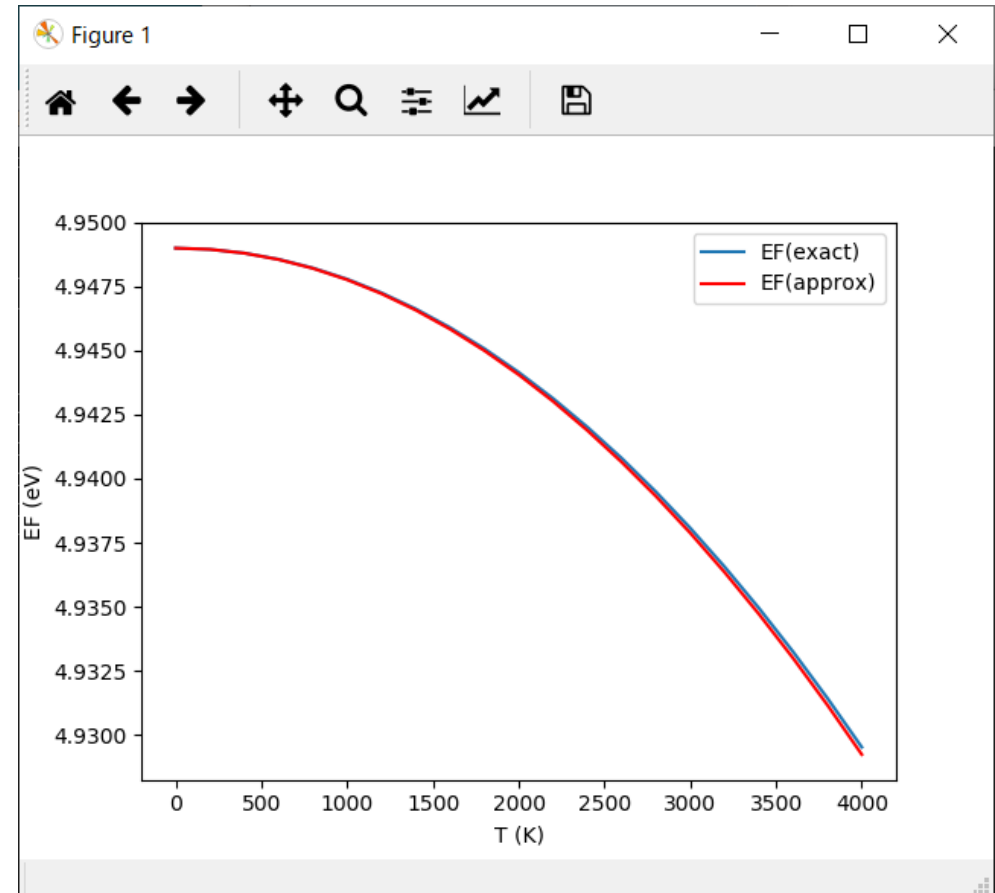
Since the variation of  $E_F(T)$  is small, the Newton method stability converges.

Compare with the approx. form  $E_F(T) = E_F(0) - \frac{\pi^2}{6} (k_B T)^2 N'(E_F(0))/N(E_F(0))$

Program: EF-T-metal.py

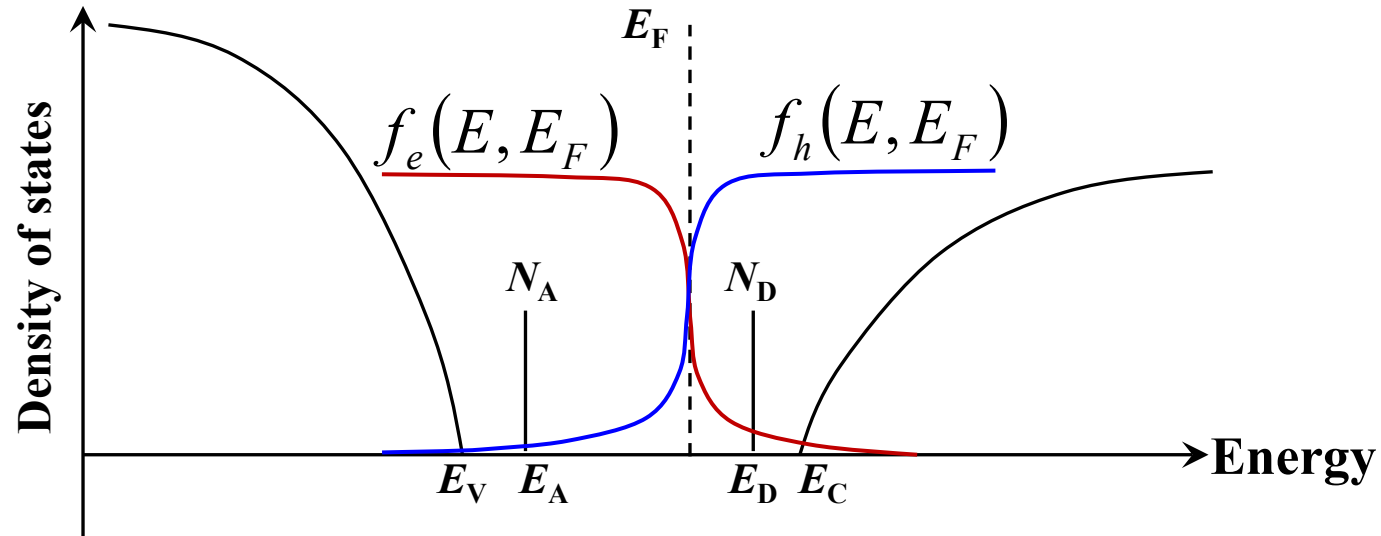
Ex.: `python EF-T-metal.py`

$T$ (K)	$E_F$ (Newton, eV)	$E_F$ (approx., eV)
0	4.948988	4.948988
600	4.948554	4.948544
1200	4.947248	4.947211
1800	4.945069	4.944990
2400	4.942013	4.941880
3000	4.938075	4.937882
3600	4.933247	4.932994
4000	4.929529	4.929243



# Density of states, $n_e$ , and $n_h$ in semiconductor

Total density of states:  $D(E) = D_e(E) + D_h(E) + D_D(E) + D_A(E)$



Valence band

$$D_h(E) = D_{V0} \sqrt{E_V - E}$$

$$D_A(E) = N_A \delta(E - E_A)$$

$$f_h(E, E_F) = \frac{1}{\exp(\beta(E_F - E)) + 1}$$

Free hole density

$$n_h = \int_{-\infty}^{E_V} f_h(E, E_F) D_h(E) dE$$

Ionized acceptor density

$$N_A^- = N_A (1 - f_h(E_A, E_F))$$

Conduction band

$$D_e(E) = D_{C0} \sqrt{E - E_C}$$

$$D_D(E) = N_D \delta(E - E_D)$$

$$f_e(E, E_F) = \frac{1}{\exp(\beta(E - E_F)) + 1}$$

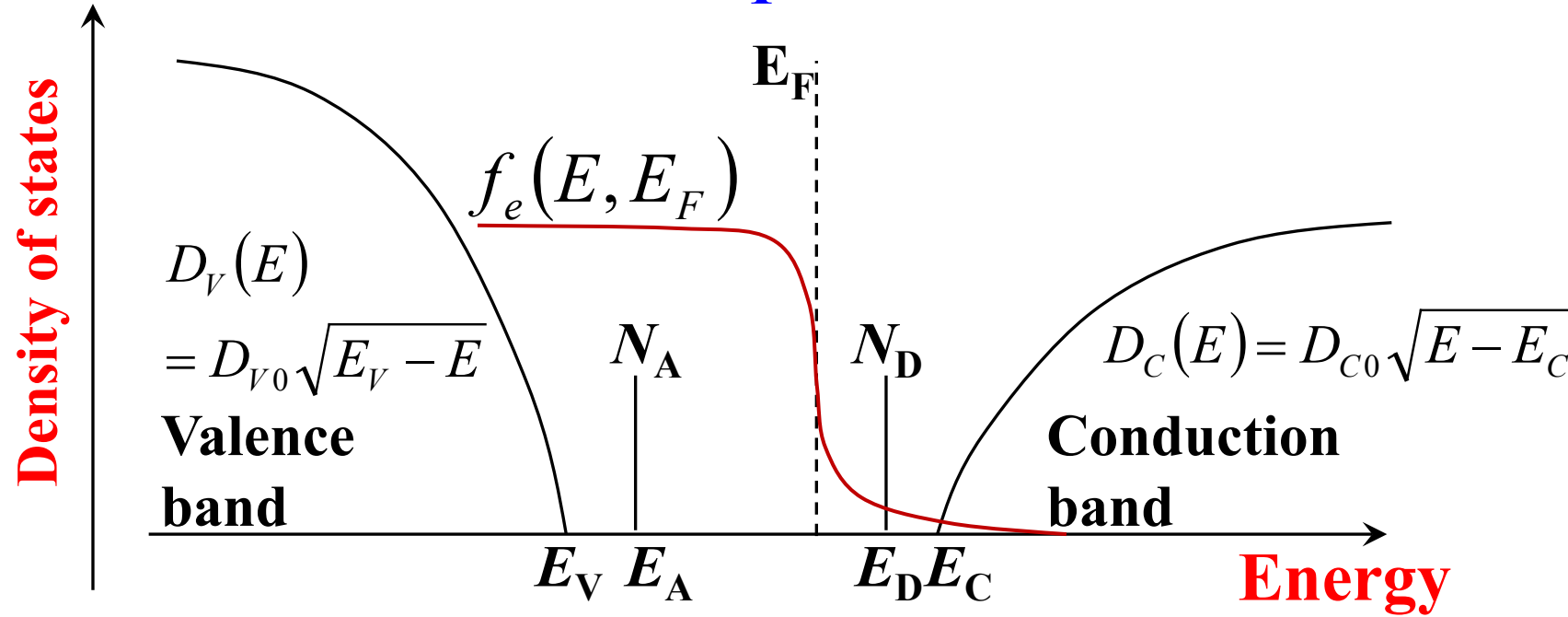
Free electron density

$$n_e = \int_{E_C}^{\infty} f_e(E) D_e(E) dE$$

Ionized donor density

$$N_D^+ = N_D (1 - f_e(E_D, E_F))$$

# How to determine $E_F$ for semiconductors



**Charge neutrality condition**

$$N_A^- + N_e = N_D^+ + N_h \quad \longrightarrow \quad E_F$$

$$N_e = \int_{E_C}^{\infty} D_C(E) f_e(E, E_F) dE$$

$$N_D^+ = N_D [1 - f_e(E_D, E_F)]$$



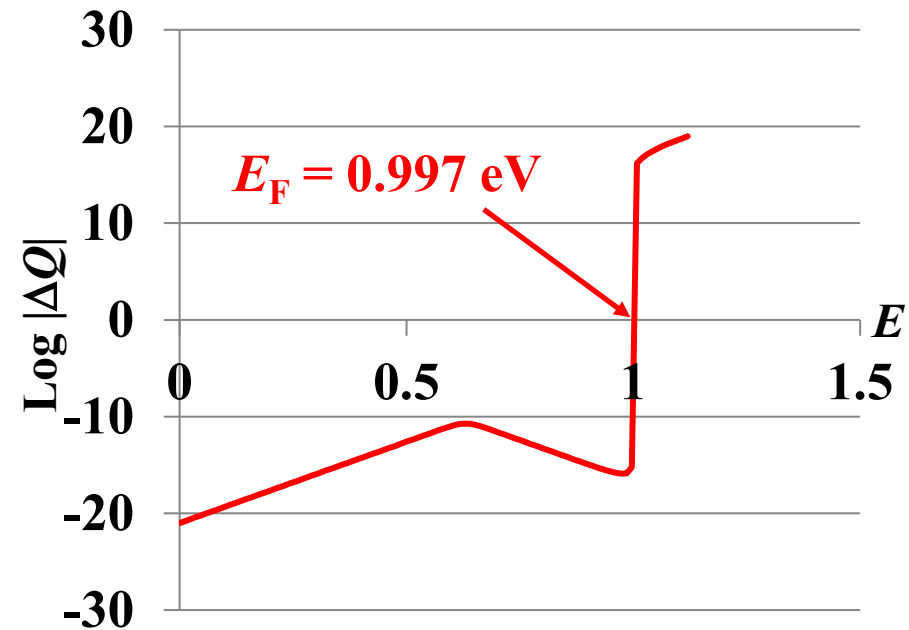
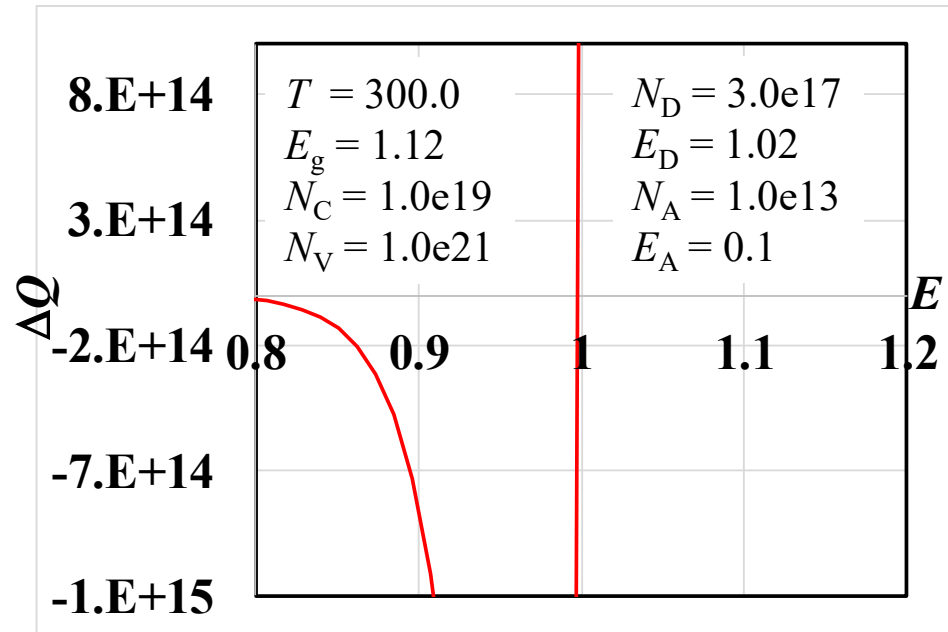
# How to calculate $E_F$ : Illustrative solution

$$N_e = \int_{E_C}^{\infty} D_C(E) f_e(E, E_F) dE \quad N_h = \int_{E_C}^{\infty} D_V(E) f_h(E, E_F) dE$$

$$N_D^+ = N_D [1 - f_e(E_D, E_F)] \quad N_A^- = N_A [1 - f_h(E_A, E_F)]$$

$$f_h(E, E_F) = 1 - f_e(E, E_F)$$

Plot  $\Delta Q = (N_A^- + N_e) - (N_D^+ + N_h)$  w.r.t.  $E_F$  and find  $\Delta Q = 0$



