BRIN
BADAN RISET
DAN INOVASI NASIONAL

Visualisasi Data dengan Python

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Pusat Riset Fisika Kuantum BRIN

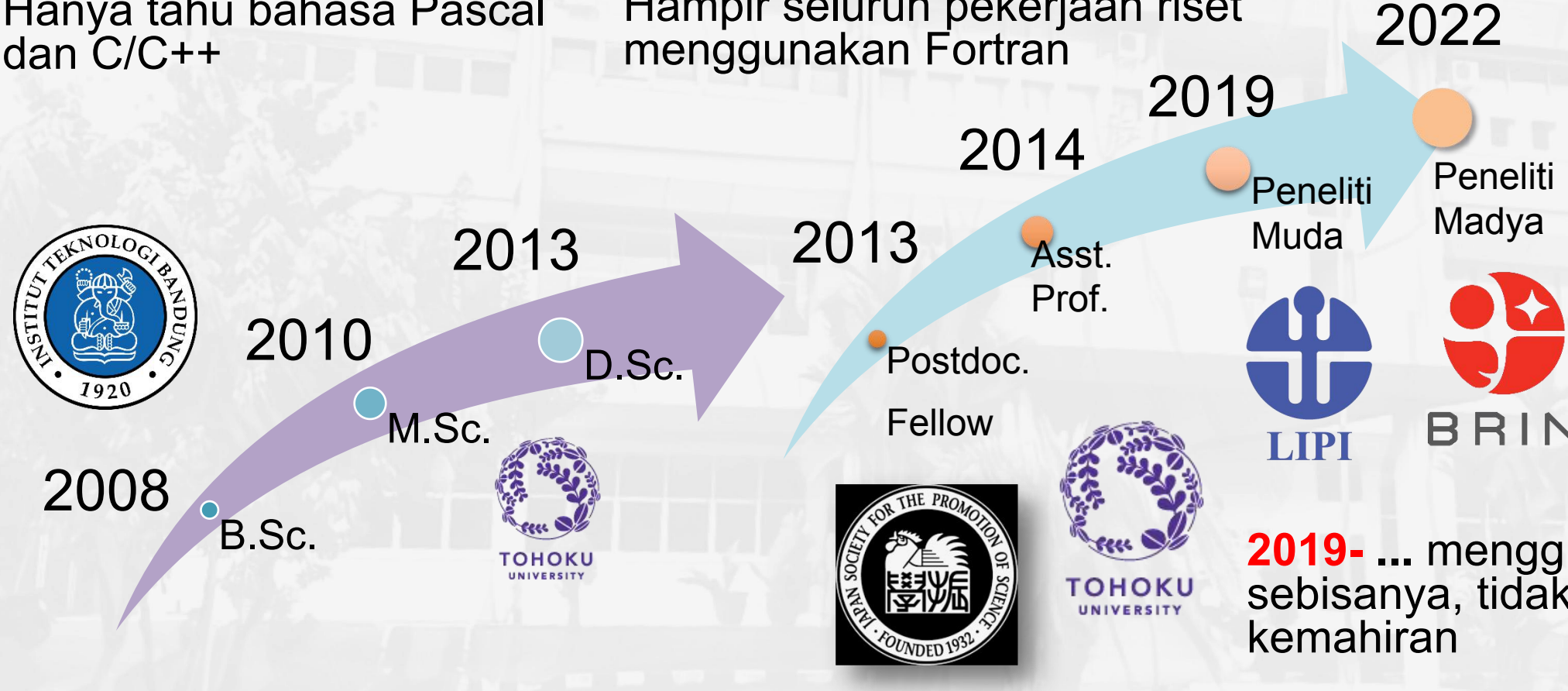
15-04-2023

Pendahuluan

Pengalaman Belajar, Berhitung, *Programming*

2004-2008
Hanya tahu bahasa Pascal dan C/C++

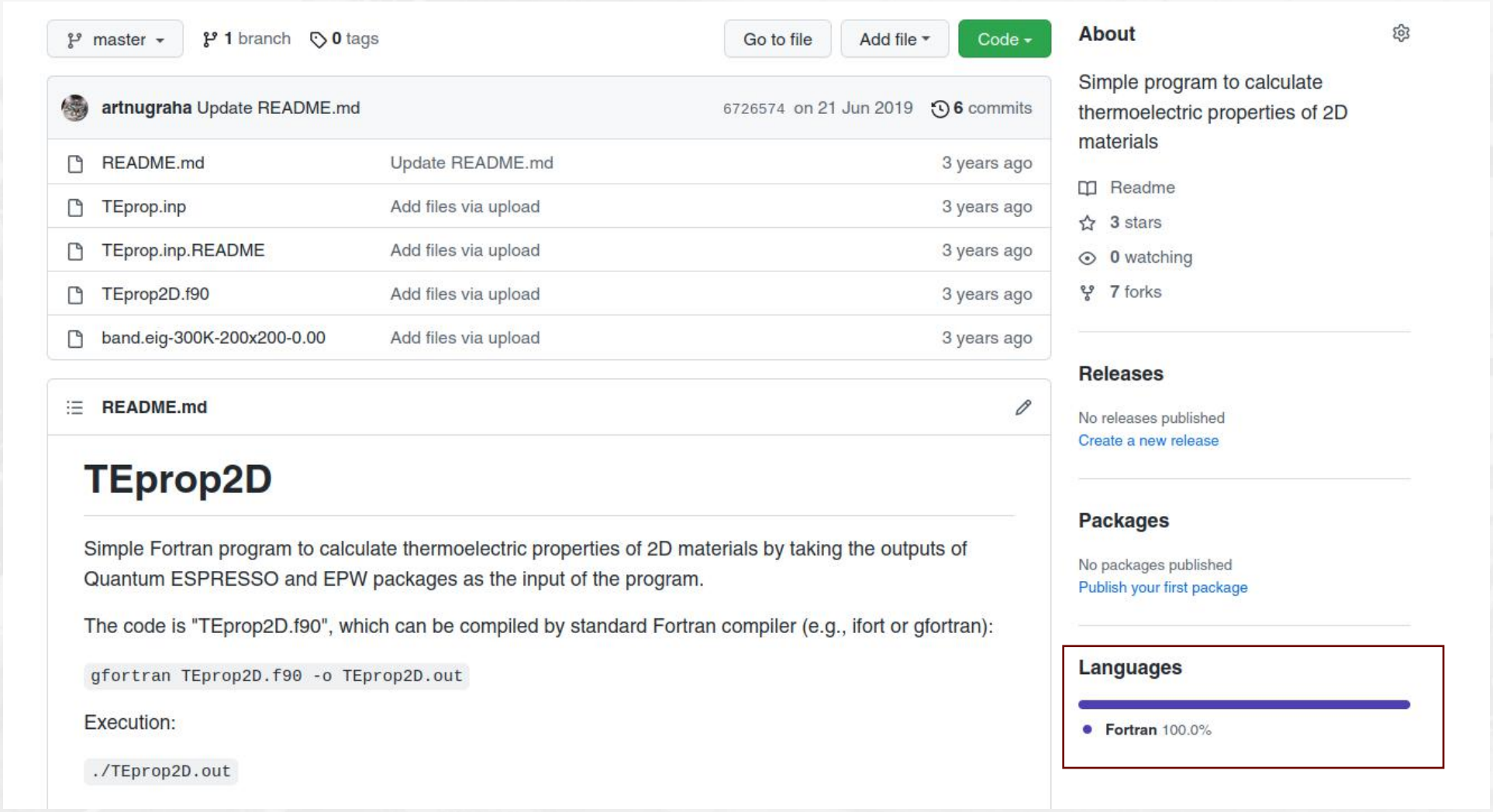
2008-2018
Hampir seluruh pekerjaan riset menggunakan Fortran



2019- ... menggunakan Python sebisanya, tidak mengincar kemahiran

Contoh Program Fortran untuk Termoelektrik

https://github.com/artnugraha/TEprop2D



master · 1 branch · 0 tags · Go to file · Add file · Code

artnugraha Update README.md — 6726574 on 21 Jun 2019 — 6 commits

README.md	Update README.md	3 years ago
TEprop.inp	Add files via upload	3 years ago
TEprop.inp.README	Add files via upload	3 years ago
TEprop2D.f90	Add files via upload	3 years ago
band.eig-300K-200x200-0.00	Add files via upload	3 years ago

README.md

TEprop2D

Simple Fortran program to calculate thermoelectric properties of 2D materials by taking the outputs of Quantum ESPRESSO and EPW packages as the input of the program.

The code is "TEprop2D.f90", which can be compiled by standard Fortran compiler (e.g., ifort or gfortran):

```
gfortran TEprop2D.f90 -o TEprop2D.out
```

Execution:

```
./TEprop2D.out
```

About

Simple program to calculate thermoelectric properties of 2D materials

Readme
3 stars
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7 forks

Releases

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Create a new release

Packages

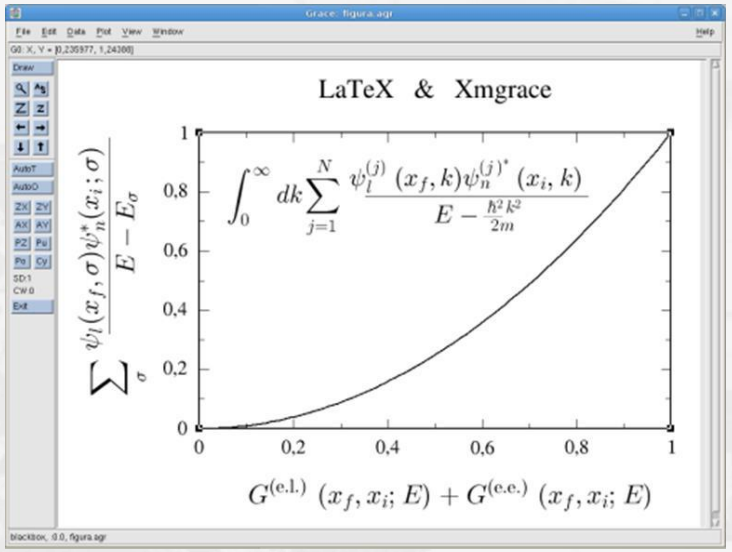
No packages published
Publish your first package