# Bisection method (二分法): Continuous func (連続関数)

Solution of  $f(x) = 0$  for (monotonic) continuous function  $f(x)$

1. Start from a range  $[x_0, x_1]$  where  $f(x_0) < 0$  &  $f(x_1) > 0$   
(or  $f(x_0) > 0$  &  $f(x_1) < 0$ )

\* **Solution exist in this range for a monotonic function**

2. Solve the equation by the following iterative procedure

Case  $f(x_0) < 0$  and  $f(x_1) > 0$ : Judge by  $f(x_0) \cdot f(x_1) < 0$

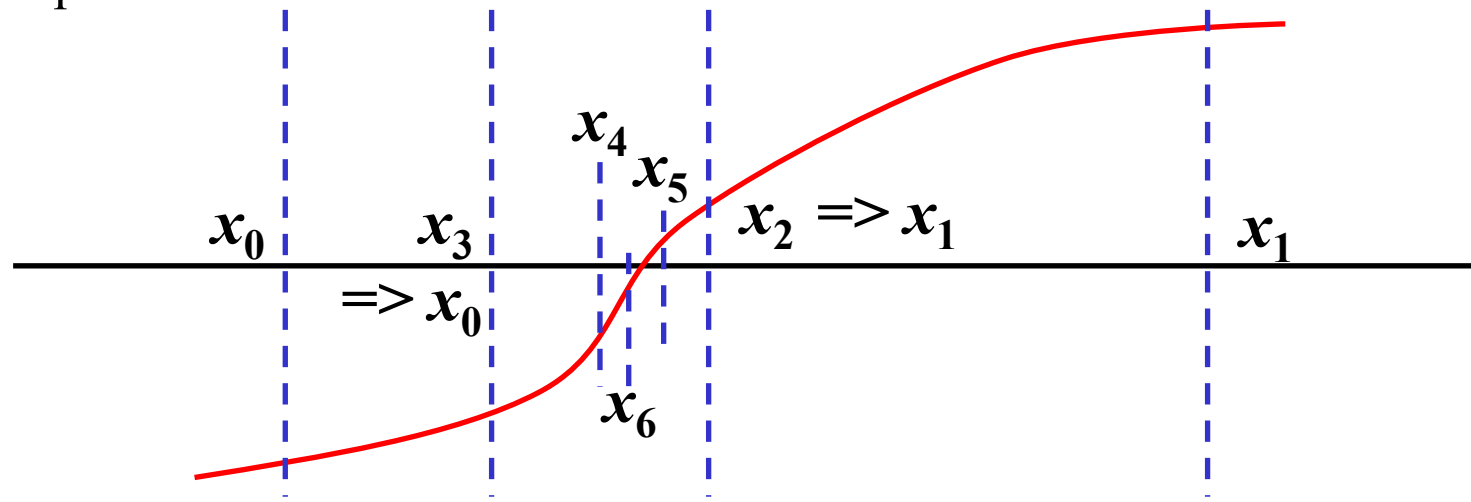
1.  $x_2 = (x_0 + x_1) / 2.0$

2. If  $f(x_2) > 0$  ( $f(x_0) \cdot f(x_2) < 0$ ),  $x_1$  is replaced with  $x_2$

If  $f(x_2) < 0$  ( $f(x_1) \cdot f(x_2) < 0$ ),  $x_0$  is replaced with  $x_2$

3. Solution  $x_2$  is obtained when  $|x_1 - x_0|$ ,  $|f(x_1) - f(x_0)|$  becomes less than EPS.

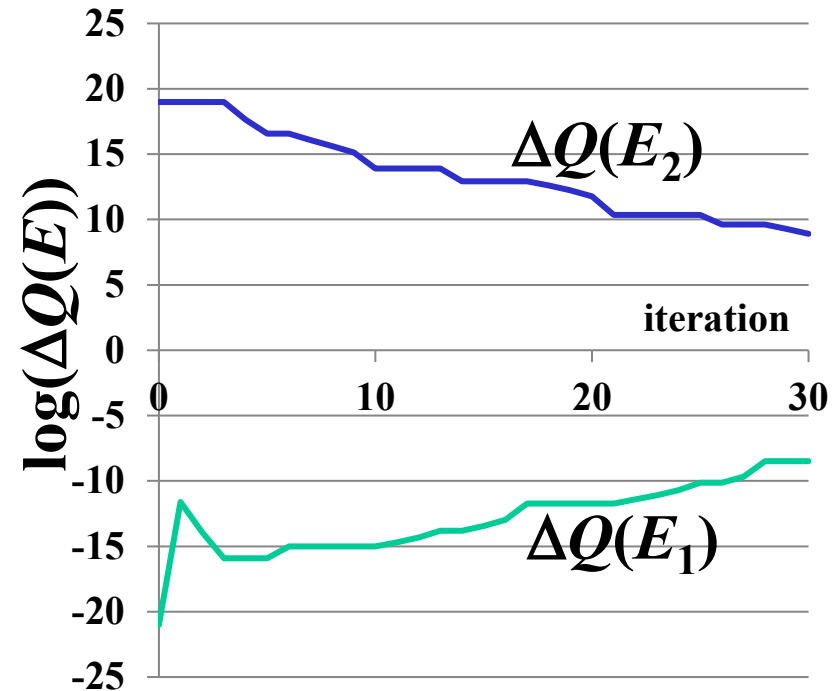
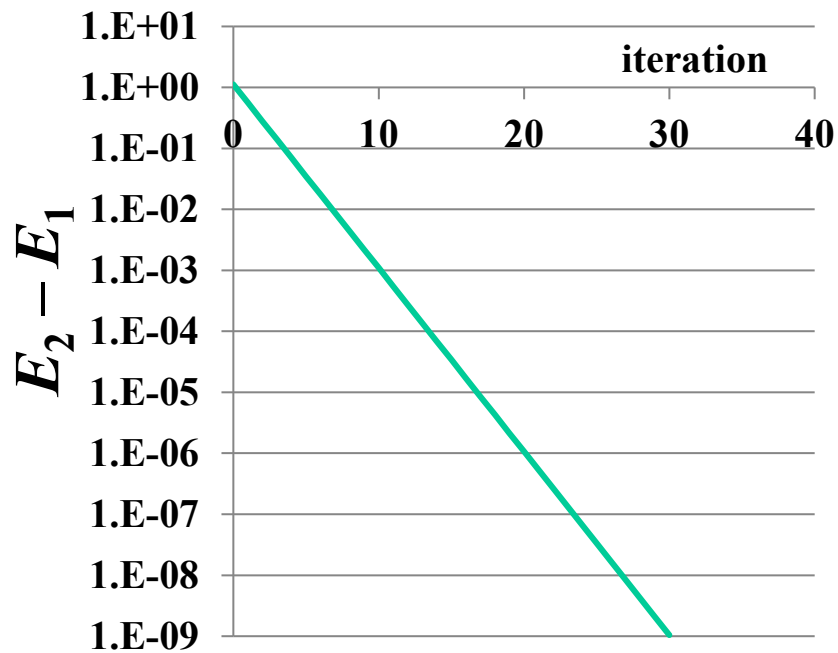
4. Repet 1 – 3



# $E_F$ by bisection method: Convergence procedure

Initial range:  $[E_1, E_2] = [E_V = 0, E_C = E_g]$

Find  $\Delta Q = (N_A^- + N_e) - (N_D^+ + N_h) = 0$



After 30 times iterations

$E_F = [0.9985173589, 0.9985173599]$

$dQ = [-3 \times 10^8, 8 \times 10^8]$

# Program: EF-T-semiconductor.py

## Program: EF-T-semiconductor.py

Usage: `python EF-T-semiconductor.py EA NA ED ND Ec Nv Nc`

Ex.: `python EF-T-semiconductor.py 0.05 1.0e15 0.95 1.0e16 1.0 1.2e19 2.1e18`

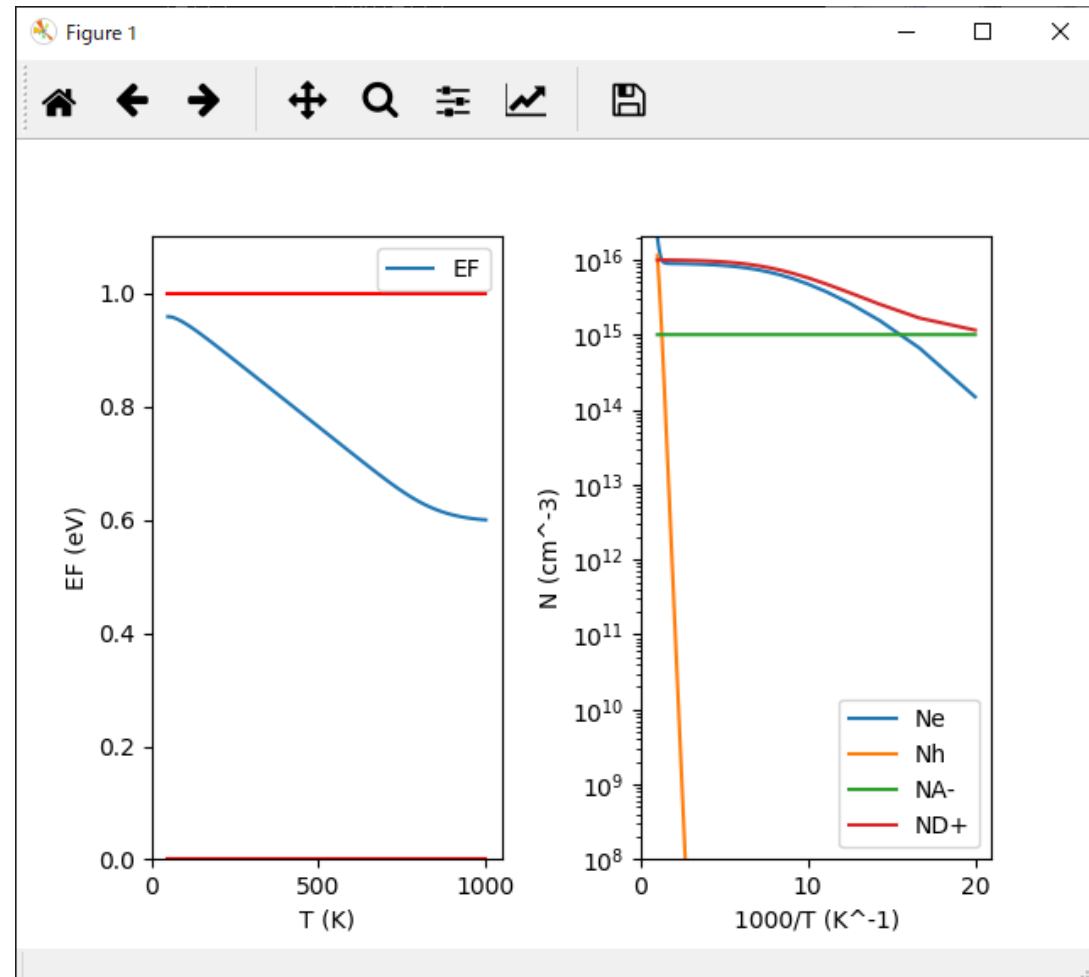
$E_c = 0$ ,  $E_v = 1.0$  eV (= band gap)

$E_A = 0.05$  eV,  $N_A = 10^{15}$  cm<sup>-3</sup>,

$E_D = 0.95$  eV,  $N_D = 10^{16}$  cm<sup>-3</sup>

$N_c = 1.2 \times 10^{19}$  cm<sup>-3</sup>

$N_v = 2.1 \times 10^{18}$  cm<sup>-3</sup>



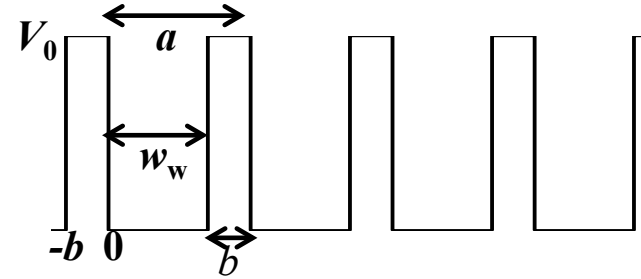
# Multi-values equation: Kronig-Penney model

Solution of  $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \phi = E\phi$

$\phi_k(x) = \exp(ikx)u(x)$ ,  $u(x+a) = u(x)$

In well:  $\phi(x) = A \exp(i\alpha x) + B \exp(-i\alpha x)$   $\alpha = \sqrt{2mE} / \hbar$

In barrier:  $\phi(x) = C \exp(\beta x) + D \exp(-\beta x)$   $\beta = \sqrt{2m(V_0 - E)} / \hbar$



Boundary condition:  $\phi_k(x)$  and  $\phi_k'(x)$  are continuous at  $x = 0$  and  $-b$

Bloch's theorem :  $\phi_k(x + a) = \lambda \phi_k(x)$ ,  $\lambda = \exp(ika)$

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ i\alpha & -i\alpha & -\beta & \beta \\ \exp(i\alpha w_w) & \exp(-i\alpha w_w) & -\lambda \exp(-\beta b) & -\lambda \exp(\beta b) \\ i\alpha \exp(i\alpha w_w) & -i\alpha \exp(-i\alpha w_w) & -\beta \lambda \exp(-\beta b) & \beta \lambda \exp(\beta b) \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The determinant of the left matrix must be 0:

$$\cos ka = \left( \frac{\beta(E)^2 - \alpha(E)^2}{2\alpha(E)\beta(E)} \sin \alpha(E)w_w \sinh \beta(E)b + \cos \alpha(E)w_w \cosh \beta(E)b \right)$$

**Scan  $E$  in possible range to find all the solutions,  
then use them for initial values  
to obtain accurate values by Newton-Raphson method**

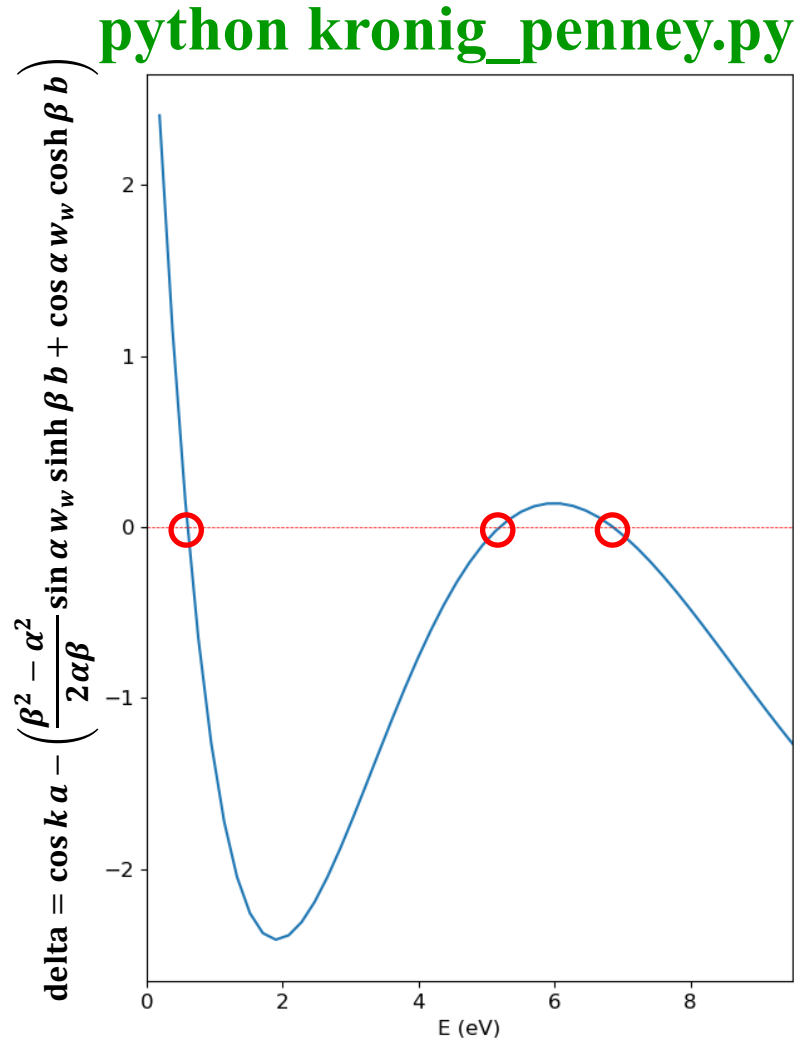


# Program: Kronig-Penney model

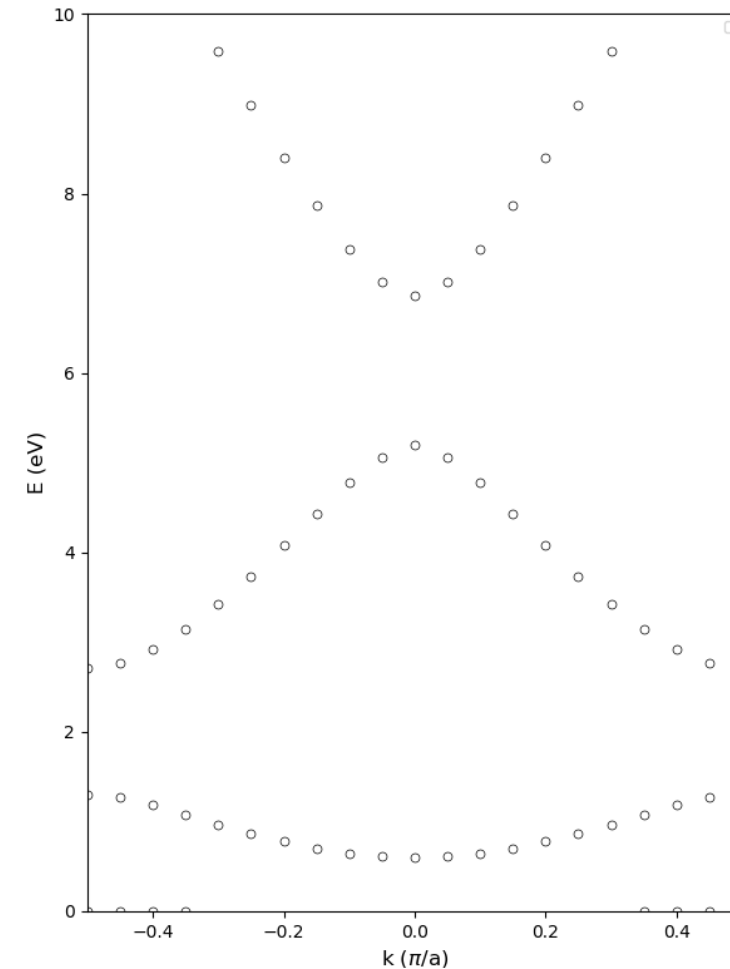
Program: `kronig_penney.py`

Lattice parameter (Si)  $a = 5.4064 \text{ \AA}$       Effective mass  $m^* = 1.0m_e$

Barrier width  $0.5 \text{ \AA}$       Barrier height  $10.0 \text{ eV}$



python `kronig_penney.py` band



# **Non-linear (NL) optimization**

## 非線形最適化

# Optimization

**Objective:** Find parameters  $\mathbf{x}_i$  to minimize or maximize  
a objective function  $F(\mathbf{x}_i)$

**Maximization problem for  $F(\mathbf{x}_i)$   
is equivalent to minimization problem for  $-F(\mathbf{x}_i)$**

**Examples:**

- **Linear least-squares method:** A linear minimization problem for L2 norm of errors
- **Curve fitting:** A non-linear minimization problem for L2 norm of errors
- **Structure relaxation:** A non-linear minimization for total energy

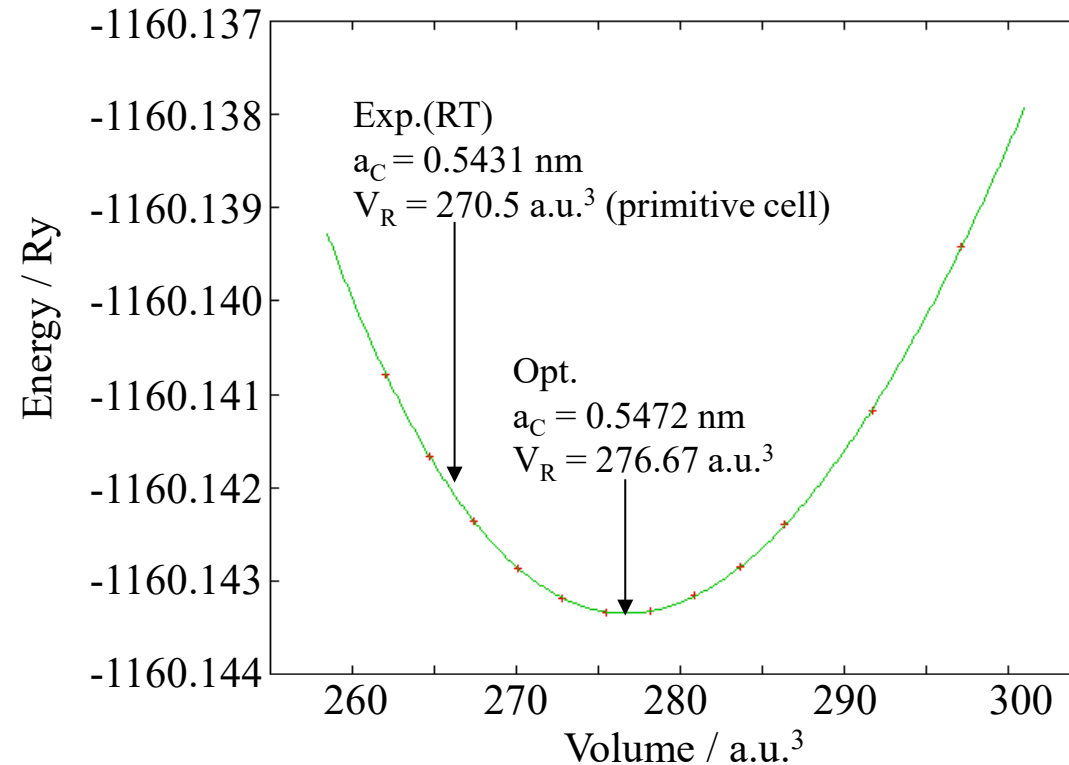
**Focus on minimization problem**

# NL optimization of crystal structure:

## Illustrative approach

安定構造: 図解による解法

Calculate total energy by quantum calculations by varying a lattice parameter  
*ex. Si*



$$E = E_{\min} + 1/2B_0(V/V_0)^2$$

$$B_0 \text{ (GPa)} = 87.57 \text{ GPa (exp: 97.88 GPa)}$$

# Profile models used for spectroscopy

## Lorentz function

$$I_L(x) = \frac{1}{1 + [(x - x_0)/w]^2}$$

**w**: half width at half maximum

## Gauss function

$$I_G(x) = \frac{1}{a_w w \pi^{1/2}} \exp\left\{-\left[(x - x_0)/(a_w w)\right]^2\right\}$$
$$a_w = (\ln 2)^{-1/2} = 0.832554611$$

## Voigt function:

E.g., observed is convolution of sample spectrum  $I_L(x)$  and apparatus function  $I_G(x)$

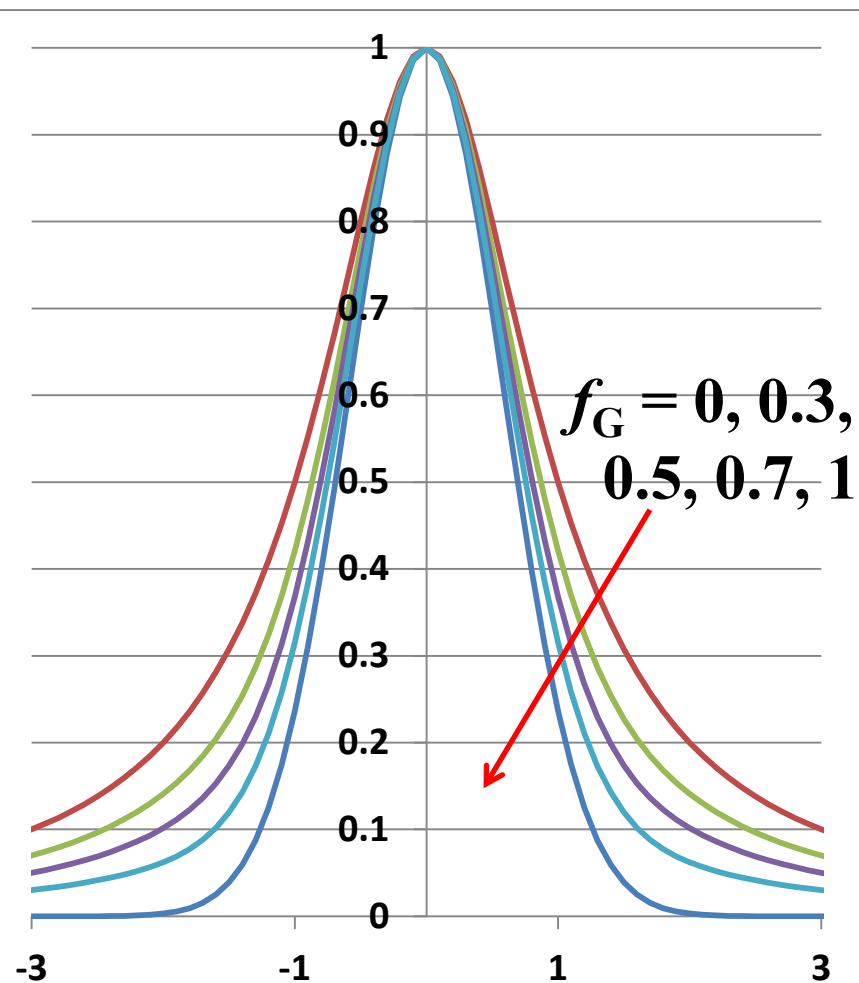
$$I_V(x) = \int_{-\infty}^{\infty} I_G(x') I_L(x - x') dx'$$
$$= \frac{a_V}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-x'^2)}{a_V^2 + (x - x')^2} dx'$$

## Pseudo-Voigt function:

Simplified Voigt function

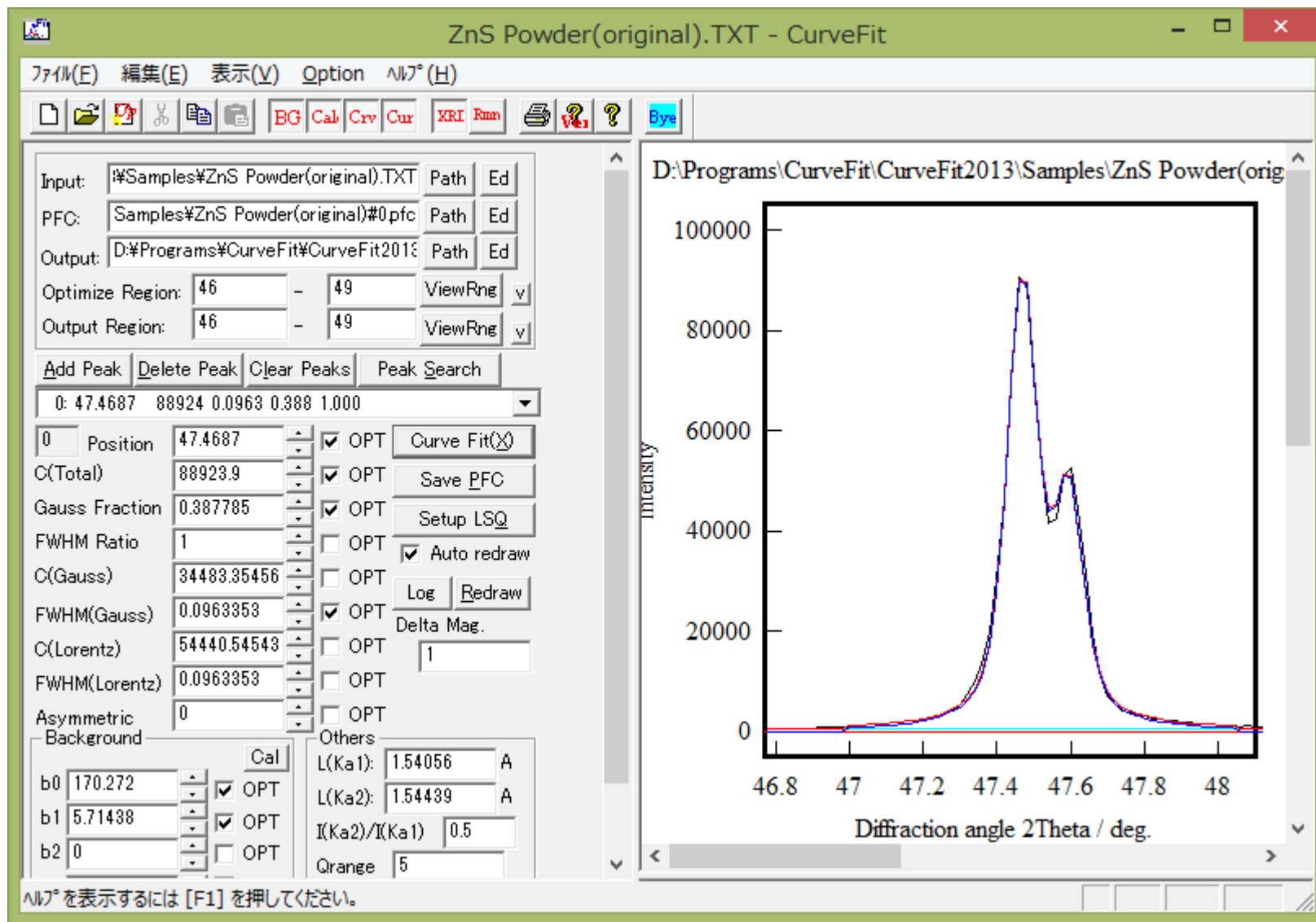
$$I_{PV}(x) = f_G I_G(x) + (1 - f_G) I_L(x)$$

**$f_G$** : Gauss fraction



# Ex.: Deconvolution of powder XRD peak

Incorporate the intensity ratio from  $K\alpha_1$  and  $K\alpha_2$  at 2:1



# Methods of non-linear (NL) optimization

To find a minimum (maximum) of **target function**  $F(x)$ :

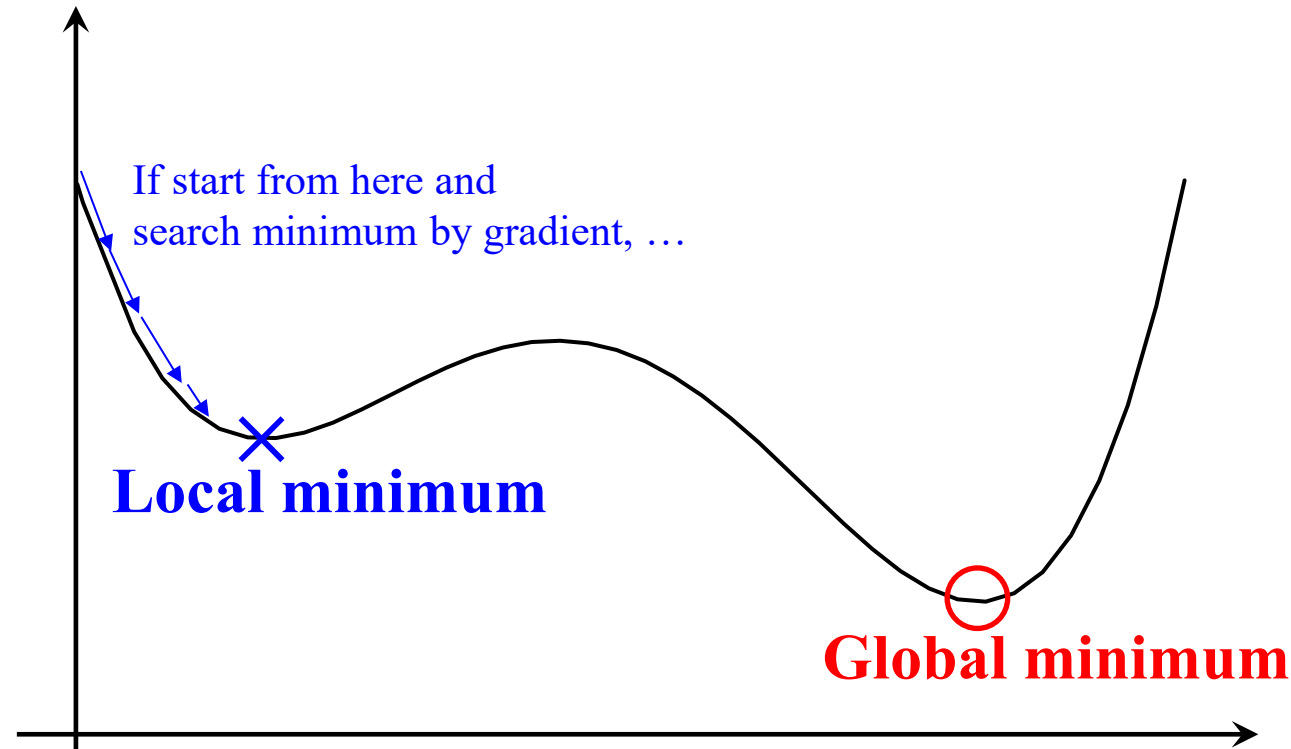
**Direct search method** (直接探索法)

Trial and errors to find a minimum,  
but following a certain defined procedures

**Gradient method** (勾配法):

Use first differential to find the direction of minimum

# Global minimum (大域的最小値) vs local minimum (極小値)



**How to avoid to be trapped by local minimum:**

1. Employ a large initial search range
2. Not use a direct value of gradient

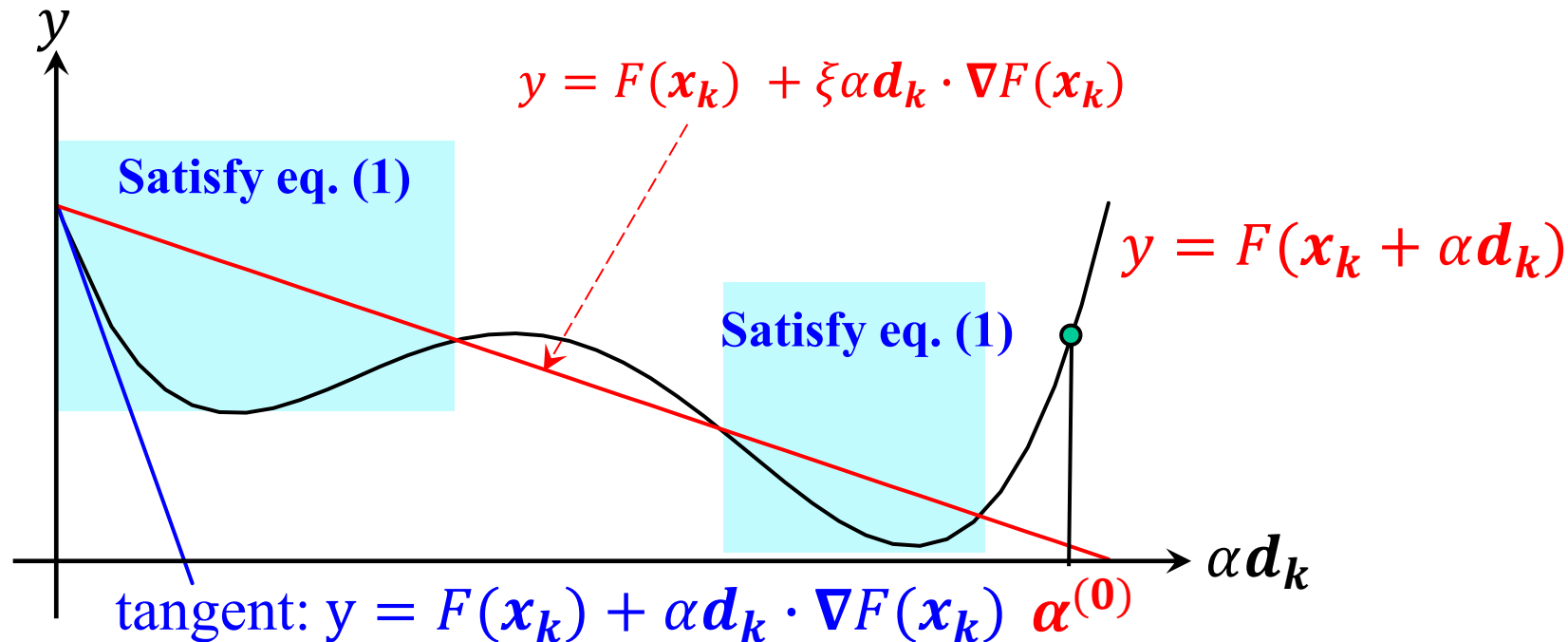


# Line search (直線探索法): Armijo condition

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

## Armijo (アルミホ) condition (eq. (1)) and algorism:

1. Provide initial  $\mathbf{x}_k$ , choose constant  $\xi$  and  $\tau$  ( $0 < \xi < 1$ ,  $0 < \tau < 1$ )
2. Find search direction  $\mathbf{d}_k$  (e.g., by steepest descent method)
3. Find  $\alpha > 0$  so as to satisfy  $F(\mathbf{x}_k + \alpha \mathbf{d}_k) \leq F(\mathbf{x}_k) + \xi \alpha \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k)$  (1)
  - (i)  $\beta_{k,0} = 1, i = 0$
  - (ii) if  $F(\mathbf{x}_k + \beta_{k,i} \mathbf{d}_k) \leq F(\mathbf{x}_k) + \xi \beta_{k,i} \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k)$  go to step 4, or go to (iii)
  - (iii)  $\beta_{k,i+1} = \tau \beta_{k,i}$  and go to (ii)
4.  $\alpha = \beta_{k,i}$