Languages

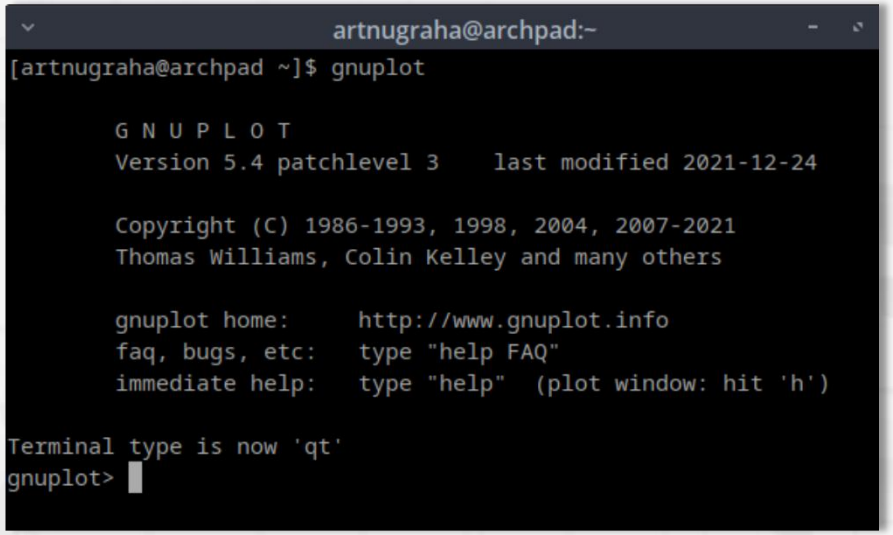
Fortran 100.0%

Pengalaman *Plotting* / Visualisasi Data

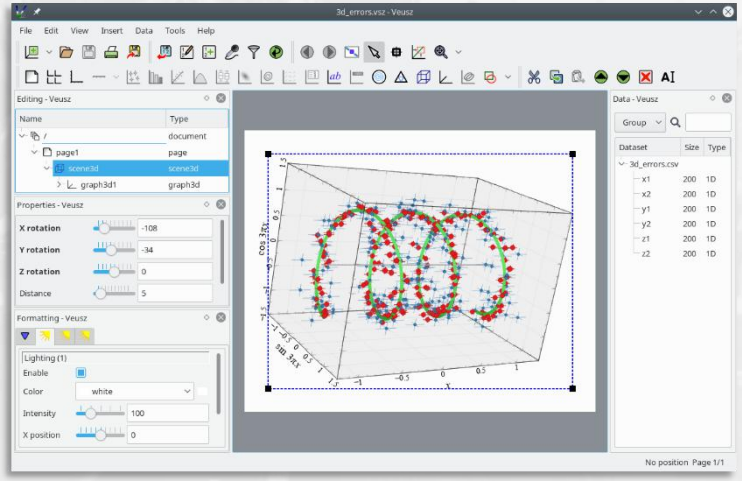
Grace/Xmgrace



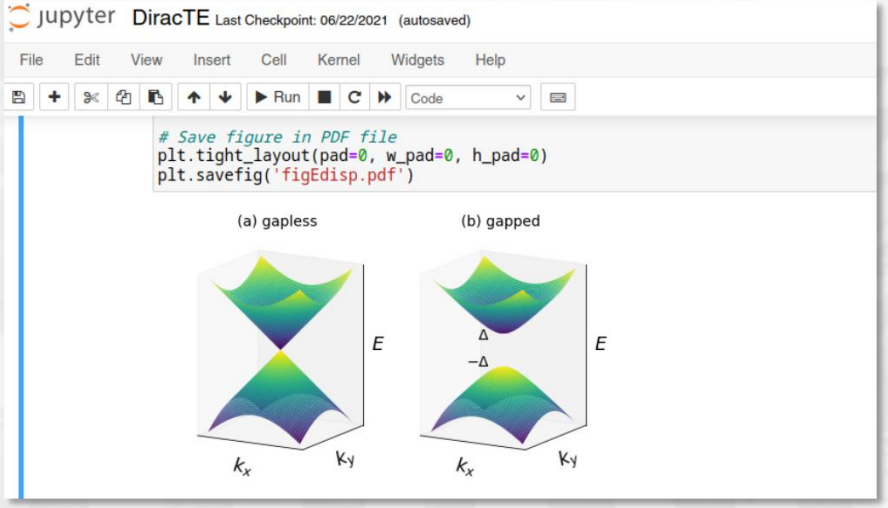
Gnuplot



Veusz



Python Matplotlib



Cara Belajar Python dan Pustaka Matplotlib

Googling tutorial Python dan Matplotlib

Rekomendasi:

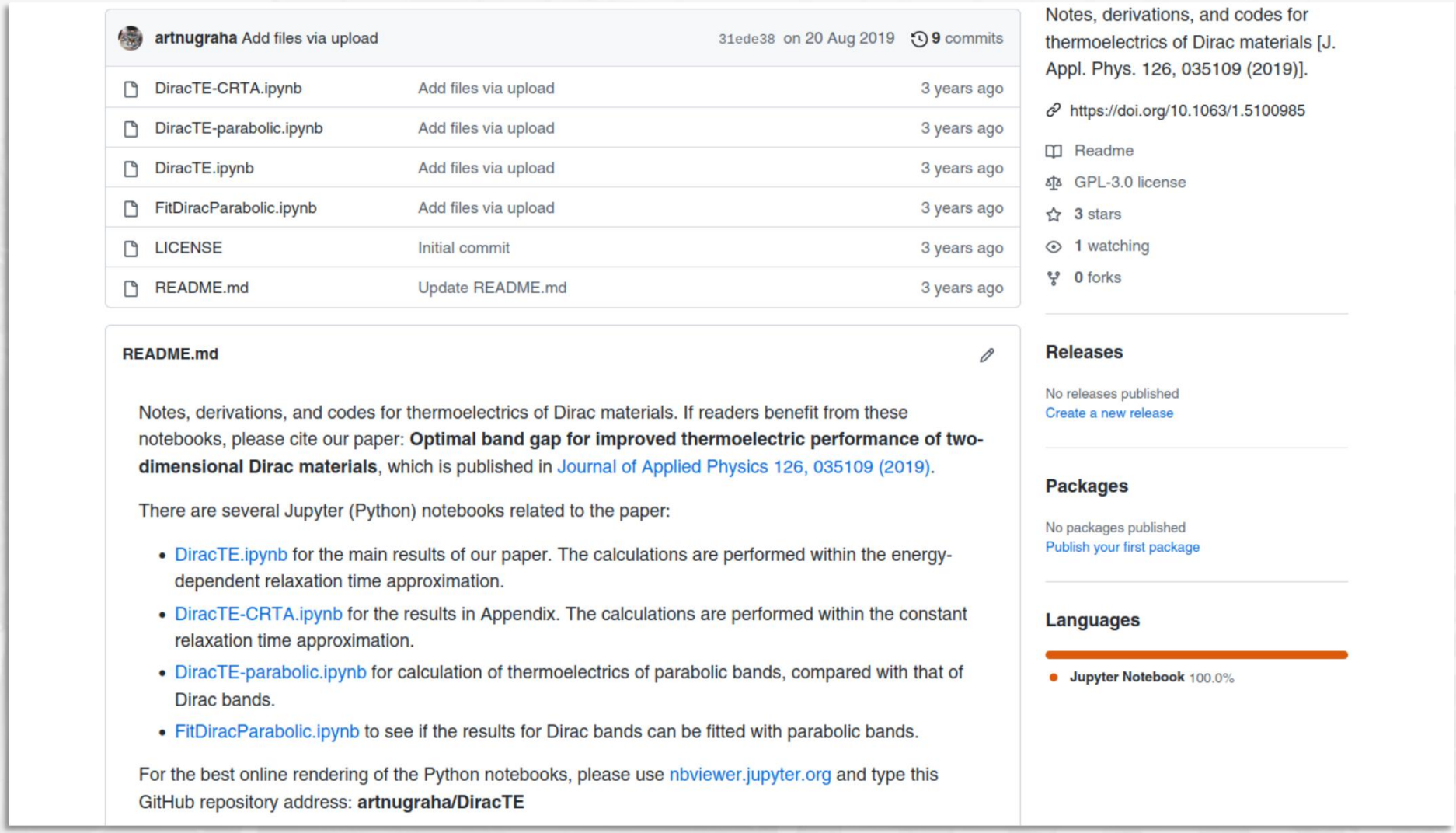
- https://www.math.ubc.ca/~pwalls/math-python/
- https://github.com/venkatesannaveen/python-science-tutorial

Praktik Langsung Kalkulasi, Visualisasi, dan Menulis Paper :-))

- https://github.com/artnugraha/DiracTE
- (pretty view:) https://nbviewer.org/github/artnugraha/DiracTE

Contoh praktik langsung sampai jadi paper

https://github.com/artnugraha/DiracTE



artnugraha Add files via upload — 31ede38 on 20 Aug 2019 — 9 commits

DiracTE-CRTA.ipynb	Add files via upload	3 years ago
DiracTE-parabolic.ipynb	Add files via upload	3 years ago
DiracTE.ipynb	Add files via upload	3 years ago
FitDiracParabolic.ipynb	Add files via upload	3 years ago
LICENSE	Initial commit	3 years ago
README.md	Update README.md	3 years ago

README.md

Notes, derivations, and codes for thermoelectrics of Dirac materials. If readers benefit from these notebooks, please cite our paper: **Optimal band gap for improved thermoelectric performance of two-dimensional Dirac materials**, which is published in Journal of Applied Physics 126, 035109 (2019).

There are several Jupyter (Python) notebooks related to the paper:

- DiracTE.ipynb for the main results of our paper. The calculations are performed within the energy-dependent relaxation time approximation.
- DiracTE-CRTA.ipynb for the results in Appendix. The calculations are performed within the constant relaxation time approximation.
- DiracTE-parabolic.ipynb for calculation of thermoelectrics of parabolic bands, compared with that of Dirac bands.
- FitDiracParabolic.ipynb to see if the results for Dirac bands can be fitted with parabolic bands.

For the best online rendering of the Python notebooks, please use nbviewer.jupyter.org and type this GitHub repository address: **artnugraha/DiracTE**

Notes, derivations, and codes for thermoelectrics of Dirac materials [J. Appl. Phys. 126, 035109 (2019)].

https://doi.org/10.1063/1.5100985

Readme
GPL-3.0 license
3 stars
1 watching
0 forks

Releases

No releases published
Create a new release

Packages

No packages published
Publish your first package

Languages

Jupyter Notebook 100.0%

Dampak Positif dari “Open Science”

Two-dimensional InSe as a potential thermoelectric material

Authors: Nguyen T Hung, Ahmad RT Nugraha, Riichiro Saito

Publication date: 2017/9/1

Journal: Applied Physics Letters

Volume: 111

Issue: 9

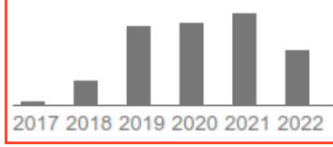
Pages: 092107

Publisher: AIP

Description: Thermoelectric properties of monolayer indium selenide (InSe) are investigated by using Boltzmann transport theory and first-principles calculations as a function of Fermi energy and crystal orientation. We find that the maximum power factor of p-type (n-type) monolayer InSe can be as large as 0.049 (0.043) W/K2m at 300 K in the armchair direction. The excellent thermoelectric performance of monolayer InSe is attributed to both its Seebeck coefficient and electrical conductivity. The large Seebeck coefficient originates from the moderate (about 2 eV) bandgap of monolayer InSe as an indirect gap semiconductor, while its large electrical conductivity is due to its unique two-dimensional density of states (DOS), which consists of an almost constant DOS near the conduction band bottom and a sharp peak near the valence band top.