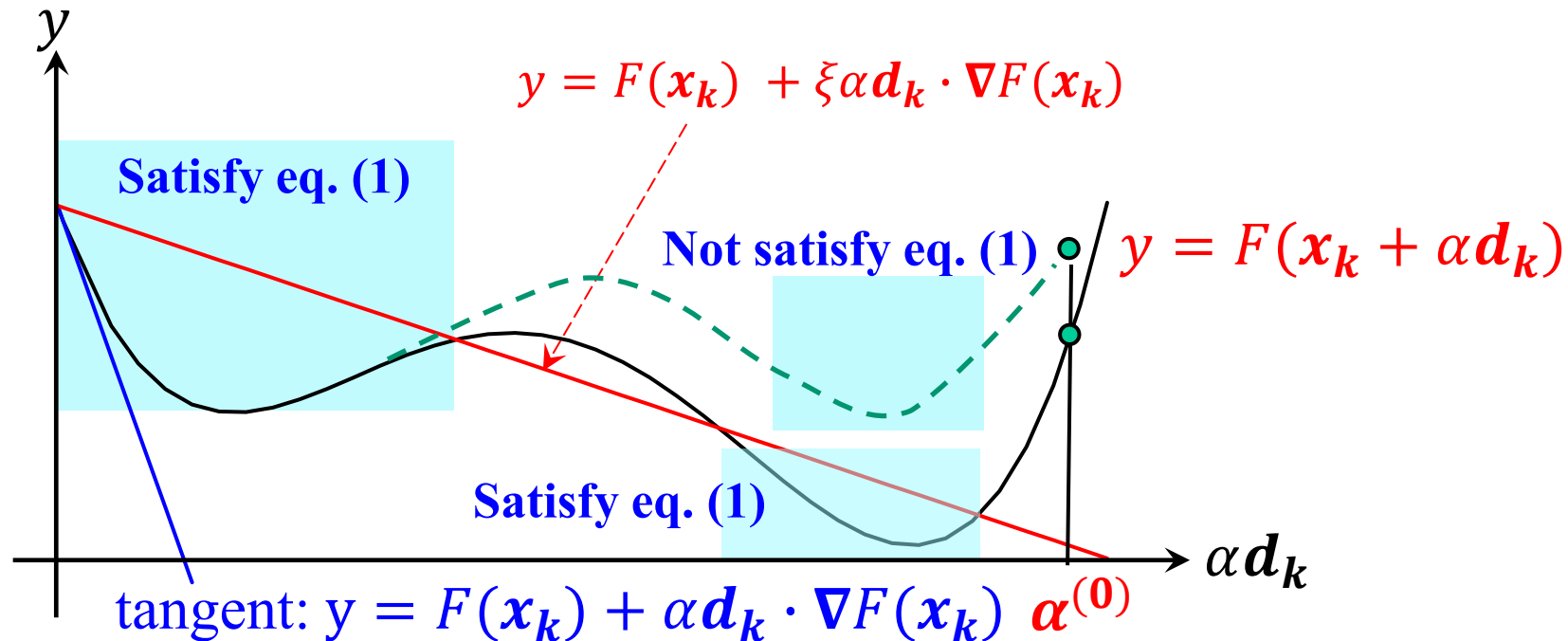


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  - (i)  $\beta_{k,0} = 1, i = 0$
  - (ii) if  $F(\mathbf{x}_k + \beta_{k,i} \mathbf{d}_k) \leq F(\mathbf{x}_k) + \xi \beta_{k,i} \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k)$  go to step 4, or go to (iii)
  - (iii)  $\beta_{k,i+1} = \tau \beta_{k,i}$  and go to (ii)
4.  $\alpha = \beta_{k,i}$



# Line search (直線探索法): Wolfe condition

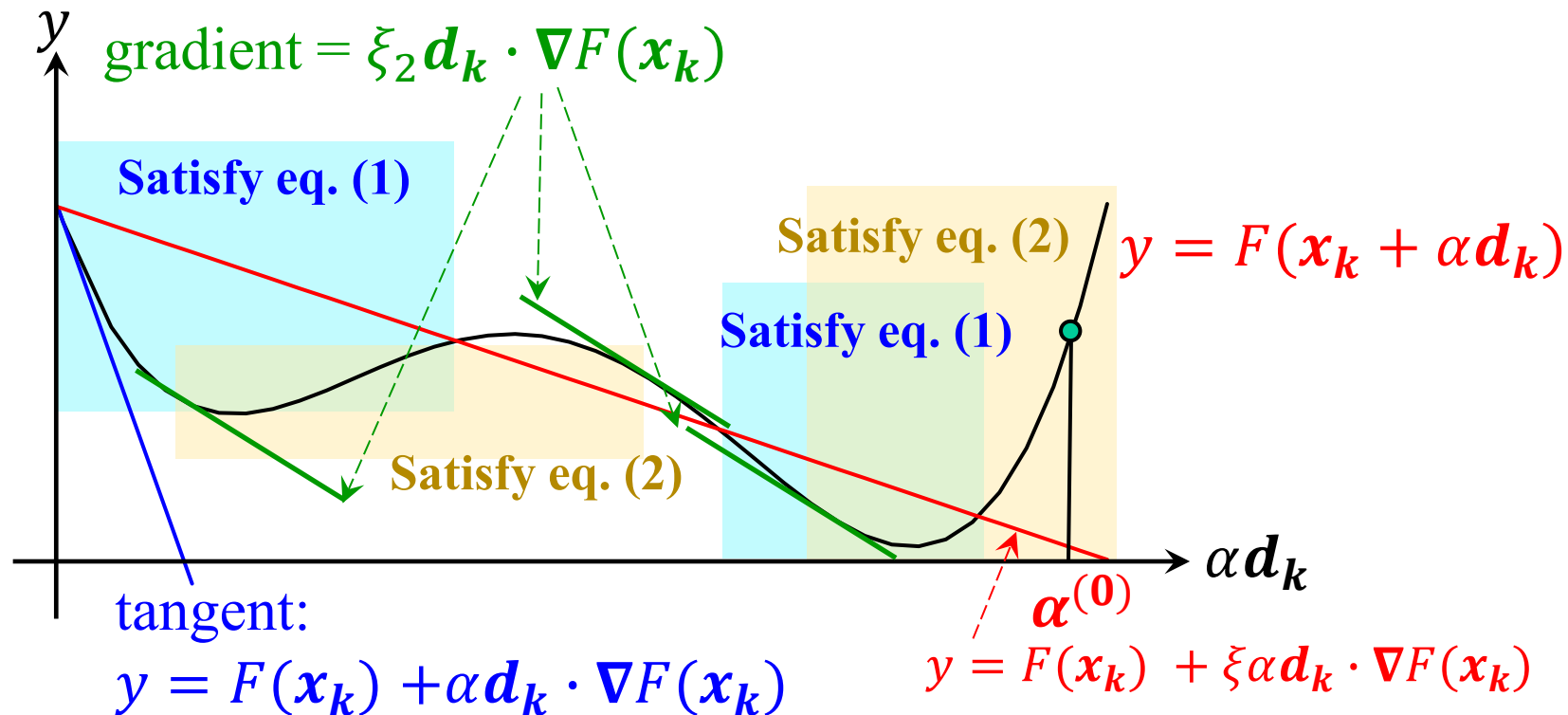
矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

## Wolfe (ウルフ) condition:

1. Find search direction  $\mathbf{d}_k$  (e.g., by steepest descent method)
2. Choose constants  $\xi_1$  and  $\xi_2$  that satisfy  $0 < \xi_1 < \xi_2 < 1$
3. Find  $\alpha > 0$  so as to satisfy:

$$F(\mathbf{x}_k + \alpha \mathbf{d}_k) \leq F(\mathbf{x}_k) + \xi \alpha \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k) \quad (1)$$

$$\xi_2 \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k) \leq \mathbf{d}_k \cdot \nabla F(\mathbf{x}_k + \alpha \mathbf{d}_k) \quad (2)$$



## Bisection method (二分法) vs Golden-section search (黄金分割探索)

### Bisection method: Find solution of $f(x) = 0$ for monotonous continuous function

Unique solution exists in the range  $[x_0^{(0)}, x_2^{(0)}]$  if  $f(x_0^{(0)})f(x_2^{(0)}) < 0$

Add  $x_1^{(0)}$  in  $[x_0^{(0)}, x_2^{(0)}]$  ( $x_0^{(0)} < x_1^{(0)} < x_2^{(0)}$ )

Case 1: If  $f(x_0^{(0)})f(x_1^{(0)}) < 0$ , solution is in  $[x_0^{(0)}, x_1^{(0)}]$

Next search range is reduced to  $x_0^{(1)} := x_0^{(0)}$ ,  $x_1^{(1)} := x_3^{(0)} = \frac{x_0^{(0)} + x_1^{(0)}}{2}$ ,  $x_2^{(1)} := x_1^{(0)}$

Case 2: If  $f(x_1^{(0)})f(x_2^{(0)}) < 0$ , solution is in  $[x_1^{(0)}, x_2^{(0)}]$

Next search range is reduced to:  $x_0^{(1)} := x_1^{(0)}$ ,  $x_1^{(1)} := x_3^{(0)} = \frac{x_1^{(0)} + x_2^{(0)}}{2}$ ,  $x_2^{(1)} := x_2^{(0)}$

### Golden-section search: Find minimum for single downward convex continuous func $f(x)$

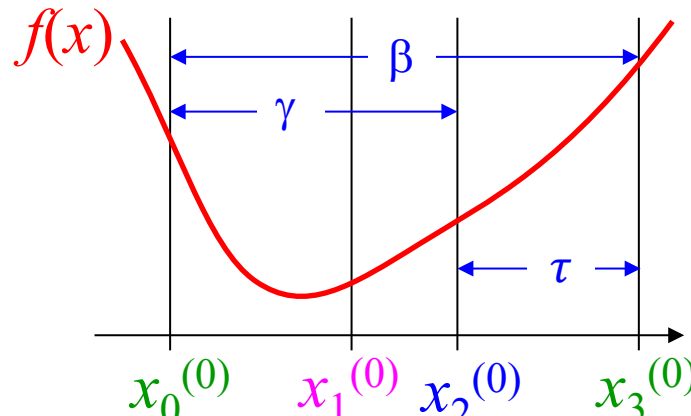
Unique solution exists in the range  $[x_0^{(0)}, x_3^{(0)}]$  if  $f(x_1^{(0)}) < f(x_0^{(0)}), f(x_3^{(0)})$  for  $x_0^{(0)} < x_1^{(0)} < x_3^{(0)}$

Add  $x_2^{(0)}$  in  $[x_0^{(0)}, x_3^{(0)}]$  ( $x_0^{(0)} < x_1^{(0)} < x_2^{(0)} < x_3^{(0)}$ )

Case 1: if  $f(x_1^{(0)}) < f(x_2^{(0)})$ , solution is in  $[x_0^{(0)}, x_2^{(0)}]$

Replace  $x_2^{(0)}$  with  $x_4^{(0)}$  in  $[x_0^{(0)}, x_1^{(0)}]$

Next search range is reduced to  $x_0^{(1)} := x_0^{(0)} < x_1^{(1)} := x_4^{(0)} < x_2^{(1)} := x_1^{(0)} < x_3^{(1)} := x_2^{(0)}$



# Golden-section search (黄金分割探索)

For downward convex continuous function, unique solution exists

in the range  $[x_0^{(0)}, x_3^{(0)}]$  if  $f(x_1^{(0)}), f(x_2^{(0)}) < f(x_0^{(0)}), f(x_3^{(0)})$  for  $x_0^{(0)} < x_1^{(0)} < x_2^{(0)} < x_3^{(0)}$

Case 1: if  $f(x_1^{(0)}) < f(x_2^{(0)})$ , solution is in  $[x_0^{(0)}, x_2^{(0)}]$

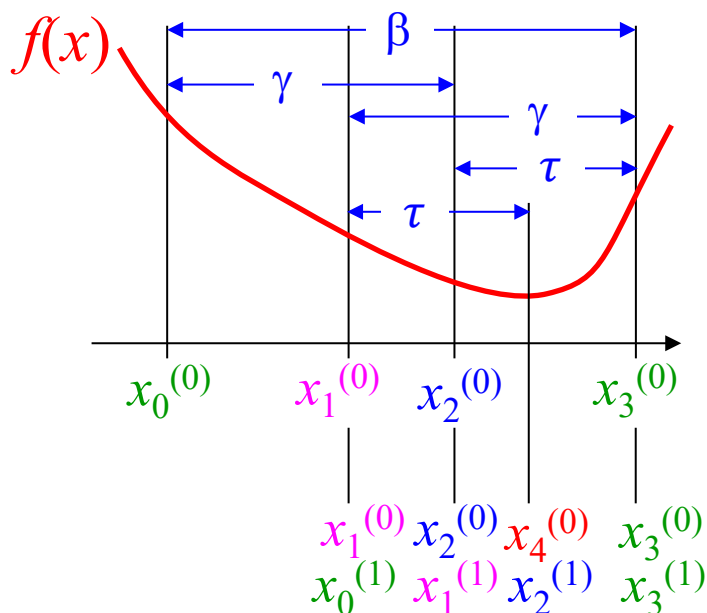
Replace  $x_2^{(0)}$  with  $x_4^{(0)}$  in  $[x_0^{(0)}, x_1^{(0)}]$

Next search range is reduced to  $x_0^{(1)} := x_0^{(0)} < x_1^{(1)} := x_4^{(0)} < x_2^{(1)} := x_1^{(0)} < x_3^{(1)} := x_2^{(0)}$

Case 2: if  $f(x_1^{(0)}) > f(x_2^{(0)})$ , solution is in  $[x_1^{(0)}, x_3^{(0)}]$

Replace  $x_0^{(0)}$  with  $x_4^{(0)}$  in  $[x_2^{(0)}, x_3^{(0)}]$

Next search range is reduced to  $x_0^{(1)} := x_1^{(0)} < x_1^{(1)} := x_2^{(0)} < x_2^{(1)} := x_4^{(0)} < x_3^{(1)} := x_3^{(0)}$



Strategy: keep the ratio of  $x_0^{(k)}, x_1^{(k)}, x_2^{(k)}, x_3^{(k)}$  constant for iteration steps

$$\beta = x_3^{(k)} - x_0^{(k)}$$

$$\gamma = x_2^{(k)} - x_0^{(k)} = x_3^{(k)} - x_1^{(k)}$$

$$\tau = \beta - \gamma$$

$$x_4^{(k)} = x_1^{(k)} + \tau$$

To keep the ratio for next step (k+1)

$$\beta : \gamma = x_3^{(k+1)} - x_0^{(k+1)} : x_2^{(k+1)} - x_0^{(k+1)}$$

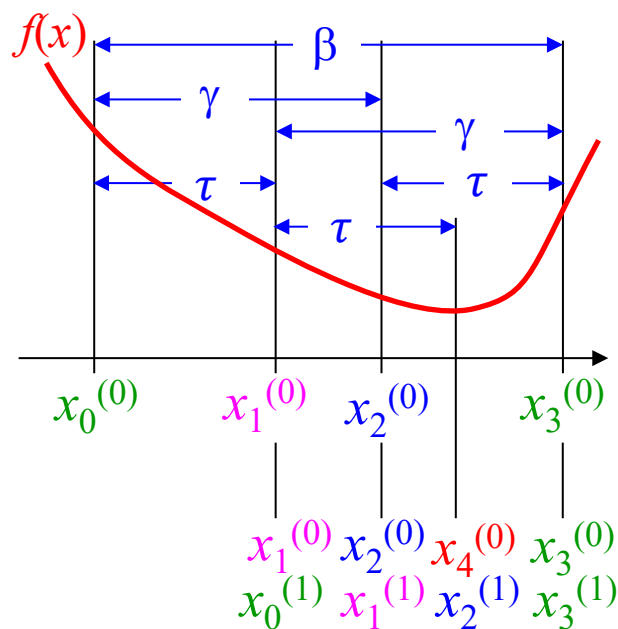
$$= x_3^{(k)} - x_1^{(k)} : x_4^{(k)} - x_1^{(k)} = \gamma : \tau$$

$$\tau = \beta - \gamma \text{ から}$$

$$\frac{\beta}{\gamma} = \frac{1+\sqrt{5}}{2} \text{ Golden number}$$

# Golden-section search (黄金分割探索)

Minimum solution of downward convex continuous function  $f(x)$



$$\frac{\beta}{\gamma} = \frac{1+\sqrt{5}}{2}$$

$$\eta = \frac{\tau}{\beta} = \frac{\beta-\gamma}{\beta} = 1 - \frac{2}{\sqrt{5}+1} = \frac{\sqrt{5}-1}{\sqrt{5}+1}$$

1. For  $x_0^{(0)} < x_1^{(0)} < x_2^{(0)} < x_3^{(0)}$ , assign initial parameters as:

$$\beta^{(0)} = x_3^{(0)} - x_0^{(0)}$$

$$\tau^{(0)} = \eta \beta^{(0)}$$

$$x_1^{(0)} = x_0^{(0)} + \tau^{(0)}$$

$$x_2^{(0)} = x_3^{(0)} - \tau^{(0)}$$

2. Terminate if  $|\beta^{(k)}| < \text{eps}$

$$3. \quad \beta^{(k+1)} = \tau^{(k)}$$

$$\tau^{(k+1)} = \eta \beta^{(k+1)}$$

4. If  $f(x_1^{(k)}) < f(x_2^{(k)})$ , substitute  $x_3^{(k)}$  for  $x_4^{(k)} = x_2^{(k)} - \tau^{(k)}$  as:

$$x_0^{(k+1)} = x_0^{(k)}, x_1^{(k+1)} = x_2^{(k)} - \tau^{(k)}, x_2^{(k+1)} = x_1^{(k)}, x_3^{(k+1)} = x_2^{(k)}$$