APL Impact Factor: 3.791

Total citations: Cited by 98



98 citations in 5 years:
“impact factor”
98/(5/2) = 39.2

Optimal band gap for improved thermoelectric performance of two-dimensional Dirac materials

Authors: Eddwi H Hasdeo, Lukas PA Krisna, Muhammad Y Hanna, Bobby E Gunara, Nguyen T Hung, Ahmad RT Nugraha

Publication date: 2019/7/19

Journal: Journal of Applied Physics

Volume: 126

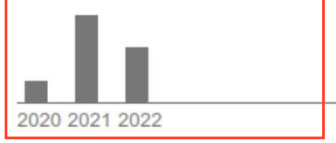
Pages: 035109

Publisher: AIP Publishing

Description: Thermoelectric properties of two-dimensional (2D) Dirac materials are calculated within linearized Boltzmann transport theory and relaxation time approximation. We find that the gapless 2D Dirac material exhibits poorer thermoelectric performance than the gapped one. This fact arises due to the cancelation effect from electron-hole contributions to the transport quantities. Opening the bandgap lifts this cancelation effect. Furthermore, there exists an optimal bandgap for maximizing figure of merit (Z T) in the gapped 2D Dirac material. The optimal bandgap ranges from 6 k B T to 18 k B T, where k B is the Boltzmann constant and T is the operating temperature in kelvin. This result indicates the importance of having narrow gaps to achieve the best thermoelectrics in 2D systems. Larger maximum Z Ts can also be obtained by suppressing the lattice thermal conductivity. In the most ideal case where the lattice thermal …

JAP Impact Factor: 2.546

Total citations: Cited by 15



15 citations in 3 years:
“impact factor”
15/(3/2) = 10

Peneliti lain bisa jadi merujuk kita hanya gara-gara keberadaan kode terbuka

Serba-Serbi Pembuatan Grafik untuk Artikel Ilmiah

Pentingnya tampilan yang menarik

"A picture speaks a thousand words"

(Gambar dari Nature's delight)

Es krim yang penuh dengan krim, enak, yummy, lembut. Mengandung cokelat chip disertai mint yang yummy. Warna-warni es dari bahan alami, menenangkan pikiran, mendinginkan kepala. Topping yang bervariasi membuat rasanya sangat nikmat, dst…

Namun hati-hati...

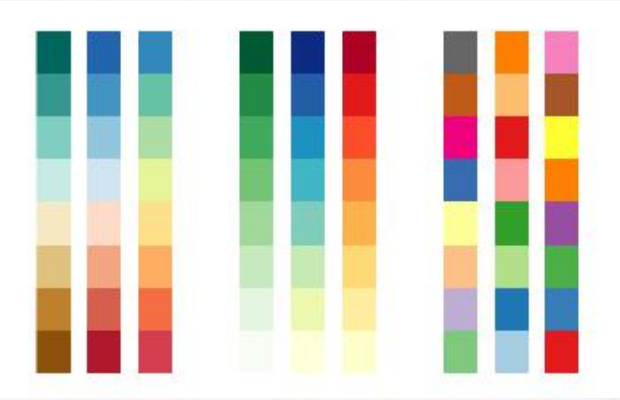
"A picture speaks a thousand words.
However, with illustration software,
the picture may tell a thousand lies."

Penggunaan perangkat lunak pengolah gambar secara berlebihan dapat mengaburkan makna data ilmiah dari gambar tersebut

Standar grafik/ilustrasi ilmiah

Standar Umum

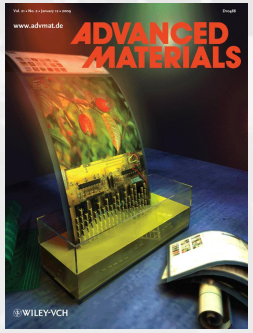
- Palet warna yang seragam
- Label sumbu cukup besar agar terbaca
- Ukuran dan jenis huruf yang konsisten
- Jangan lupa mencantumkan SATUAN!
- …

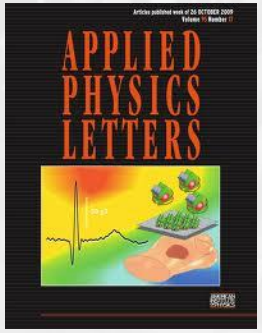


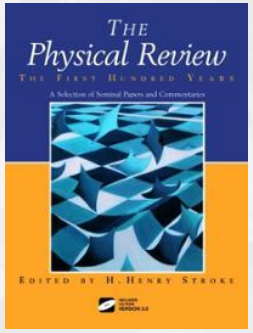
Serif vs Sans-Serif

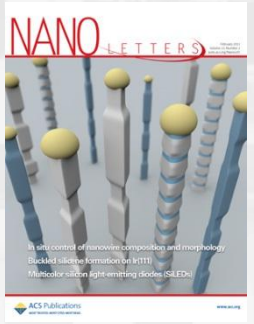
Standar Khusus

- Tipe artikel: paper ilmiah atau artikel populer atau lainnya
- Setiap jurnal memiliki spesifikasi masing-masing



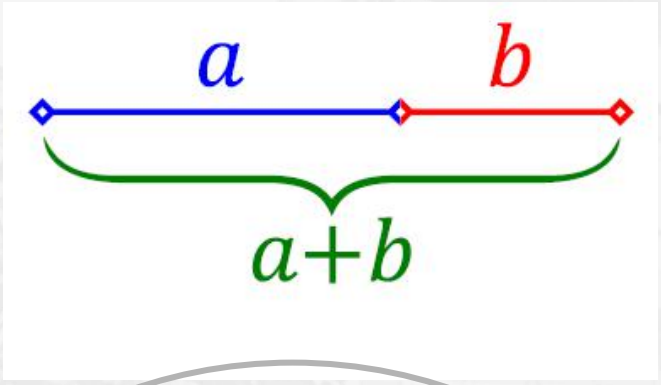




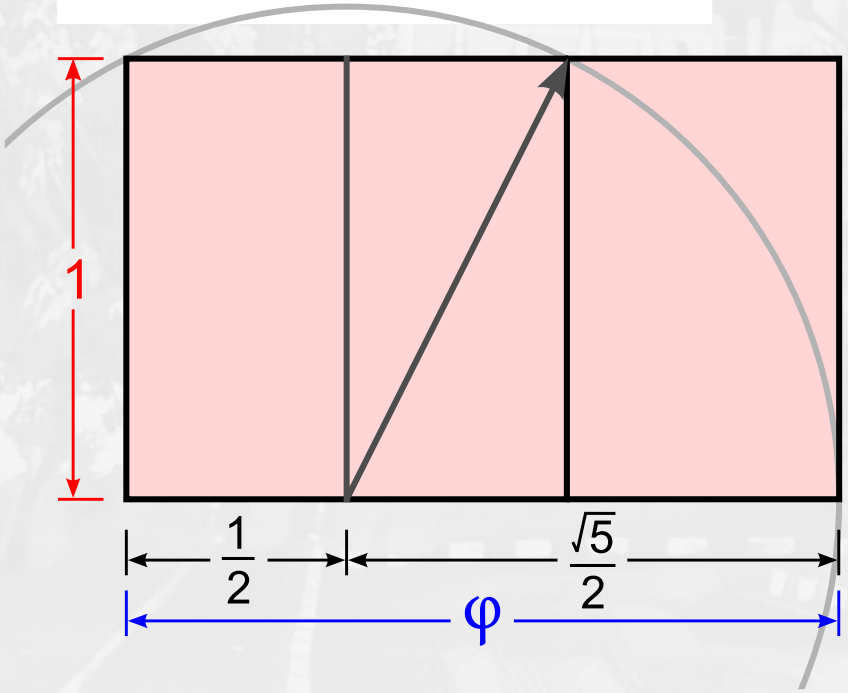


Golden ratio (kalau mau pakai...)

Berikan proporsi yang baik untuk setiap ilustrasi



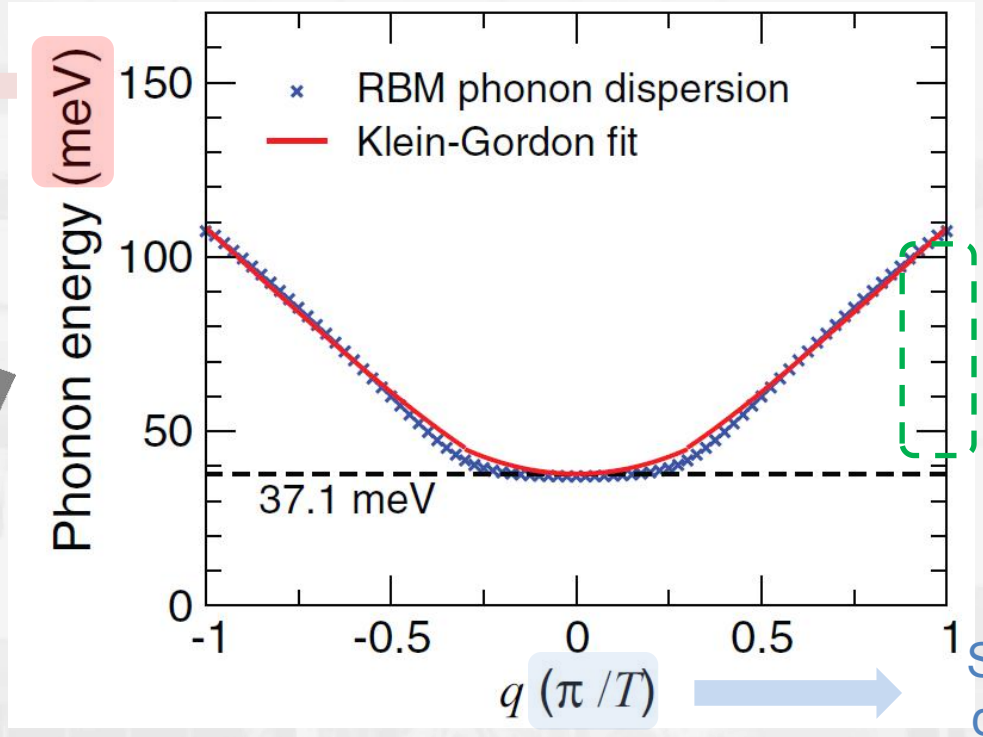
$$\varphi = \frac{a}{b} = \frac{a+b}{a} \approx 1.618\ldots$$



Golden ratio (kalau mau pakai...)