If  $f(x_1^{(k)}) > f(x_2^{(k)})$ , substitute  $x_0^{(k)}$  for  $x_4^{(k)} = x_2^{(k)} + \tau^{(k)}$  as:

$$x_0^{(k+1)} = x_1^{(k)}, x_1^{(k+1)} = x_2^{(k)}, x_2^{(k+1)} = x_1^{(k)} + \tau^{(k)}, x_3^{(k+1)} = x_3^{(k)}$$

Go to step 1

# Methods of non-linear (NL) optimization

To find a minimum (maximum) of **target function**  $F(x)$ :

**Direct search method** (直接探索法)

Trial and errors to find a minimum,  
but following a certain defined procedures

**Gradient method** (勾配法):

Use first differential to find the direction of minimum

# Steepest descent method (SD, 最急降下法)

Search minimum/maximum only by first derivatives

Objective function (multi-variable,  $x_j$ ):  $F(x_j)$

Concept: Minimum/Maximum may be found in the direction  $(\partial F(x_j)/\partial x_i)$

$$x_i^{(k+1)} = x_i^{(k)} - \alpha \partial F(x_j^{(k)})/\partial x_i$$

Need to choose/find an appropriate  $\alpha$  so as to take the minimum  $F(x_j^{(k)})$

Variations to choose  $\alpha$ :

(i) Simple: Choose small  $\alpha$

(ii) Direct search (直接探索)

Armijo / Wolfe condition



# Steepest Descend (SD) method (最急降下法)

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

Search minimum only by first derivatives. Simplest one among gradient methods

- SD:  $S^2$  would decrease in the vector  $-(df/dx_i)dx_i$

$$x_i^{(k+1)} = x_i^{(k)} - \alpha(df/dx_i)$$

$\alpha_k$  may be a small constant step

or determined by a line search method

ex. in right figure:

$$S^2 = f(x_i) = 5x_1^2 + x_2^2, \text{ initial } x_1 = 0.7, x_2 = 1.5$$

- SD method

$\alpha = 0.3$ : Diverged (not shown in the graph)

0.2, 0.15: Converged, but oscillated

0.1: Reach final solution by one cycle calculation

0.01: Not oscillated, but slowly converged

- Newton method

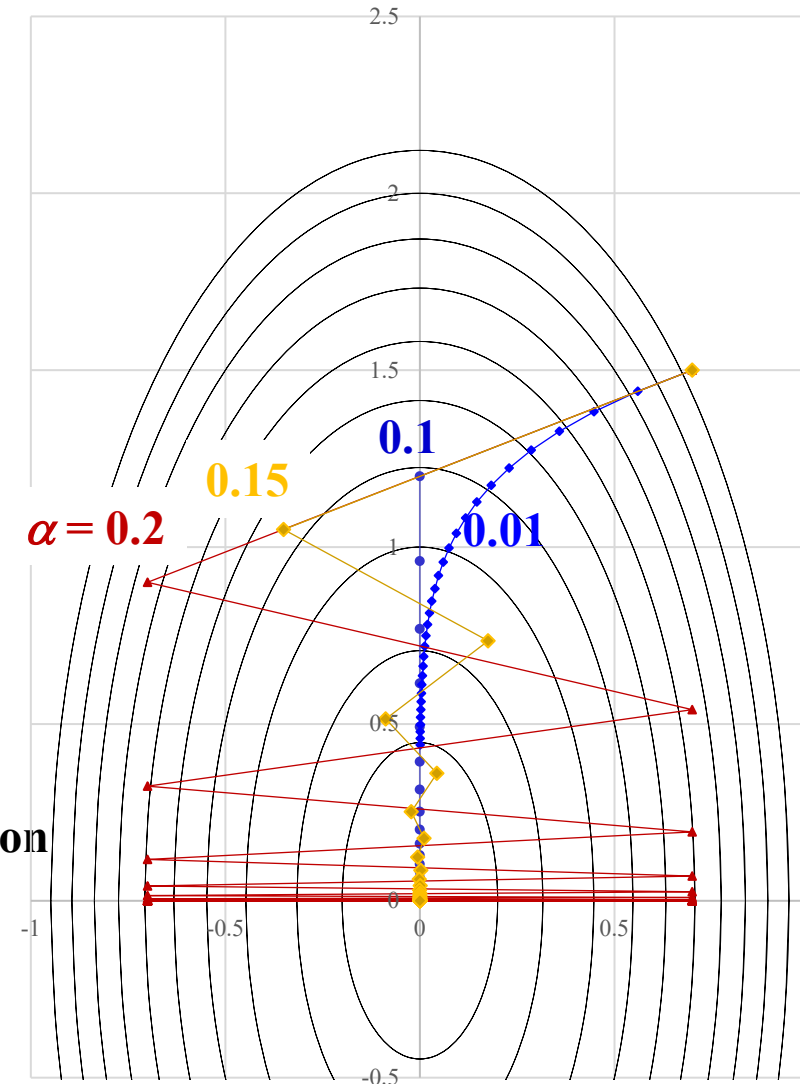
One cycle calculation provides the final solution  
for quadratic problems

楕円問題の場合は一度目の計算で最適値に到達

**Problem:** If  $S^2$  is highly anisotropic, the SD direction  
would be different largely from the minimization

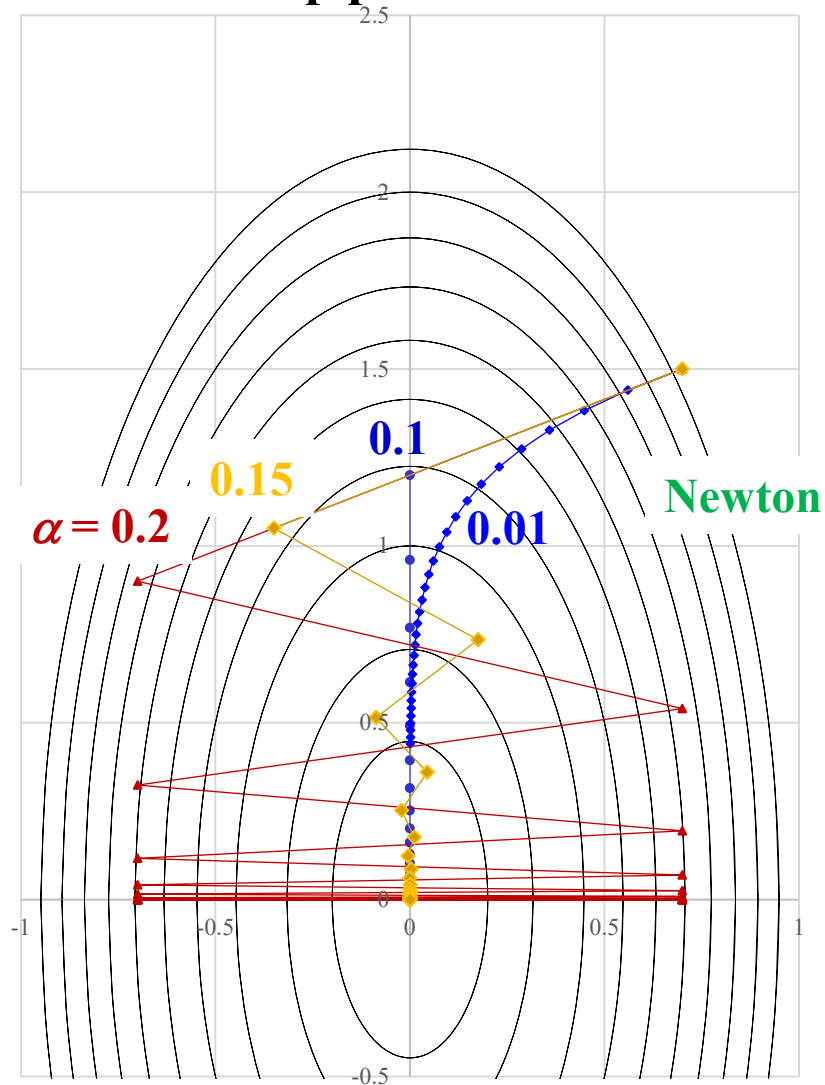
**direction**  $S^2$  が大きく非対称な場合、最急勾配方向は最小値方向とは  
大きく異なることがある

=> **Conjugate Gradient (CG) method** (共役勾配法)

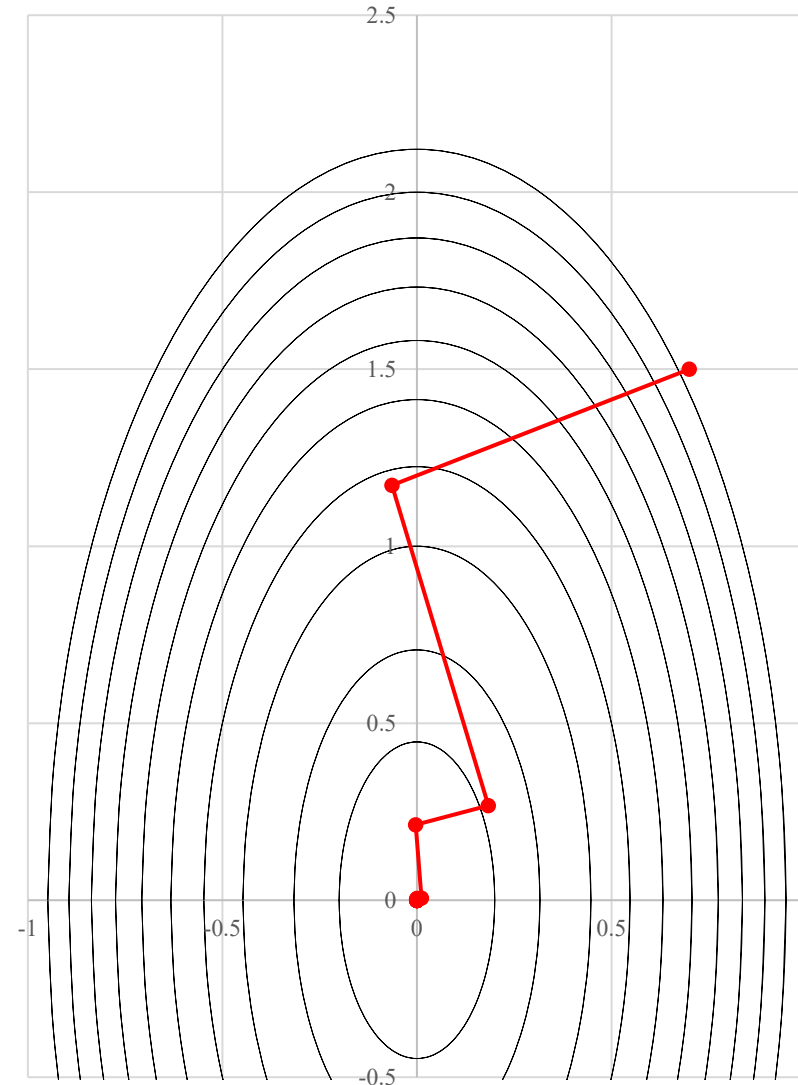


# Steepest descend method

Without direct search:  
use fixed step parameter



With direct search



# SD method in Deep Learning

- All batch data are divided to mini batches, and apply SD to each mini batch

**Example:**

$$S^2 = f(a, b; x_1, x_2) = ax_1^2 + bx_2^2, \quad a = 5, b = 1$$

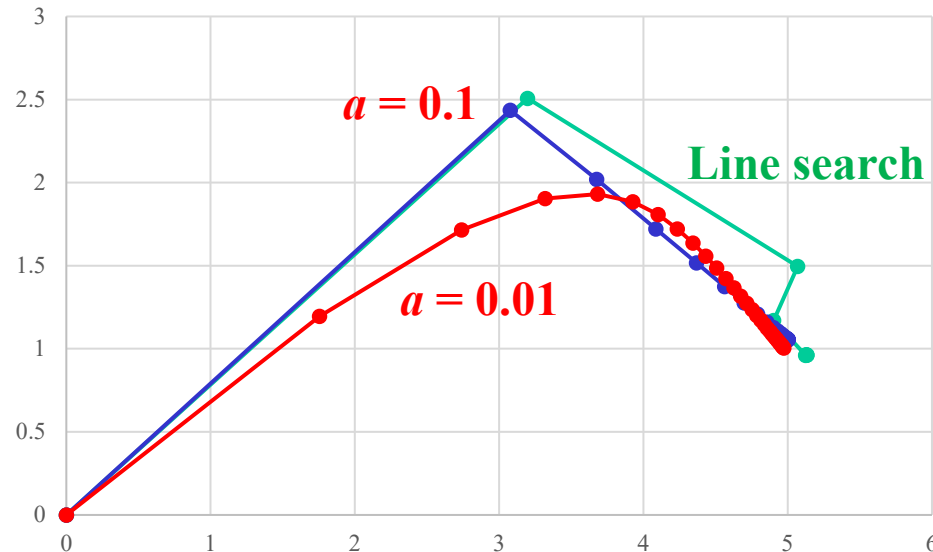
1000 batch data  $(x_{1i}, x_{2i}, f(x_i))$  are generated at random

(note: the data were re-generated for different runs)

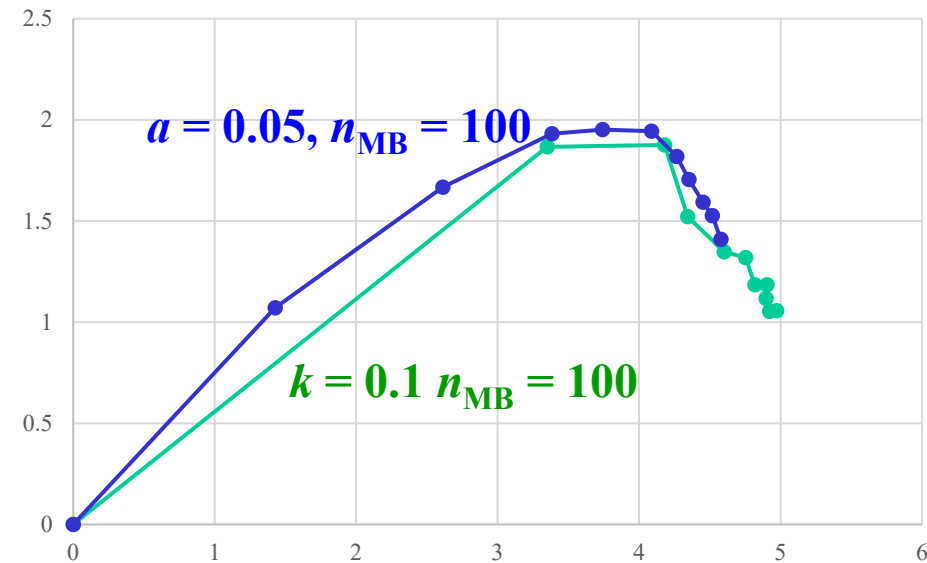
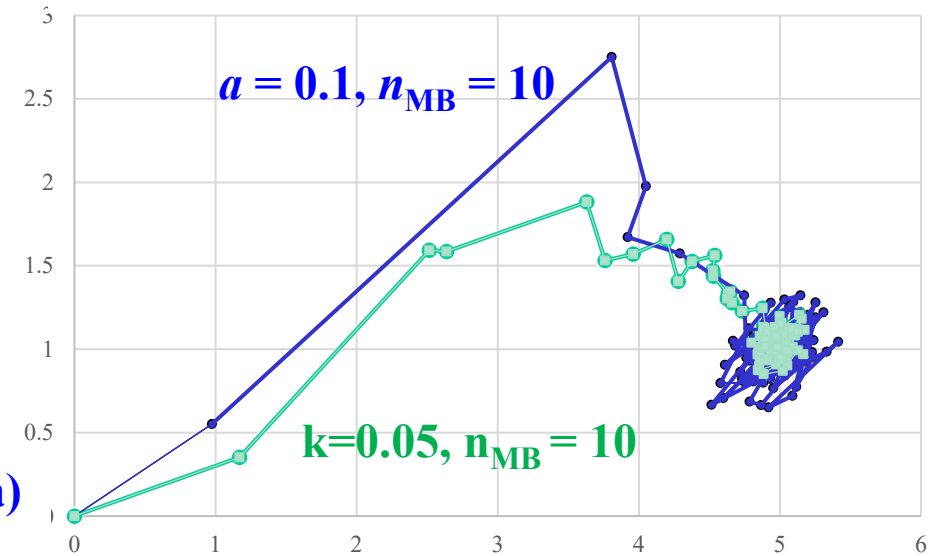
Speculate  $a$  and  $b$

Initial  $a = 0, b = 0$

**SD (Convergence iterations with all batch data)**



**DL: SD method**



# Multiple variable Newton-Raphson method

Extend to **multiple variable optimization**: Minimize  $F(x_j)$

$$f_k(x_j) = \partial F(x_j) / \partial x_k = 0$$

To solve  $f_k(x_j) = 0$  ( $k, j = 1, 2, \dots, N$ )

$$f_k(x_j + \delta x_j) \sim f_k(x_j) + \sum_{k'} \delta x_{k'} \partial f_k(x_j) / \partial x_{k'} = 0$$

$$\Rightarrow x_{j,1} = x_{j,0} - (\partial f_k(x_j) / \partial x_{k'})^{-1} (f_k) = x_{l,0} - (F''_{kk'})^{-1} (F'_k)$$

$$F''_{kk'} = \frac{\partial^2 F(x_j)}{\partial x_k \partial x_{k'}} \quad \text{Hessian matrix (ヘッセ行列)}$$

(ヘッセ行列の固有値をヘッシアンと呼ぶ)