Jangan lupa sertakan SATUAN!

b



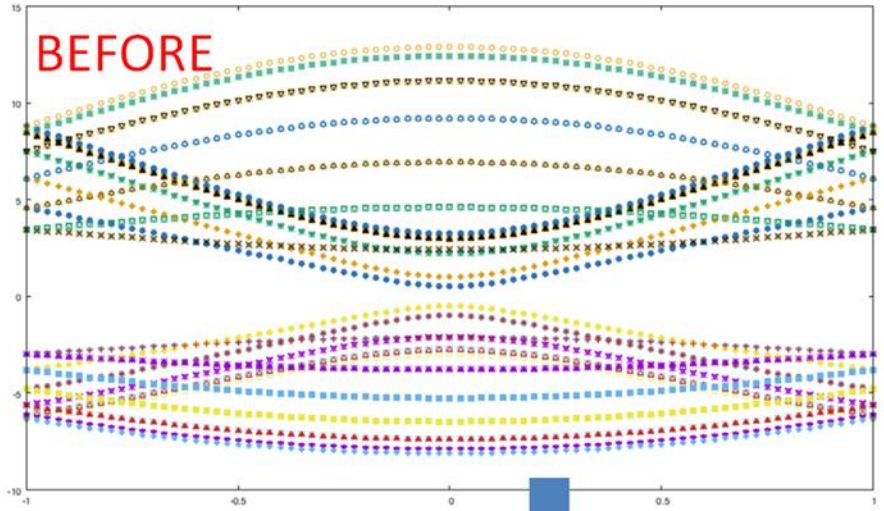
"Tick marks" u/ membantu estimasi nilai besaran

SATUAN boleh dalam variabel

a

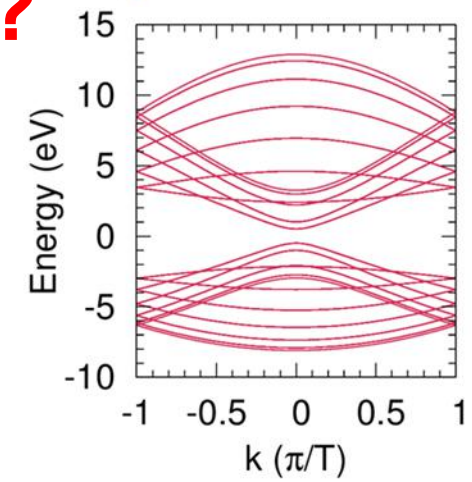
Gunakan huruf yang konsisten dengan ukuran yang jelas terbaca
Upayakan a/b sedekat mungkin dengan golden ratio
Hindari informasi redundan pada legenda
Format upayakan Vector (EPS, PDF)

Contoh perbaikan grafik sederhana



AFTER polished ?

- Label sumbu lebih terbaca
- Besaran dengan satuan dicantumkan
- “Tick marks” jelas
- Pilihan warna tidak aneh-aneh

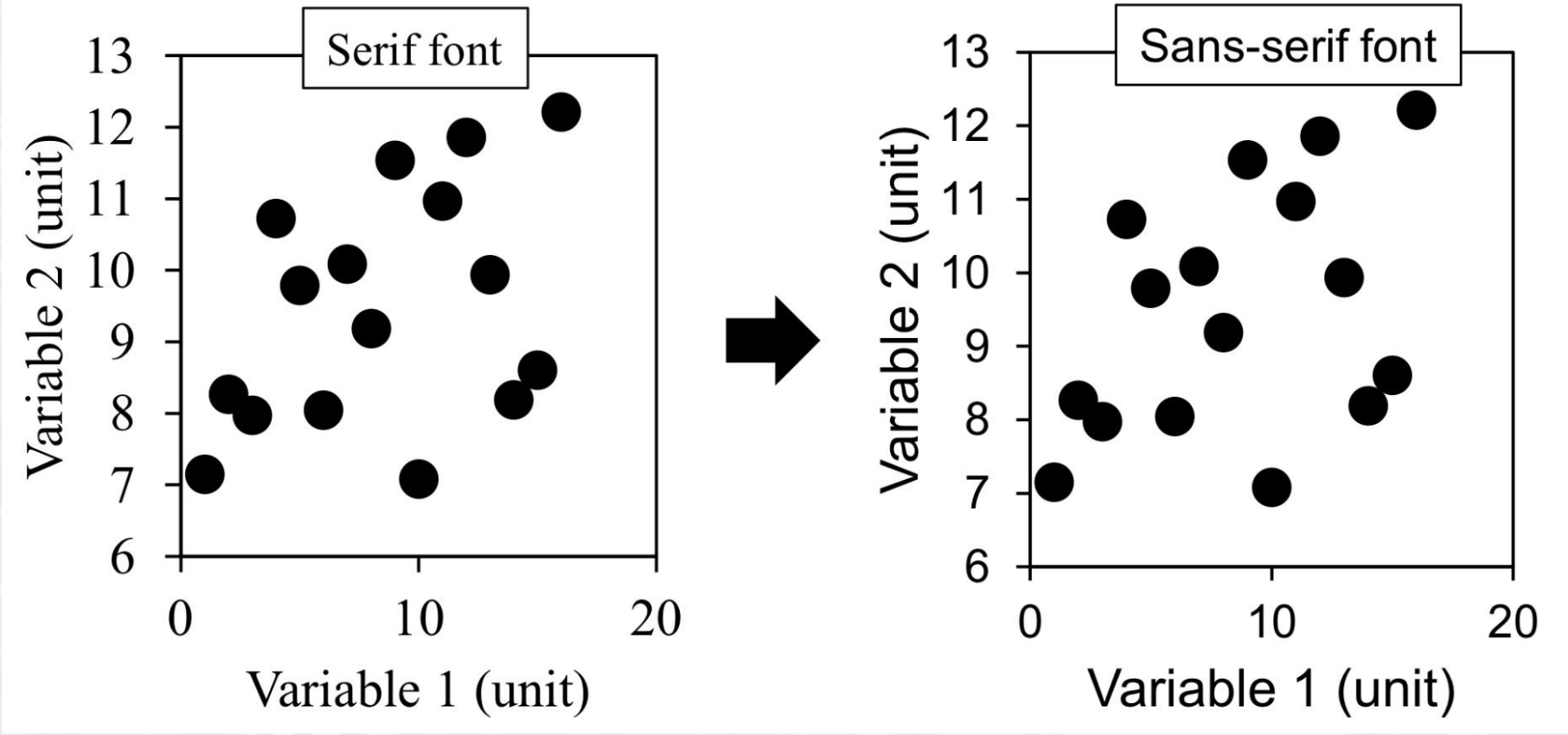


Seorang mahasiswa menggambar pita energi *carbon nanotube* sebagai fungsi *k* atau *wavector* dari elektron. Hasilnya seperti pada gambar terlihat “wah”, tetapi tidak memberikan informasi apapun.

Pada dasarnya kita tidak perlu memberi warna-warni yang berlebihan pada setiap garis yang tidak memiliki “makna khusus” atau “nilai kepentingan” tertentu.

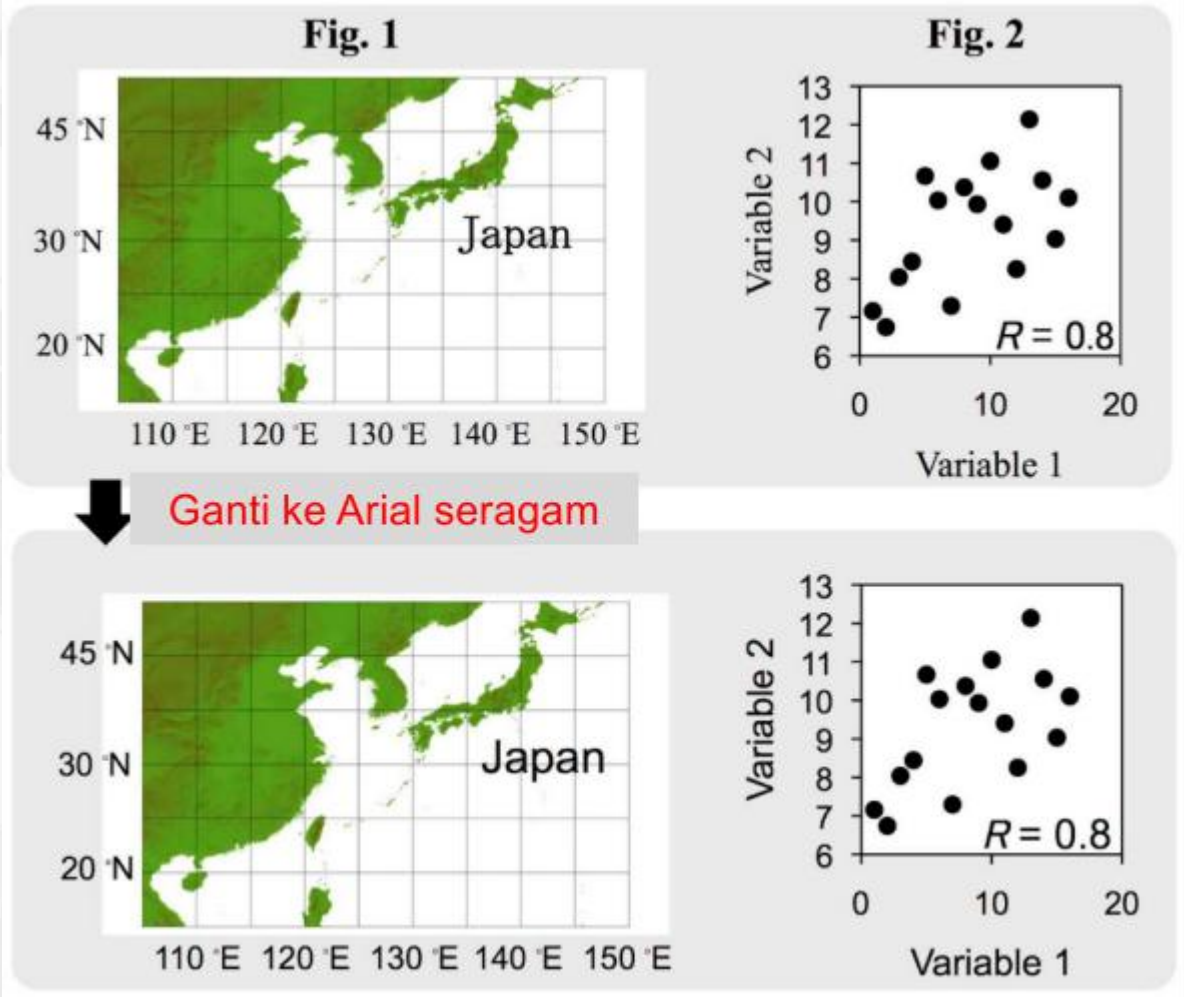
Pilihan huruf

Gunakan font Sans-serif (Helvetica atau Arial biasanya lebih disukai).



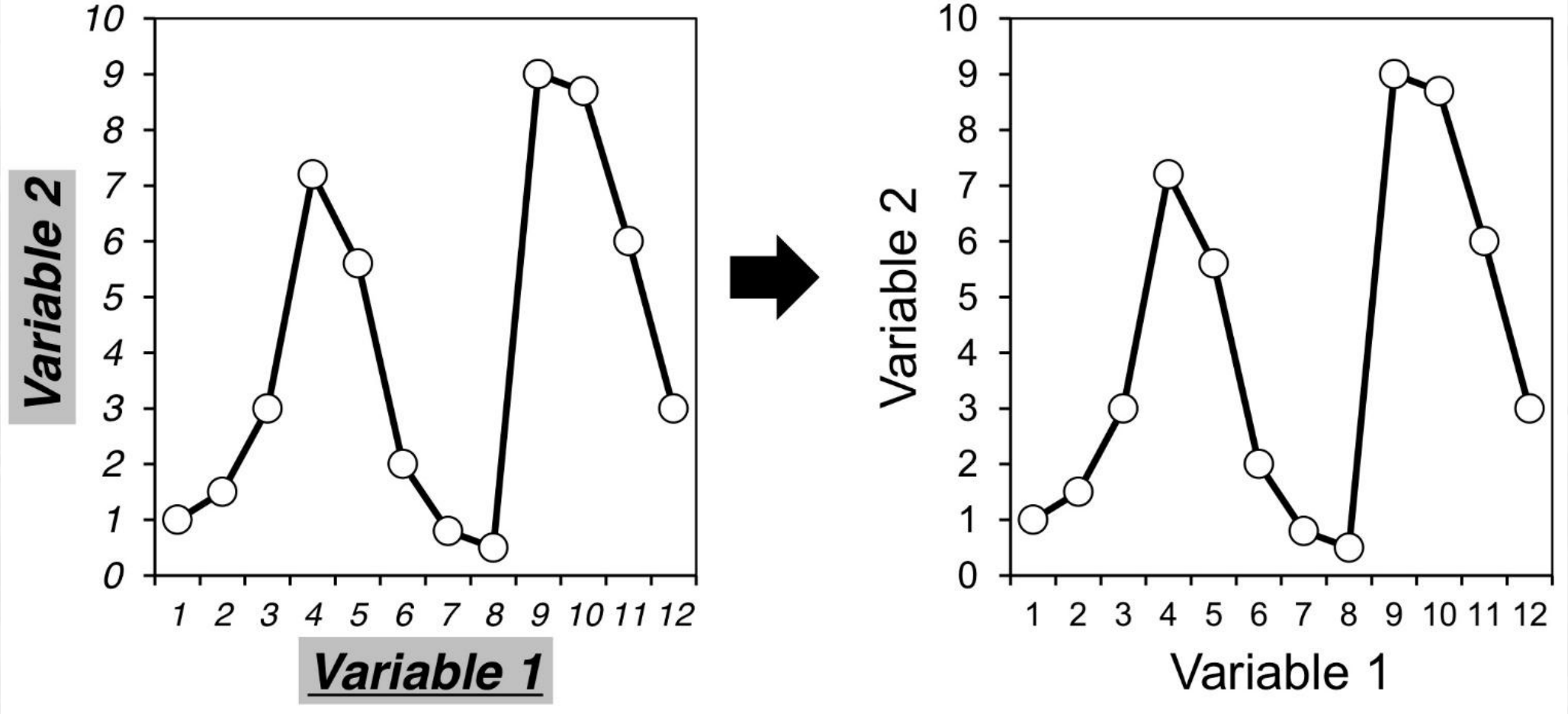
Pilihan huruf

Sebisa mungkin seragamkan jenis huruf, kecuali jika dibutuhkan untuk rumus matematis



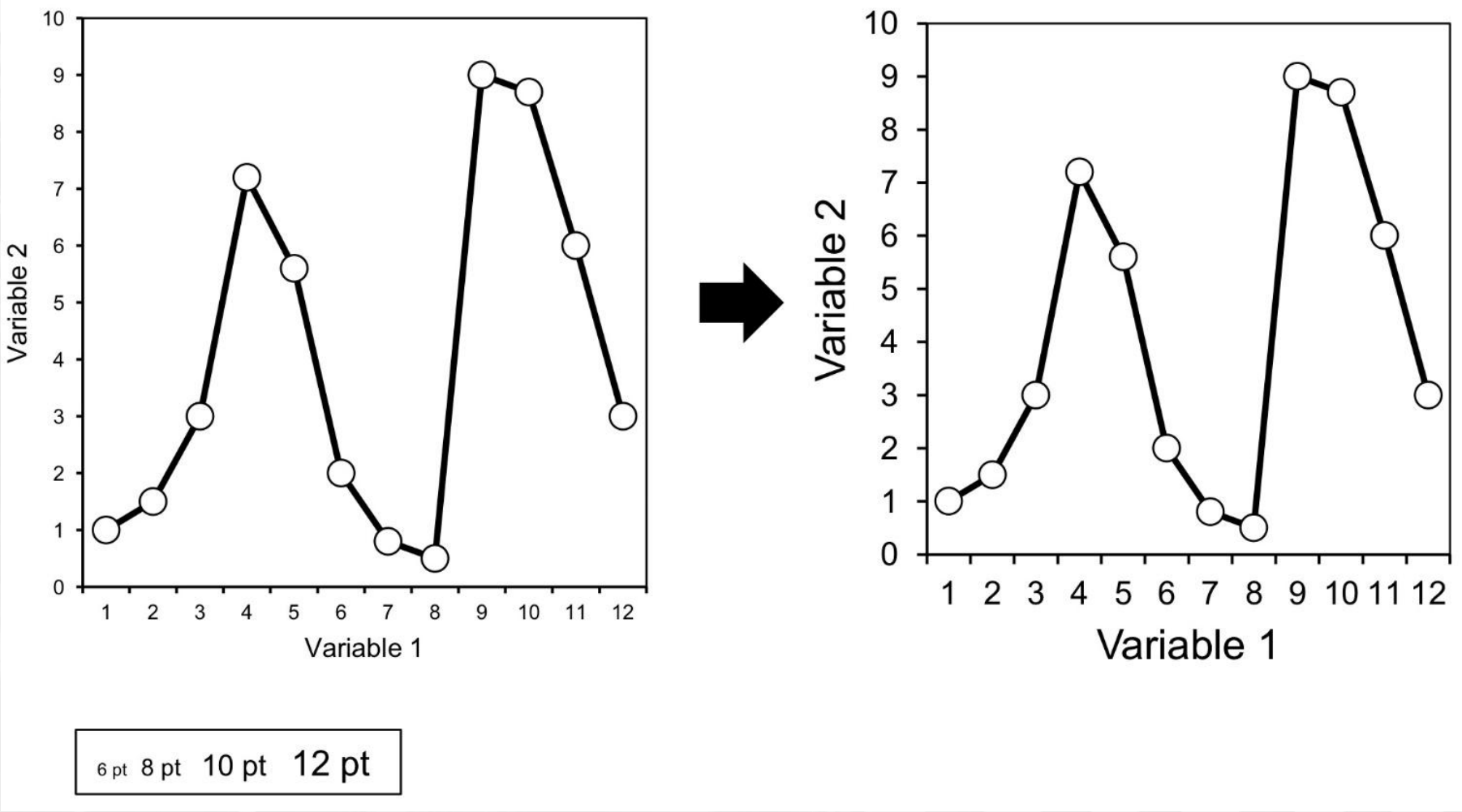
Pilihan huruf

Tidak perlu memiringkan atau menggarisbawahi huruf tertentu jika tidak ada kepentingan