Hessian matrix is not always positive definite (正定値であるとは限らない)

(Maximum, Saddle point 極大値、鞍点)

$\Rightarrow F''$  does not always give decreasing direction

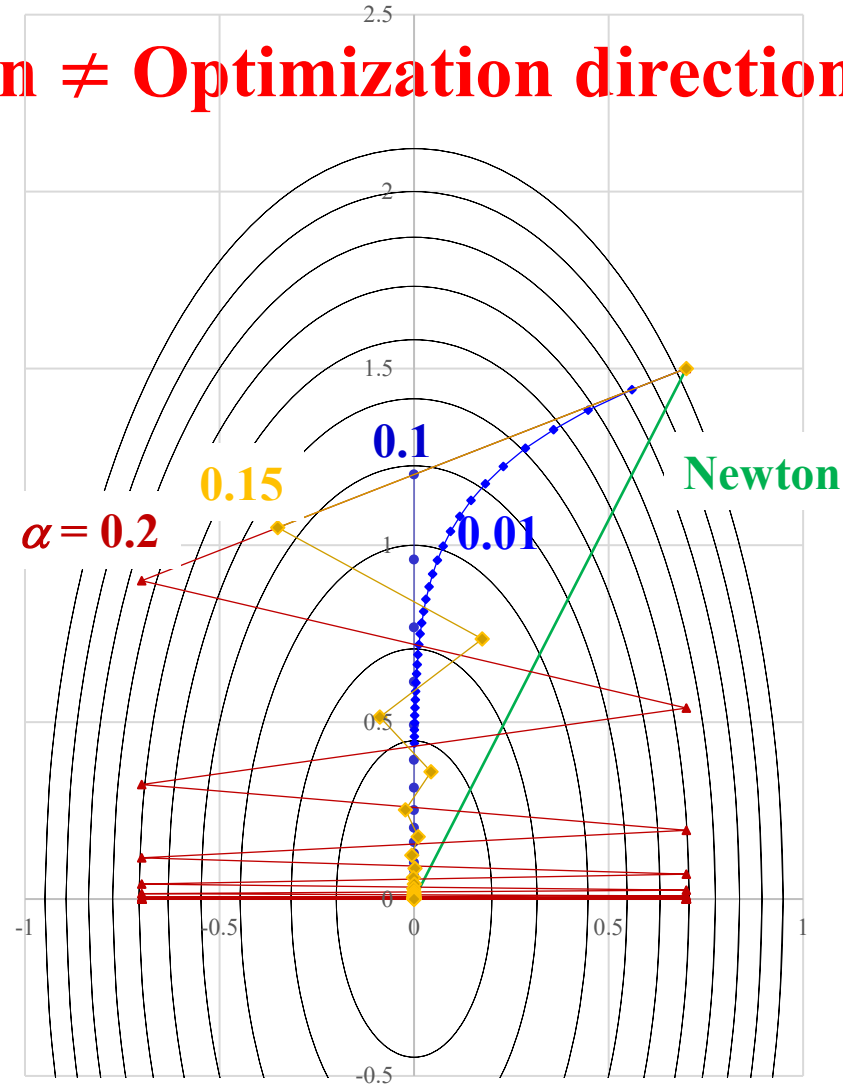
**Convert  $F''$  to positive definite and suppress divergence**

$$x_{l,1} = x_{l,0} - (F''_{kk'} + \lambda I)^{-1} (F'_k)$$

$\lambda$ : **Damping Factor**

# SD vs. Newton-Raphson methods

**Steepest direction  $\neq$  Optimization direction**

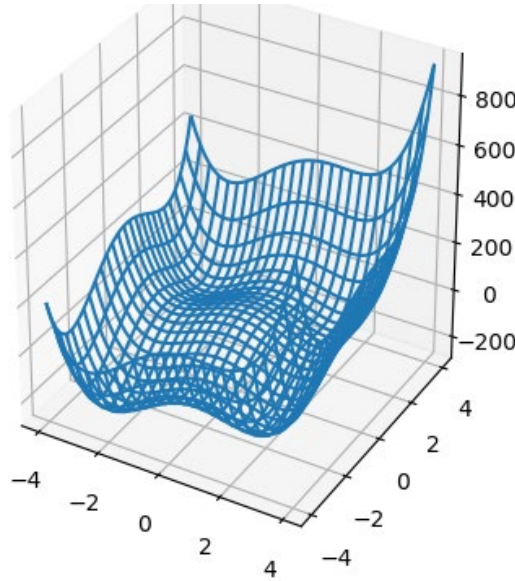


**Improve SD method to follow optimization directions**

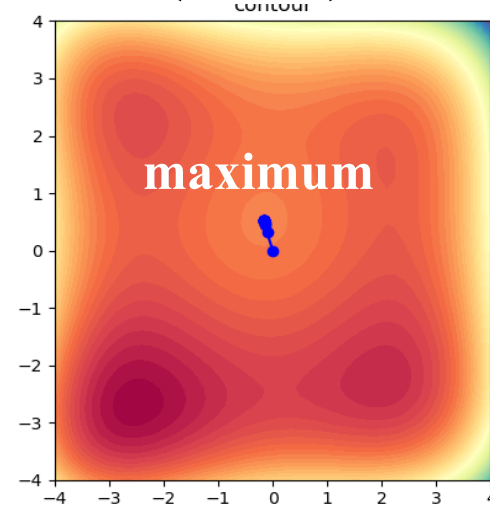
# Program: optimize-newton-raphson2d.py

$$F(x,y) = -3.0 - 10x - 30x^2 + 1.5x^3 + 3x^4 + 30y - 30y^2 + 3y^4 + 3xy^2$$

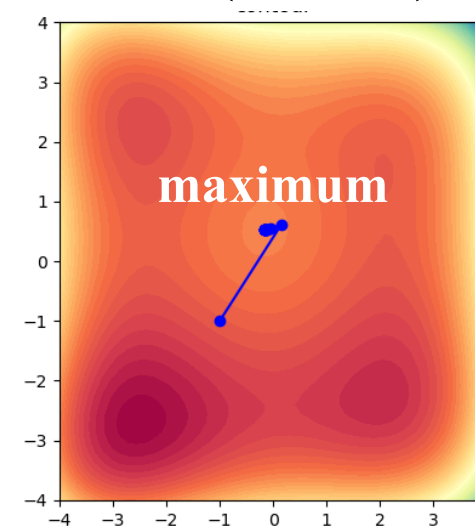
Usage: python optimize-newton-raphson2d.py  $x_0$   $y_0$



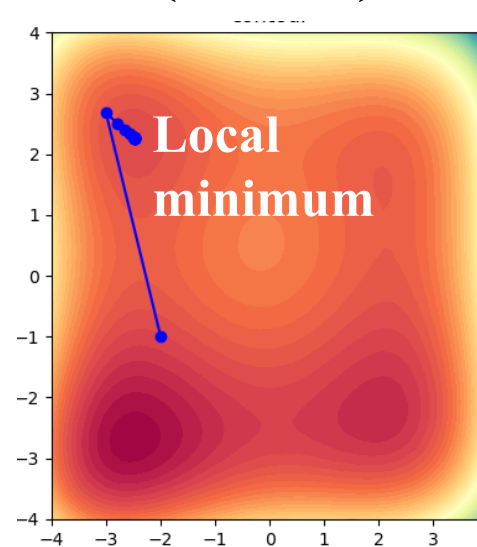
From (0.0 0.0) Newton



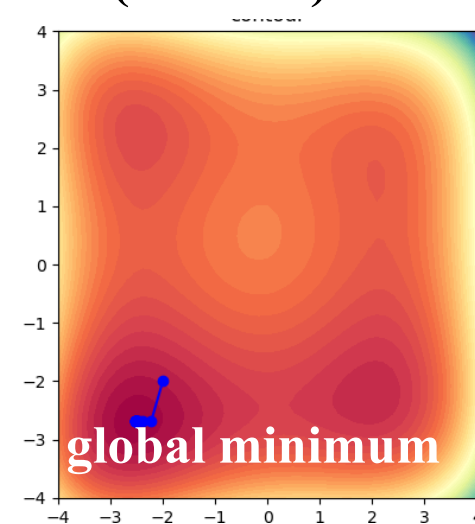
From (-1.0 -1.0)



From (-2.0 -1.0)



From (-2.0 -2.0)



# Quasi-Newton method (準Newton法)

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

Target function to minimize:  $F(x_j)$

Iteration:  $x_j^{(i+1)} = x_j^{(i)} - (\partial^2 F / \partial x_k \partial x_{k'})^{-1} (\partial F / \partial x_k)$

$F''_{kk'} = \partial^2 F / \partial x_k \partial x_{k'}$ : Hessian (ヘッセ) matrix

## Issues of Newton method:

- (1) Calculation of Hessian matrix is very high cost as it is a 2D matrix
- (2) Eigen value of Hessian matrix can be negative => lead to maximum
- (3) Easy to diverge

## Quasi-Newton method:

- (1,2) Hessian matrix is approximated from 1<sup>st</sup> differentials
- (3) Line search algorithm is applied along the search direction  
 $-(\partial^2 F / \partial x_k \partial x_{k'})^{-1} (\partial F / \partial x_k)$

# Davidon-Fletcher-Powell (DFP) method

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

$$F(x_j^{(k)} + \alpha d) = F(x_j^{(k)}) + \alpha \nabla F(x_j^{(k)})^T d + \frac{1}{2} \alpha^2 d^T B^{(k)} d \sim 0$$

Search direction  $d$  is determined from  $B^{(k)} d = -\nabla F(x_j^{(k)})$

**DFP method:** The first formulation of quasi-Newton method

$$s^{(k)} = x^{(k+1)} - x^{(k)}, \quad y^{(k)} = \nabla F(x_j^{(k+1)}) - \nabla F(x_j^{(k)})$$

$$\begin{aligned} B^{(k+1)} &= B^{(k)} + \frac{(y^{(k)} - B^{(k)} s^{(k)}) \cdot y^{(k)T} + y^{(k)} \cdot (y^{(k)} - B^{(k)} s^{(k)})^T}{s^{(k)T} \cdot y^{(k)}} \\ &\quad - \frac{s^{(k)T} \cdot (y^{(k)} - B^{(k)} s^{(k)})}{(s^{(k)T} \cdot y^{(k)})^2} y^{(k)} \cdot y^{(k)T} \\ &= B^{(k)} - \frac{B^{(k)} s^{(k)} \cdot y^{(k)T} + y^{(k)} \cdot (B^{(k)} s^{(k)})^T}{s^{(k)T} \cdot y^{(k)}} + \left( 1 + \frac{s^{(k)T} B^{(k)} s^{(k)}}{s^{(k)T} \cdot y^{(k)}} \right) \end{aligned}$$



# Broyden-Fletcher-Goldfarb-Shanno (BFGS) method

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

**BFGS method:** Regarded as most efficient among quasi-Newton methods

$$s^{(k)} = x^{(k+1)} - x^{(k)}, \quad y^{(k)} = \nabla F(x_j^{(k+1)}) - \nabla F(x_j^{(k)})$$

$$B^{(k+1)} = B^{(k)} - \frac{B^{(k)} s^{(k)} (B^{(k)} s^{(k)})^T}{s^{(k)T} B^{(k)} s^{(k)}} + \frac{y^{(k)} y^{(k)T}}{s^{(k)T} \cdot y^{(k)}}$$

## Algorithm:

STEP 0: Provide initial values  $x^{(0)}$  and initial matrix  $B^{(0)}$  (can be unit matrix)

STEP 1: Search direction  $d^{(k)}$  is determined from  $B^{(k)} d = -\nabla F(x_l^{(k)})$

STEP 2: Step width  $\alpha^{(k)}$  is determined by **line search algorism**

STEP 3: Calculate  $x^{(k+1)} = x^{(k)} + \alpha^{(k)} d^{(k)}$

STEP 4: End if self-consistency is achieve.

If not, go to STEP 5

STEP 5: Calculated  $s^{(k)}$  and  $y^{(k)}$ , and then  $B^{(k+1)}$ , and go to STEP 1

# Conjugate Gradient method (共役勾配法)

矢部博, 工学基礎 最適化とその応用, 数理工学社 (2006)

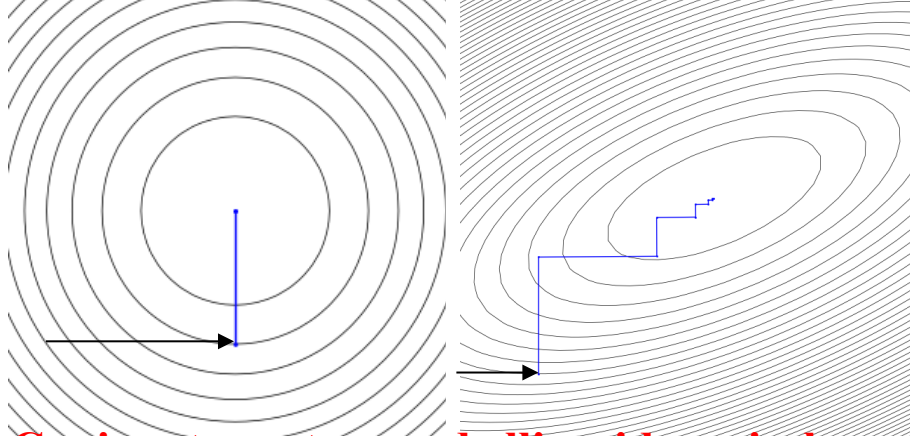
Vectors  $u$  and  $v$  satisfy  $u^T A v = 0$  for a matrix  $A$ :  $u$  and  $v$  are conjugate with each other

- For quadratic function, repetition of the conjugate direction will find the minimum in finite cycles if exact line search is employed

共役な探索方向に沿って正確な直線探索を実行  $\Rightarrow$  有限回の反復で2次関数の最小解に到達

Case contour is a circle, one cycle calculation reaches the minimum

等高線が円の場合、一回の探索で最小値に到達できる



Conjugate vectors and ellipsoid – circle conversion

$$u^T P^T P v = u^T A v = 0$$

1. Give initial value  $x_0$
2. Initial direction  $d$  is determined by SD  
$$d = -\nabla f$$

3. Find  $x_{k+1}$  using appropriately chosen  $\alpha_k$   
$$x_{k+1} = x_k + \alpha_k d_k$$
  
 $\alpha_k$  may be a small constant step or determined by a line search method

4. Search direction is updated by

$$y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

$$d_{k+1} = -\nabla f(x_{k+1}) + \frac{\nabla f(x_{k+1})^T y_k}{d_k^T y_k} d_k$$

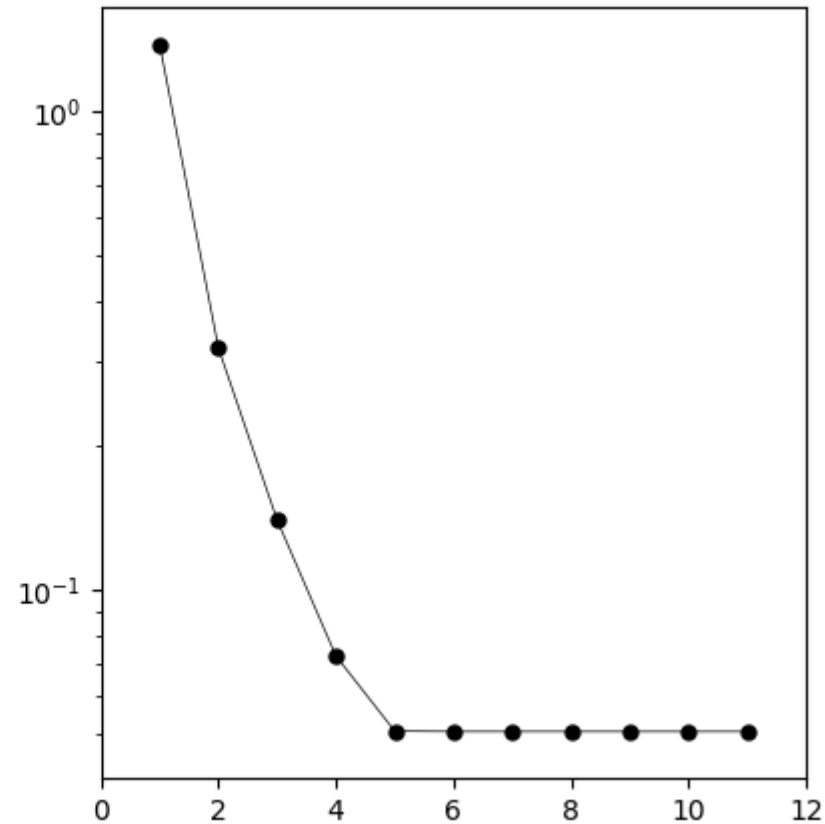
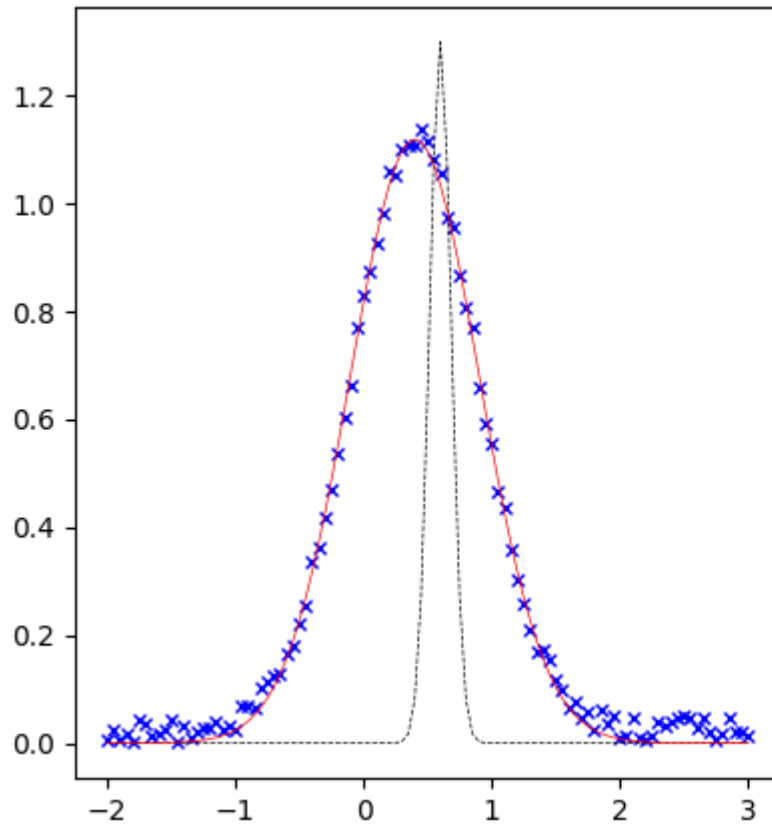
5. Repeat 3 – 4 to reach convergence

As the freedom of cg directions is the number of parameters ( $n_{\text{param}}$ ), need to go back to 2 to reset  $d_k$  at some interval (typically  $n_{\text{param}}$ , necessary for  $n_{\text{param}} = 2$ ).