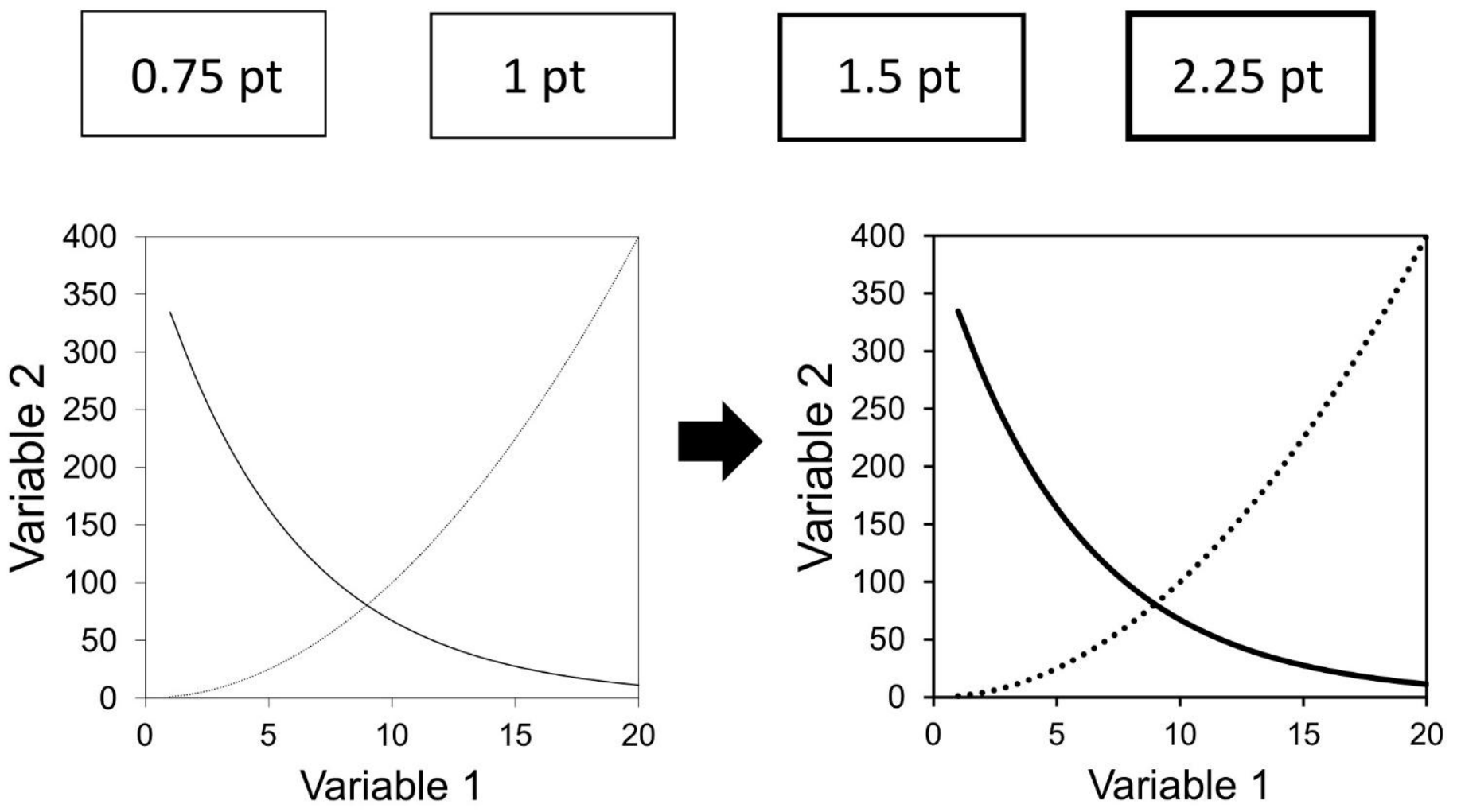
Ukuran huruf

Ukuran huruf minimal untuk pencetakan adalah 10 pt



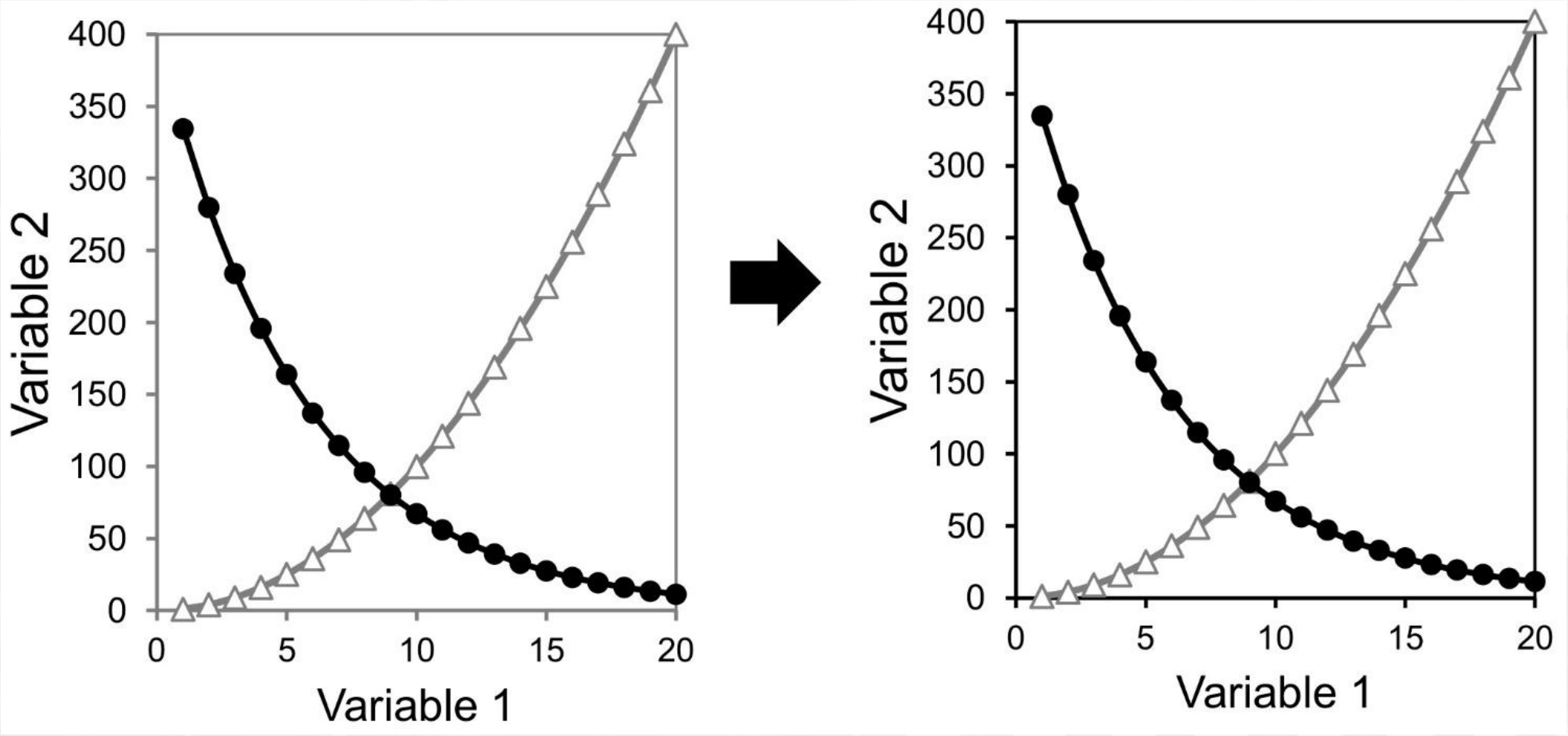
Ketebalan garis

Ketebalan garis paling minimal adalah 0,75 pt.



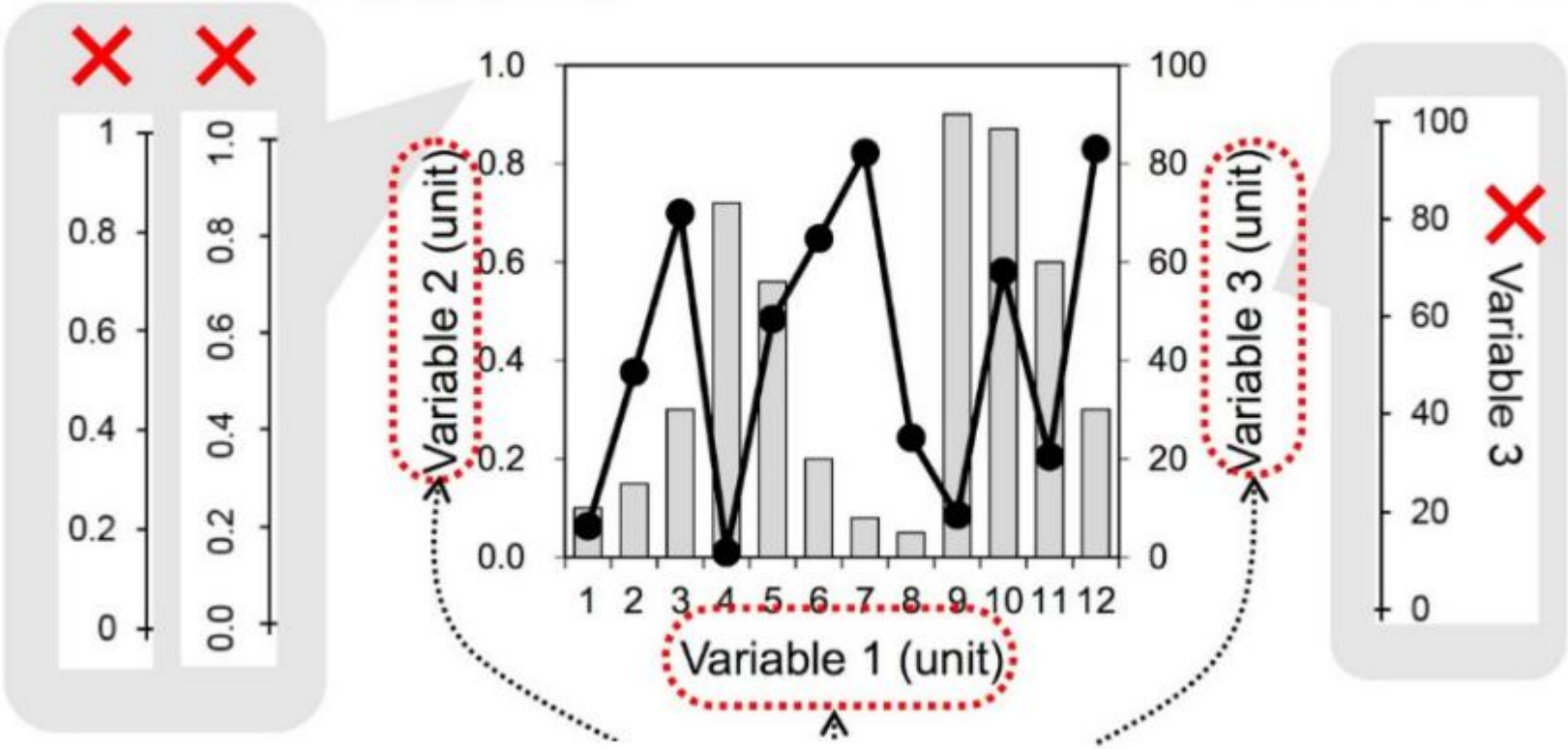
Warna garis

Gunakan warna hitam untuk *frame* maupun *border*, kecuali jika suatu saat dibutuhkan



Pelabelan sumbu grafik

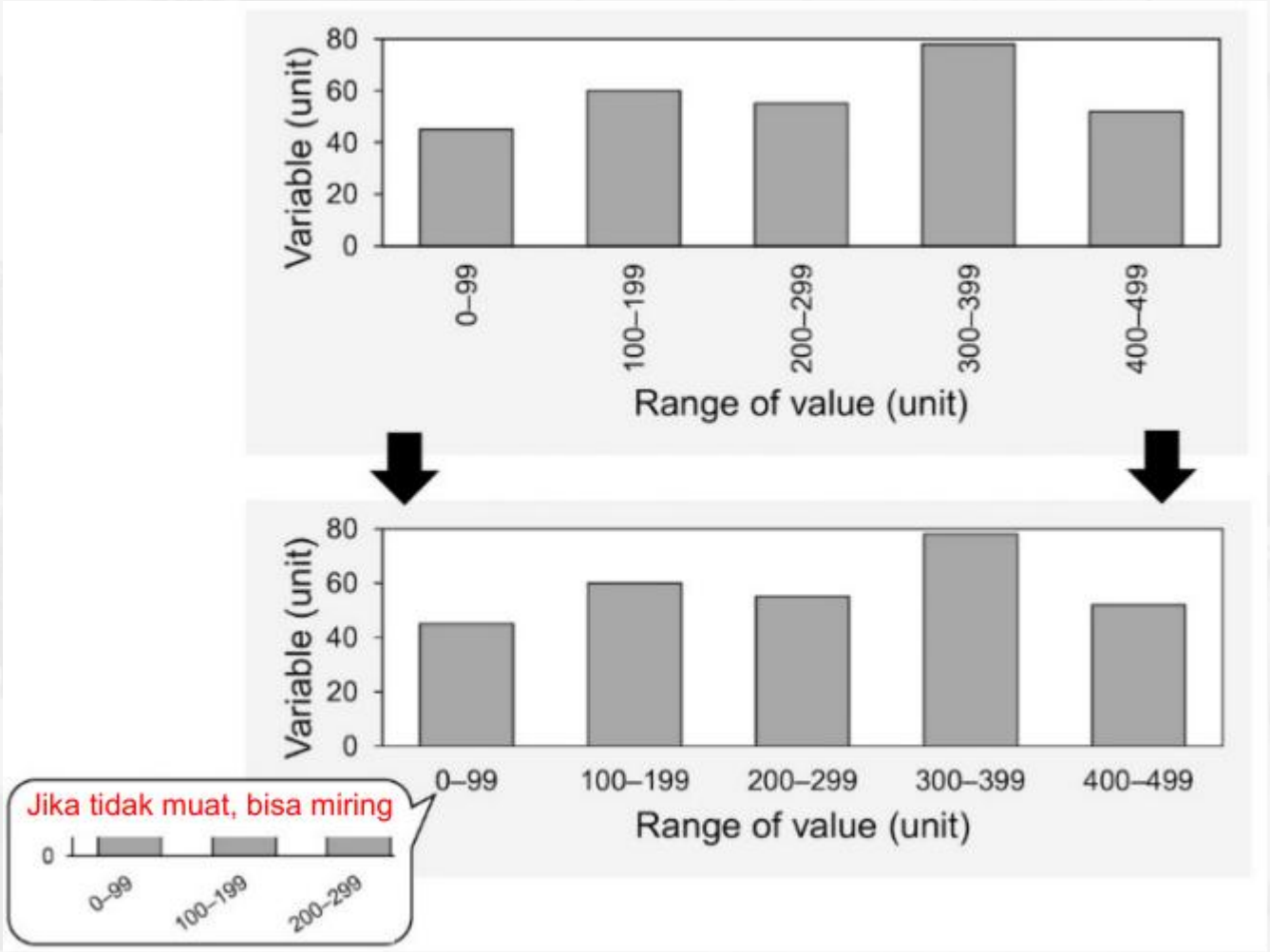
Ada arah label tertentu yang dilazimkan dalam komunitas ilmiah



Setiap sumbu harus memiliki label dekat dengan nilai besaran

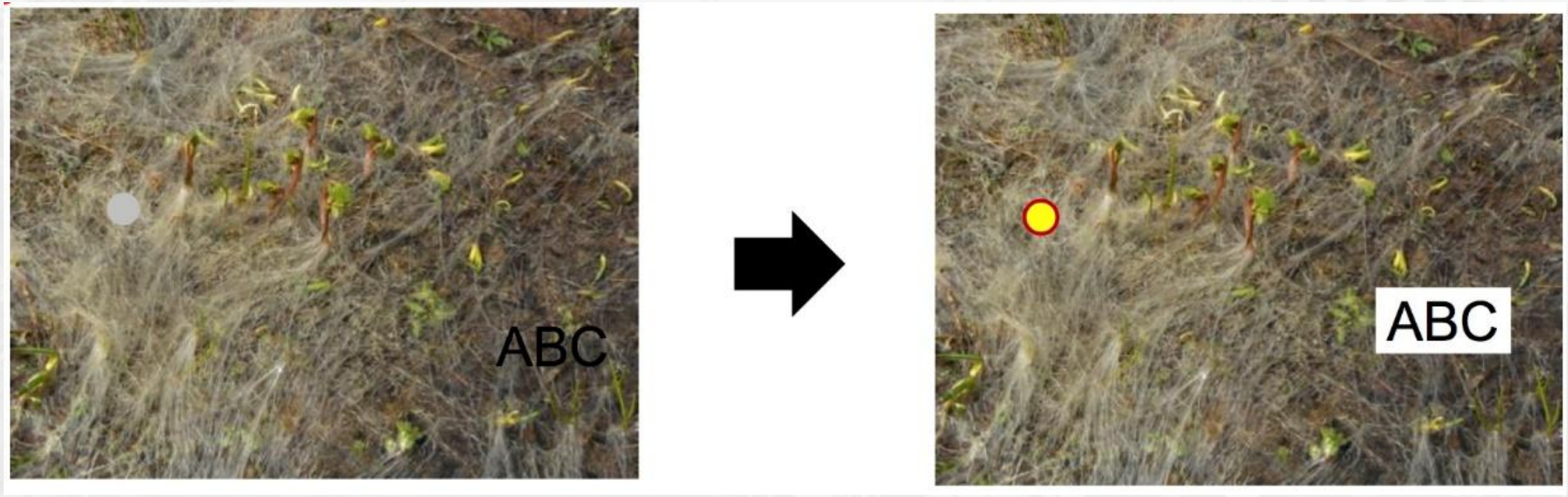
Pelabelan sumbu grafik

Nilai besaran berupa rentang sebisa mungkin ditampilkan horizontal



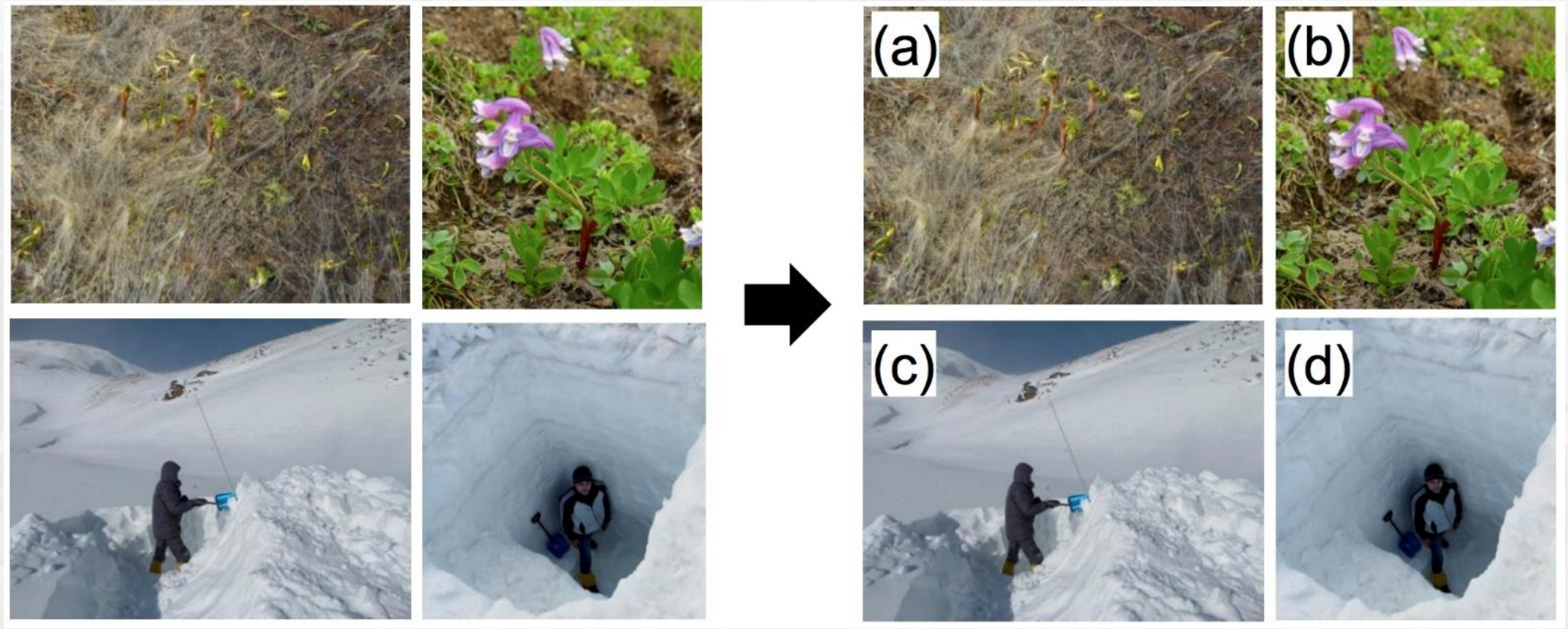
Tambahan teks atau simbol pada foto

Jika menambahkan teks/simbol di atas foto atau gambar yang padat warna, perlu perhatikan pilihan latar belakang dari teks/simbol



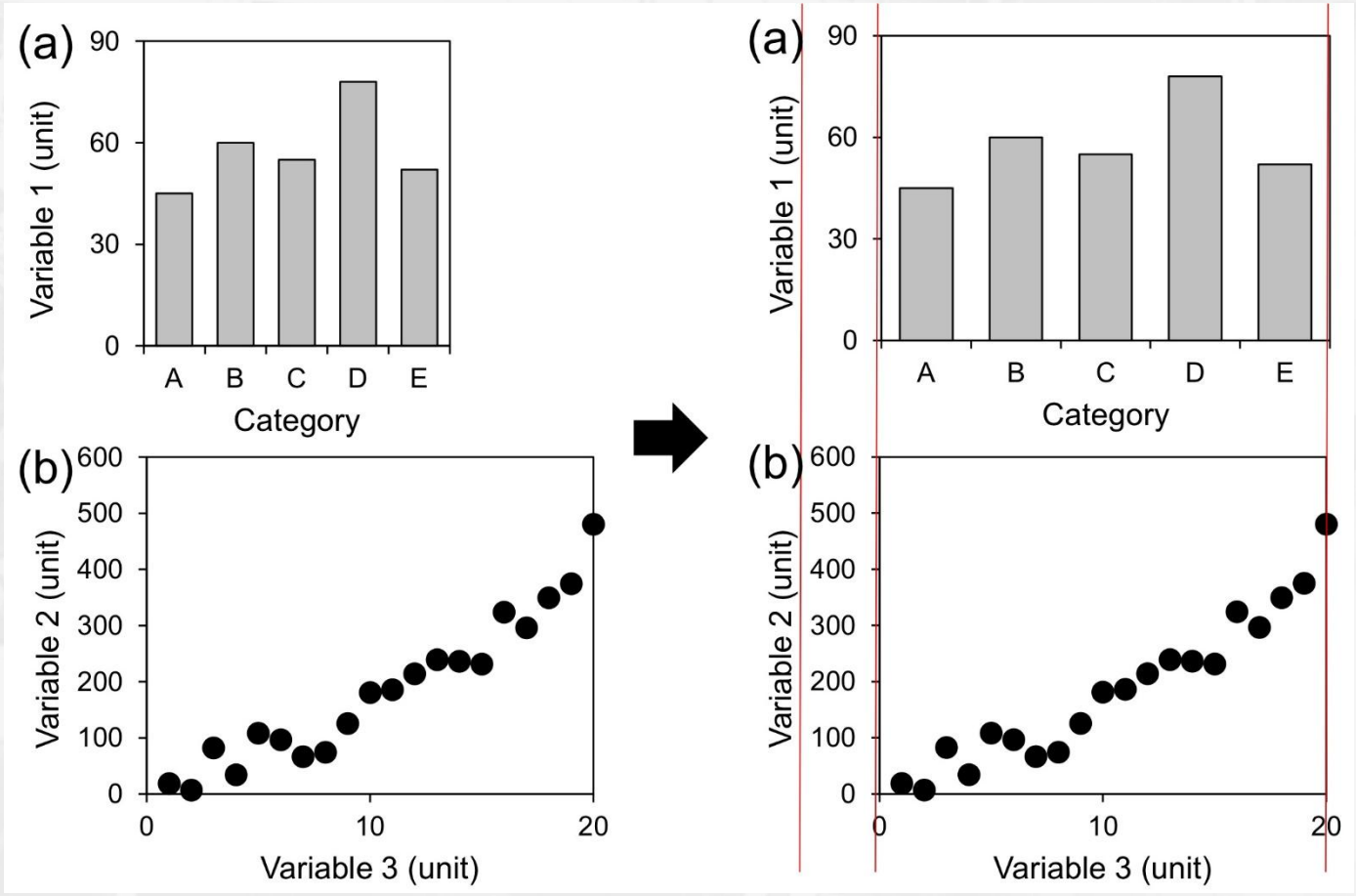
Gambar dengan beberapa panel

Label ada di setiap panel, sebisa mungkin gunakan huruf kecil minimal 10 pt dalam tanda kurung, letakkan di kiri atas, sejajarkan secara vertikal dan horizontal.