## Ex.: Curve fit

Usage: `python peakfit.py mode input_file method I0 x0 w`

`python peakfit.py sim peak.xlsx` (initial values: `method = cg`, `I0 = 1.3`, `x0 = 0.6`, `w = 0.1`)

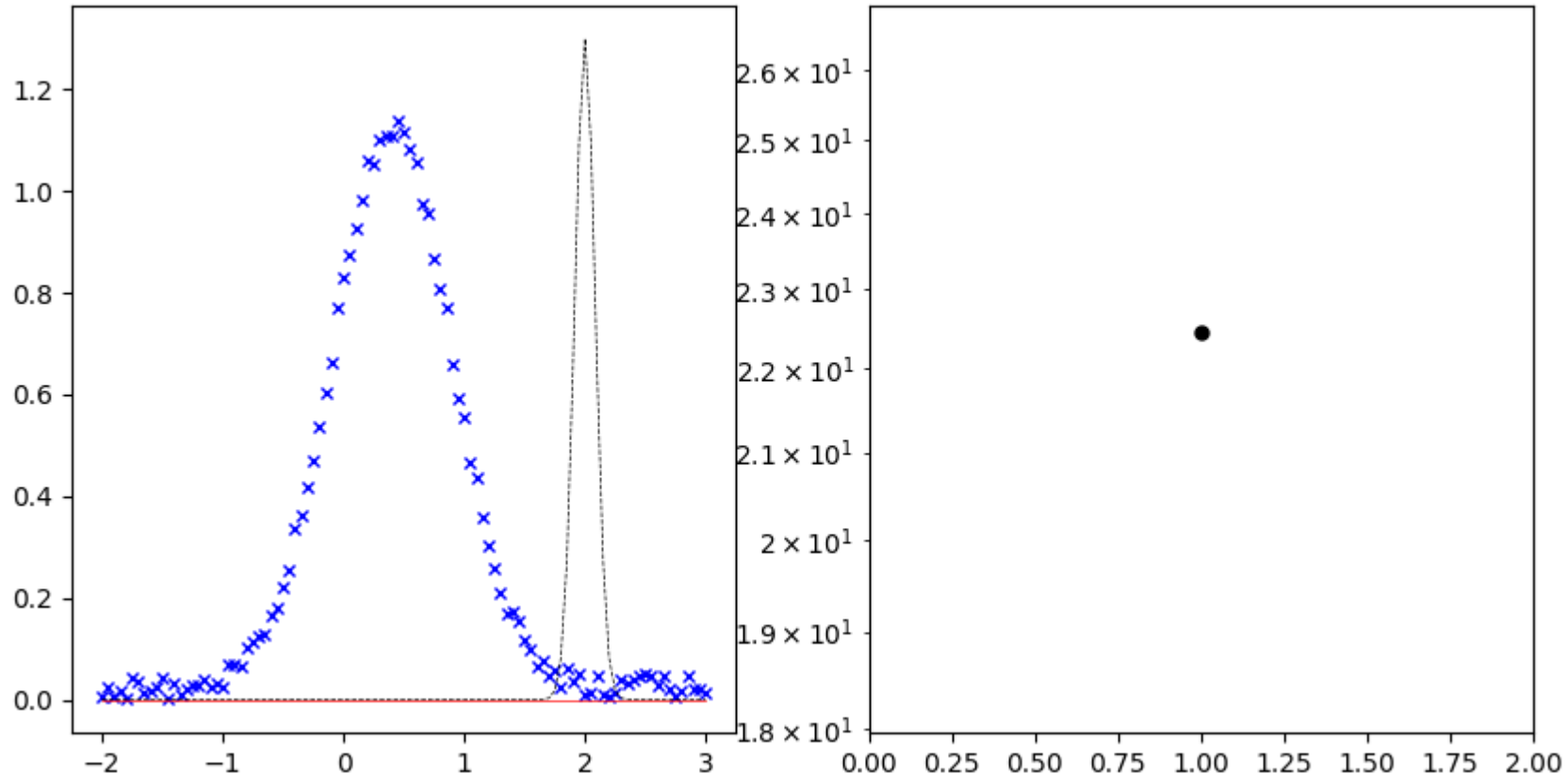


# Not optimized

python peakfit.py fit peak.xlsx cg 1.3 2.0 0.1

method: cg

initial values:  $I_0 = 1.3$ ,  $x_0 = 2.0$ ,  $w = 0.1$

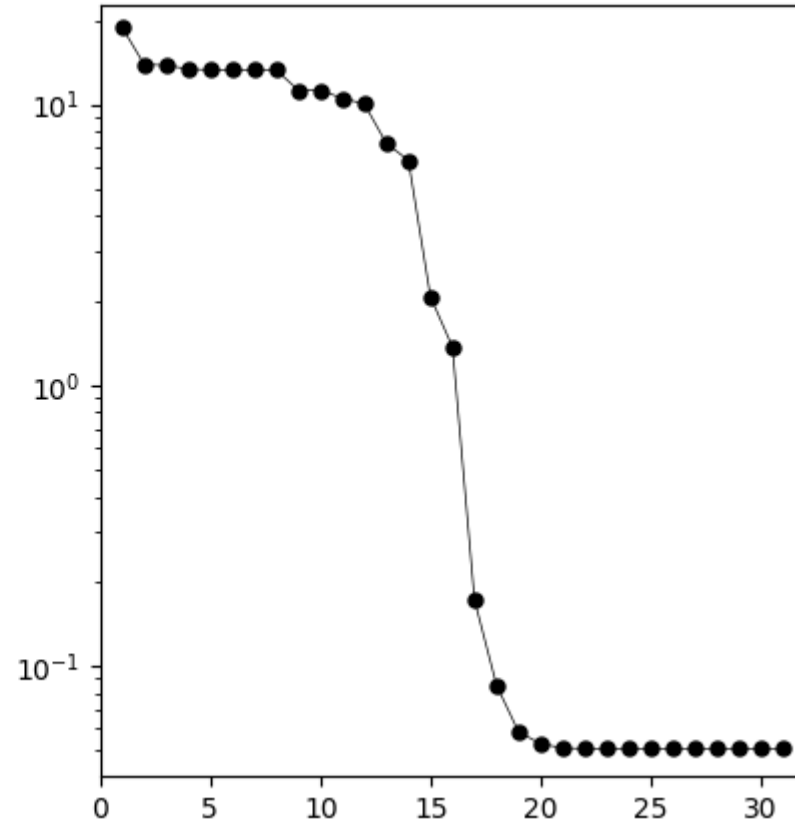
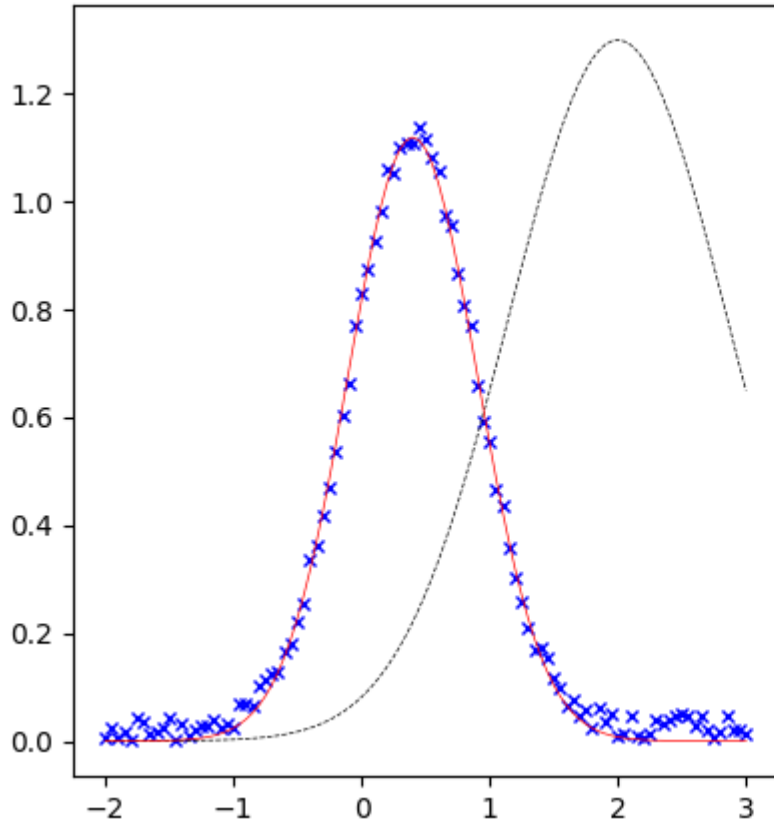


# Converged

python peakfit.py fit peak.xlsx cg 1.3 2.0 1.0

method: cg

initial values:  $I_0 = 1.3$ ,  $x_0 = 2.0$ ,  $w = 1.0$



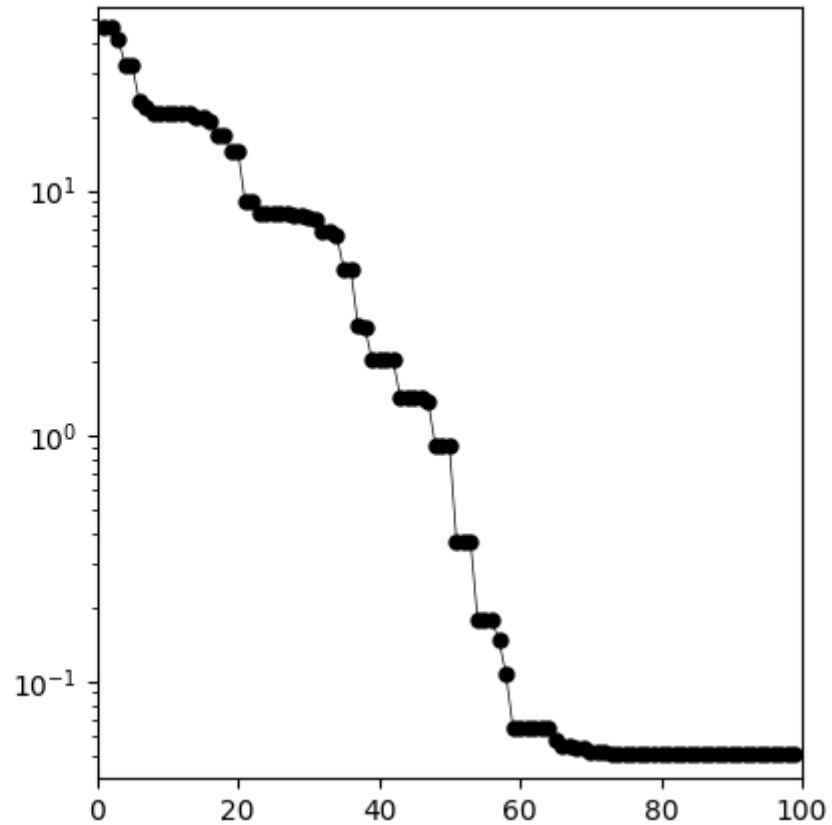
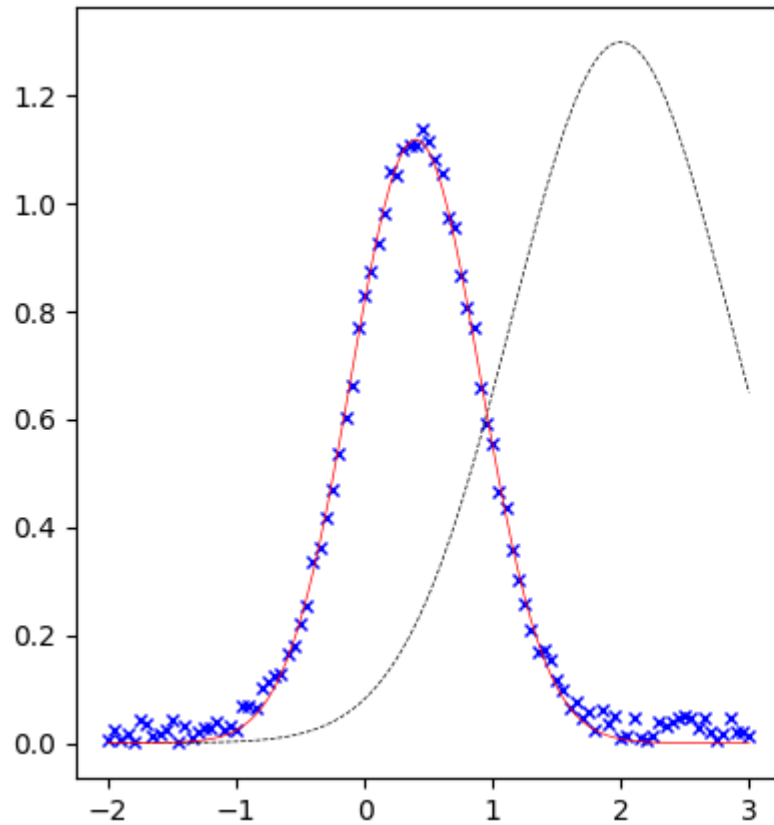
**The result may be converged if  $w$  is wide enough to cover some region of the curve, even if the initial peak position is out of the FWHM of the target peak**

# Converged

python peakfit.py fit peak.xlsx nelder-mead 1.3 2.0 1.0

method: nelder-mead (SIMPLEX)

initial values:  $I_0 = 1.3$ ,  $x_0 = 2.0$ ,  $w = 1.0$



# Marquart method (マーカート法)

Minimize a square sum of  $m$  functions  $f_j(x_i)$  with  $N$  parameters

$$F(x_i) = \sum_{j=1}^m f_j(x_i)^2$$

Approximate by

$$f_j(x_i + \delta x_i) \sim f_j(x_i) + \left( \frac{\partial f_j}{\partial x_k} \right) (\delta x_i) = f_j(x_i) + \mathbf{A} \delta x_i \quad A_{jk} = \frac{\partial f_j}{\partial x_k}$$

$$F(x_i + \delta x_i) \sim F(x_i) + 2 \sum_{j,k} f_j A_{jk} \delta x_k + \sum_{j,k,k'} A_{jk} A_{ik'} \delta x_k \delta x_{k'}$$

$$\frac{\partial F(x_i)}{\partial \delta x_k} \sim 2 \sum_j \left( A_{jk} f_j + \sum_k A_{ik} A_{jk} \delta x_j \right) = 0$$

$$\delta x = -(\mathbf{A}^t \mathbf{A})^{-1} \mathbf{A}^t (f_j) \quad \text{Gauss-Newton method}$$

## Levenberg-Marquart method

$$\delta x = -(\mathbf{A}^t \mathbf{A} + \lambda I)^{-1} \mathbf{A}^t (f_j) \quad \lambda: \text{dumping factor}$$

$$\delta x = -(\mathbf{A}^t \mathbf{A} + \lambda \text{diag}(\mathbf{A}^t \mathbf{A}))^{-1} \mathbf{A}^t (f_j) \quad \text{e.g. chosen proportional to diagonal sum of } \mathbf{A}^t \mathbf{A}$$

# Simplex method (単体法, Amoeba法)

(Nelder-Mead algorithm)

服部力、名取亮、小国力 監修、Fortranによる数値計算ソフトウェア、丸善株式会社 (1989年)

*Simplex: Polyhedron formed by  $(n+1)$  vertexes in  $n$ -dimension space*

(単体:  $n$ 次元空間で  $(n+1)$  個の頂点で作る多面体)

**Minimize  $F(\mathbf{x}_i)$**

1.  $(n+1)$  initial values  $\mathbf{x}_i$  ( $i = 1, 2, \dots, n+1$ )  $\Rightarrow$  Sort  $F(\mathbf{x}_i)$  so that  $F(\mathbf{x}_i) > F(\mathbf{x}_{i'})$  ( $i < i'$ )

$$\mathbf{x}_h = \mathbf{x}_1, \mathbf{x}_1 = \mathbf{x}_{n+1}$$

2. Average except the maximum vertex  $\mathbf{x}_i$   $\mathbf{x}_G = \sum_{i=2}^{n+1} \mathbf{x}_i / n$

3. New  $x$  will be examined along the line  $\mathbf{x}_1 - \mathbf{x}_G$  by the following selections

(i) Reflection (鏡映) :  $\mathbf{x}_R = (1 + \alpha)\mathbf{x}_G - \alpha\mathbf{x}_1$  ( $\alpha > 0$ , ex. 1.0)

(ii) Expansion (拡大) :  $\mathbf{x}_E = \gamma\mathbf{x}_R + (1 - \gamma)\mathbf{x}_G$  ( $\gamma > 0$ , ex. 2.0)

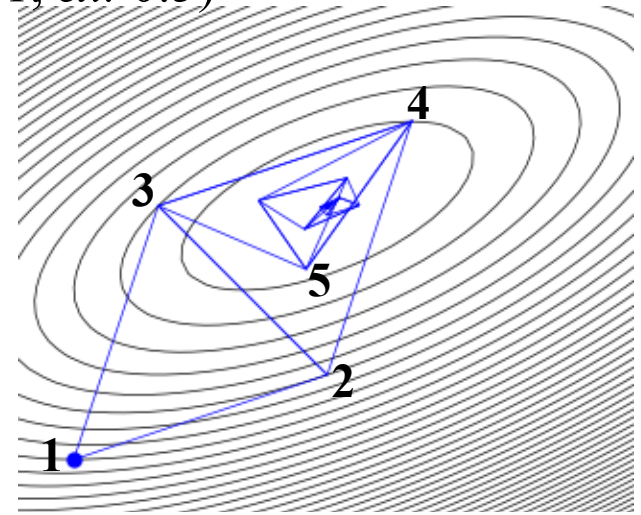
(iii) Contraction (収縮) :  $\mathbf{x}_C = \beta\mathbf{x}_1 + (1 - \beta)\mathbf{x}_G$  ( $0 < \beta < 1$ , ex. 0.5)

(iv) Reduction (縮小) :  $\mathbf{x}_{RD} = (\mathbf{x}_1 + \mathbf{x}_i) / 2$

4. Replace  $\mathbf{x}_1$  with the  $x$  in (i) – (iv) that firstly satisfies

$$F(\mathbf{x}) < F(\mathbf{x}_1)$$

5. Repeat 2 - 4

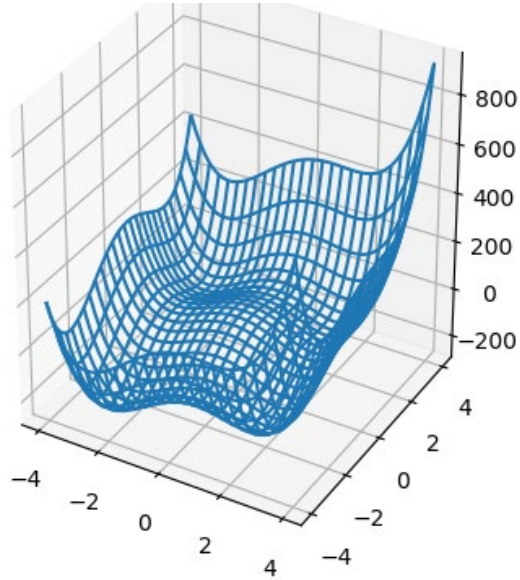




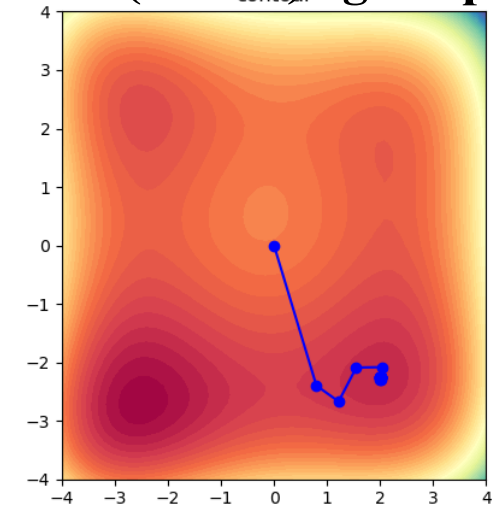
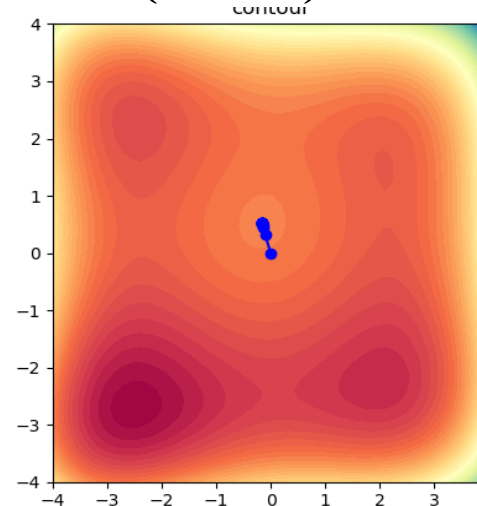
# Comparison

$$F(x,y) = -3.0 - 10x - 30x^2 + 1.5x^3 + 3x^4 + 30y - 30y^2 + 3y^4 + 3xy^2$$

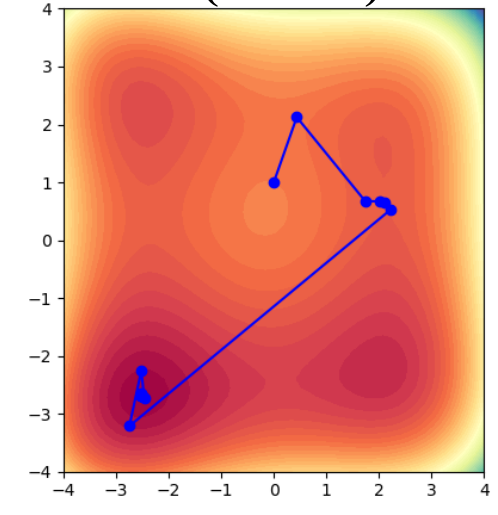
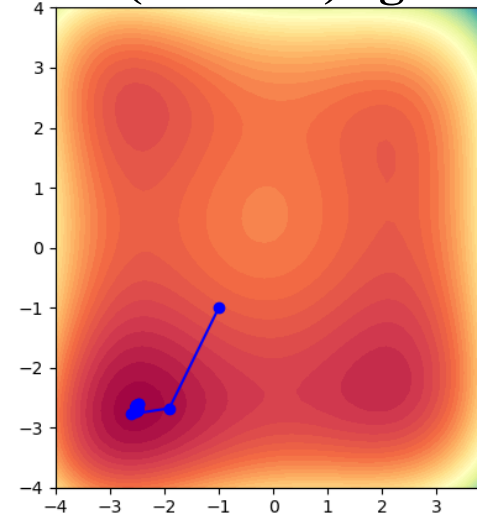
Programs: `optimize-sd-cg2d-linesearch.py`, `optimize-newton-raphson2d.py`



From (0.0 0.0) Newton From (0.0 0.0) cg simple



From (-1.0 -1.0) cg simple From (0.0 1.0) SD armijo



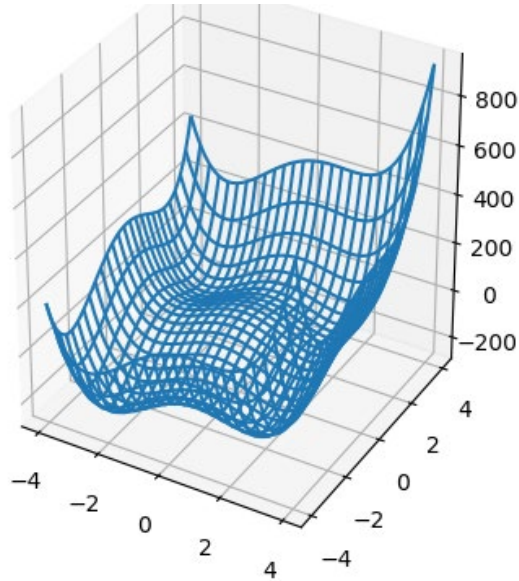
e.g.,

`optimize-sd-cg2d-linesearch.py -1.0 -1.0 sd armijo`

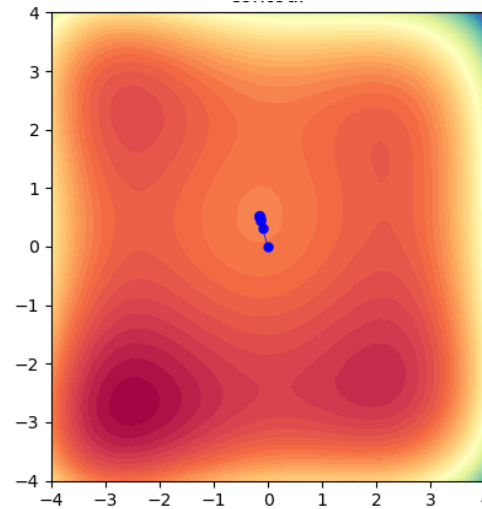
# Optimize.py for Simplex method (not working without tklib)

$$F(x,y) = -3.0 - 10x - 30x^2 + 1.5x^3 + 3x^4 + 30y - 30y^2 + 3y^4 + 3xy^2$$

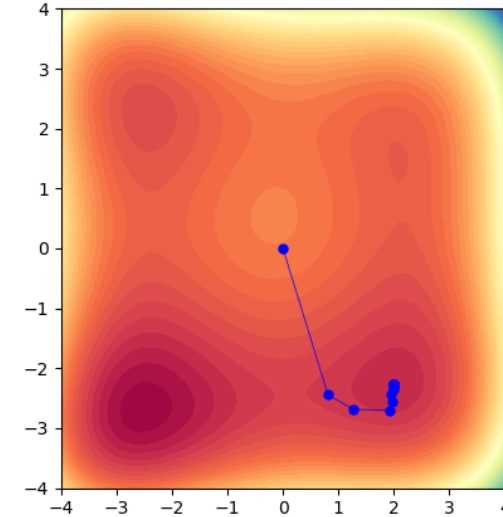
e.g.: python optimize.py 0.0 1.0 simplex



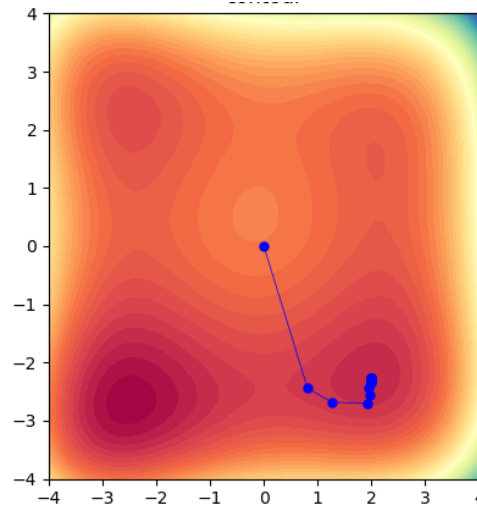
From (0.0 0.0) Newton



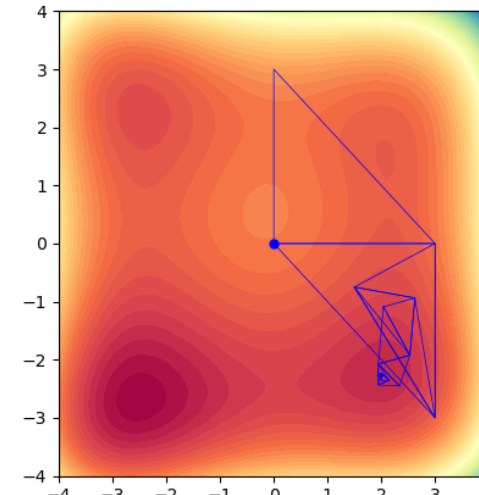
From (-1.0 -1.0) DFP golden



From (0.0 0.0) BFGS golden



From (0.0 1.0) Simplex



## Main algorism:

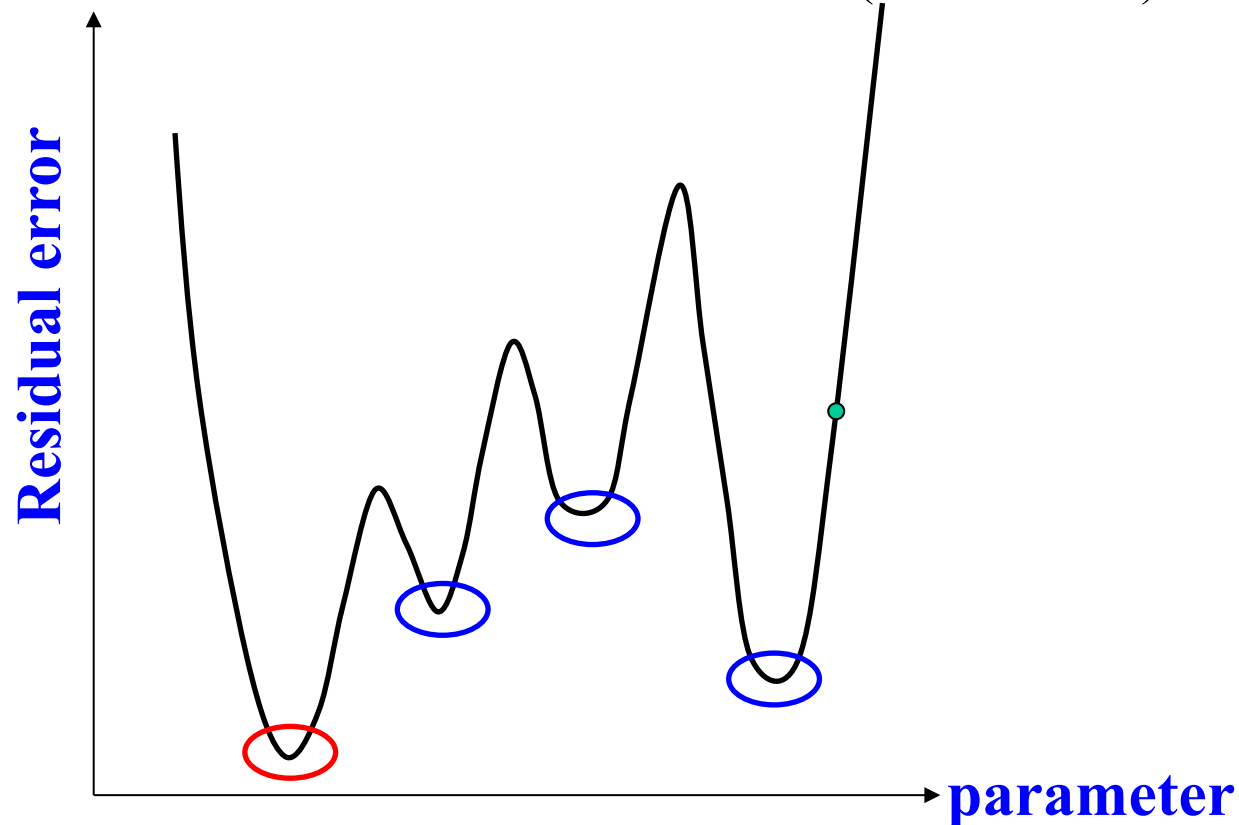
newton, sd, cg, broyden, dfp, bfgs  
simplex

## Direct search:

exact, one, simple  
armijo, golden

# Notes for NL optimization

- Solutions may be more than one
- Final solution is not obtained by one step calculation
- **Convergence must be confirmed**
- **Confirm the solution is the global minimum** (大域最小値)
  - ⇔ **Often fall in a local minimum** (局所極小値)



# Features of NL optimization algorithms

Convergence	A	B
Speed	×	○
Stability	○	×
Global convergence	○	×
For:	Initial cycles	Later cycles for fast convergence

**A : Simplex (単体法)**

**A,B: with line search algorithm:**

**Conjugate Gradient (CG, 共役勾配法)**

**Steepest Descent (SD, 最急降下法)**

**Quasi Newton methods**

▪ **Davidson-Fletcher-Powell (DFP)**

▪ **Broyden-Fletcher-Goldfarb-Shanno (BFGS)**

**B : Newton-Raphson method**

# Methods of non-linear (NL) optimization

To find a minimum (maximum) of **target function  $F(x)$** :

**Gradient method (勾配法):** Use first differential to find the direction of minimum

- **Newton-Raphson method:**

Use 1<sup>st</sup> and 2<sup>nd</sup> differentials to efficiently find minimum

- **Quasi-Newton method (準Newton法):**

2<sup>nd</sup> differential matrix is approximated from 1<sup>st</sup> differentials.

Line search method is combined to improve global convergence.

- **Steepest Descent method (最急降下法):**

Only 1<sup>st</sup> differentials are used to search minimum

- **Conjugate Gradient method (共役勾配法):**

Search direction is corrected by conjugate gradient of 1<sup>st</sup> differentials

- **Marquart method**

For least-squares fitting of  $f_j(x_i)$ , 2<sup>nd</sup> differential matrix is build from 1<sup>st</sup> differentials of  $f_j(x_i)$

**Direct search method (直接探索法)**

- **Simplex method (単体法)**

Search minimum by trial-and-error with a defined procedure

# Features of NL optimization

- **Newton-Raphson method: Gradient method**  
Use second derivatives (Hessian matrix)  
Fast convergence, easily diverged, complex program  
May reach to a maximum if Hessian matrix is not positive definite.
- **Quasi Newton method: DFP, BFGS, Broyden etc**  
Hessian matrix is iteratively approximated from 1st differentials.  
Better convergence by combining with linear search algorithms.
- **Steepest Descent:**  
Use first derivatives only  
Simple program, Slower convergence than NR and CG
- **Conjugate Gradient:**  
Use conjugate direction for efficient search  
Better convergence than NR, faster than SD, complex program
- **Marquart:**  
Use first derivatives of  $f_j(x_i)$   
Simple program, Slower convergence than NR
- **Simplex: Direct search**  
Trial and error with a pre-determined selections of next candidate parameters  
Very slow but good convergence