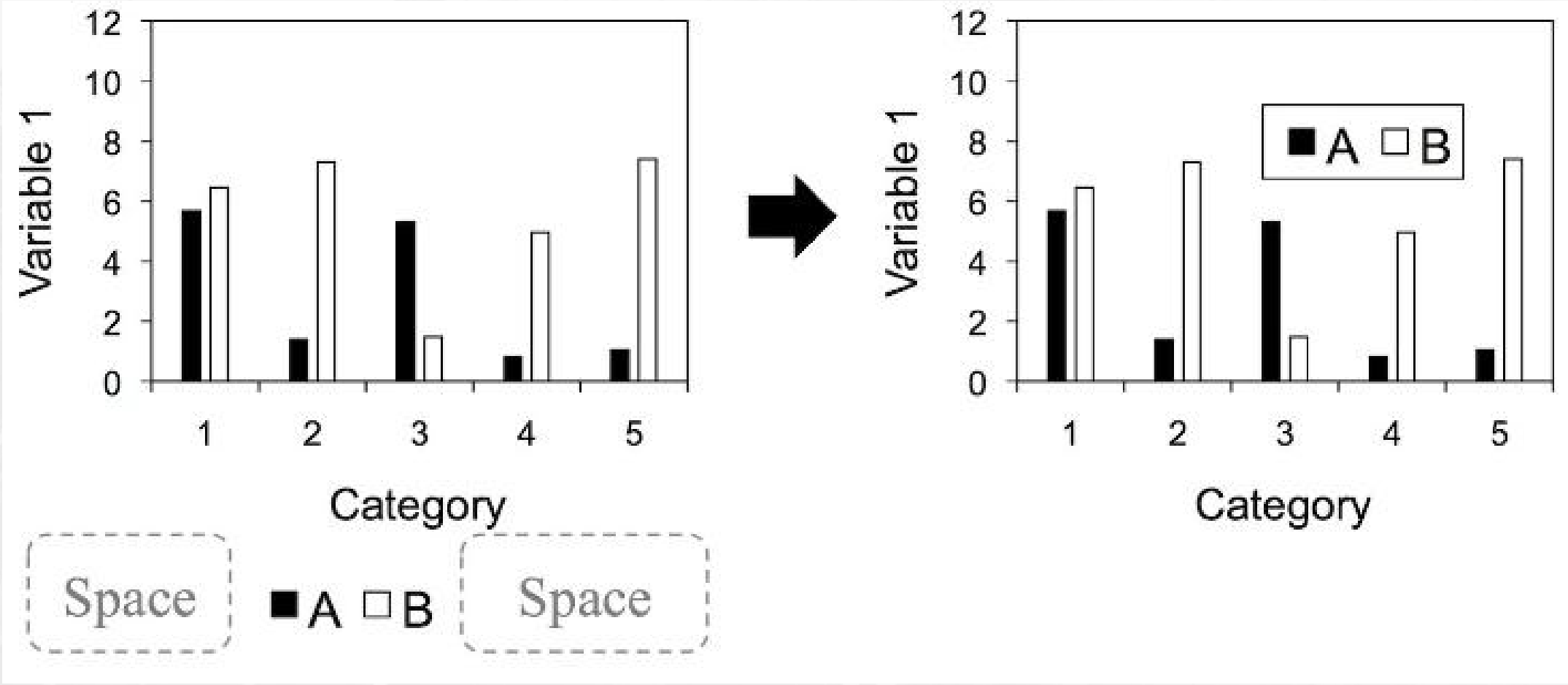
Gambar dengan beberapa panel

Ukuran panel upayakan seseragam mungkin



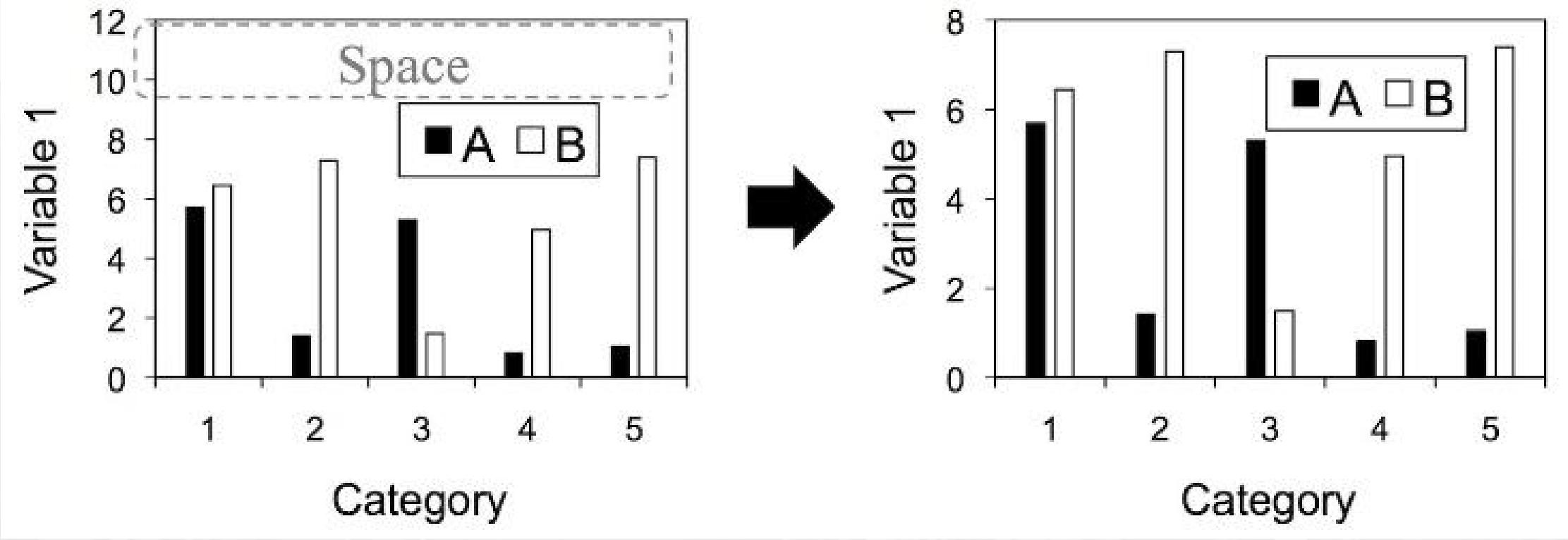
Pengaturan ruang agar tak mubazir

Atur posisi legenda



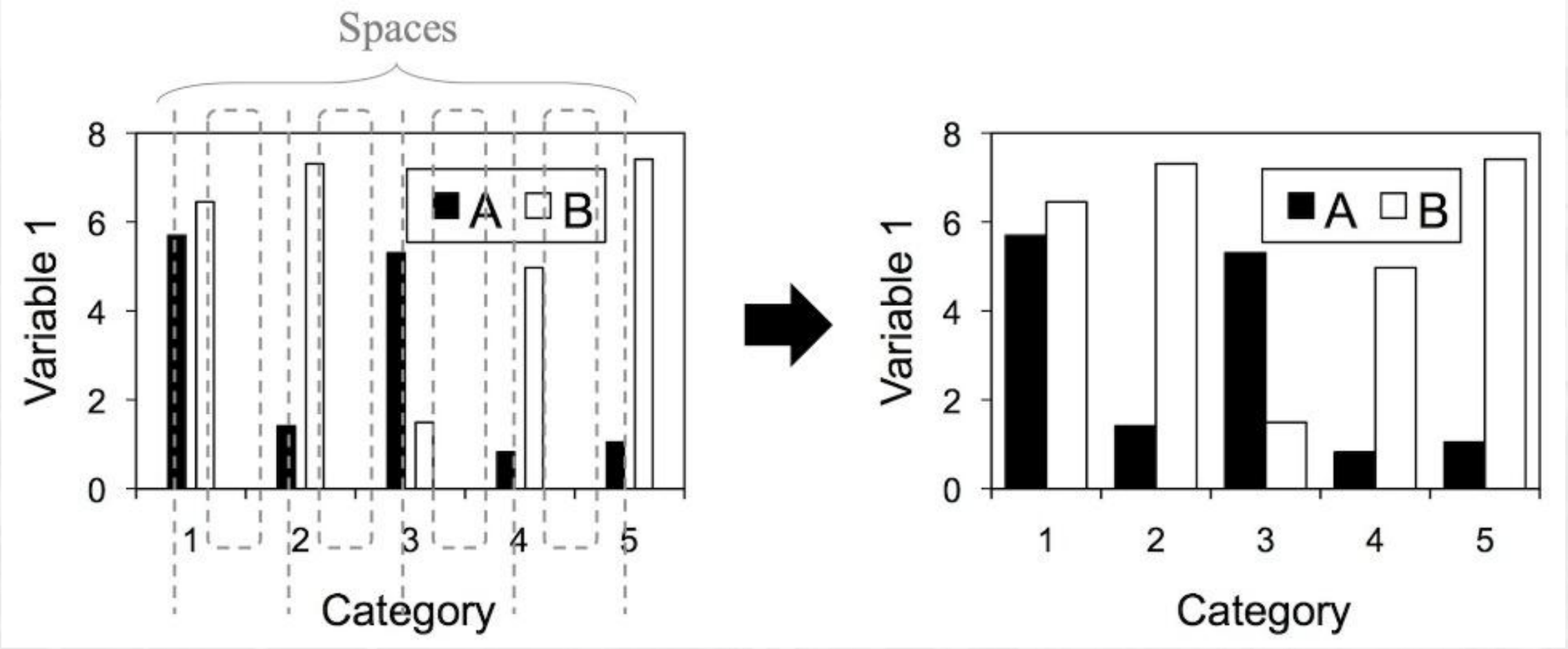
Pengaturan ruang agar tak mubazir

Buang ruang kosong



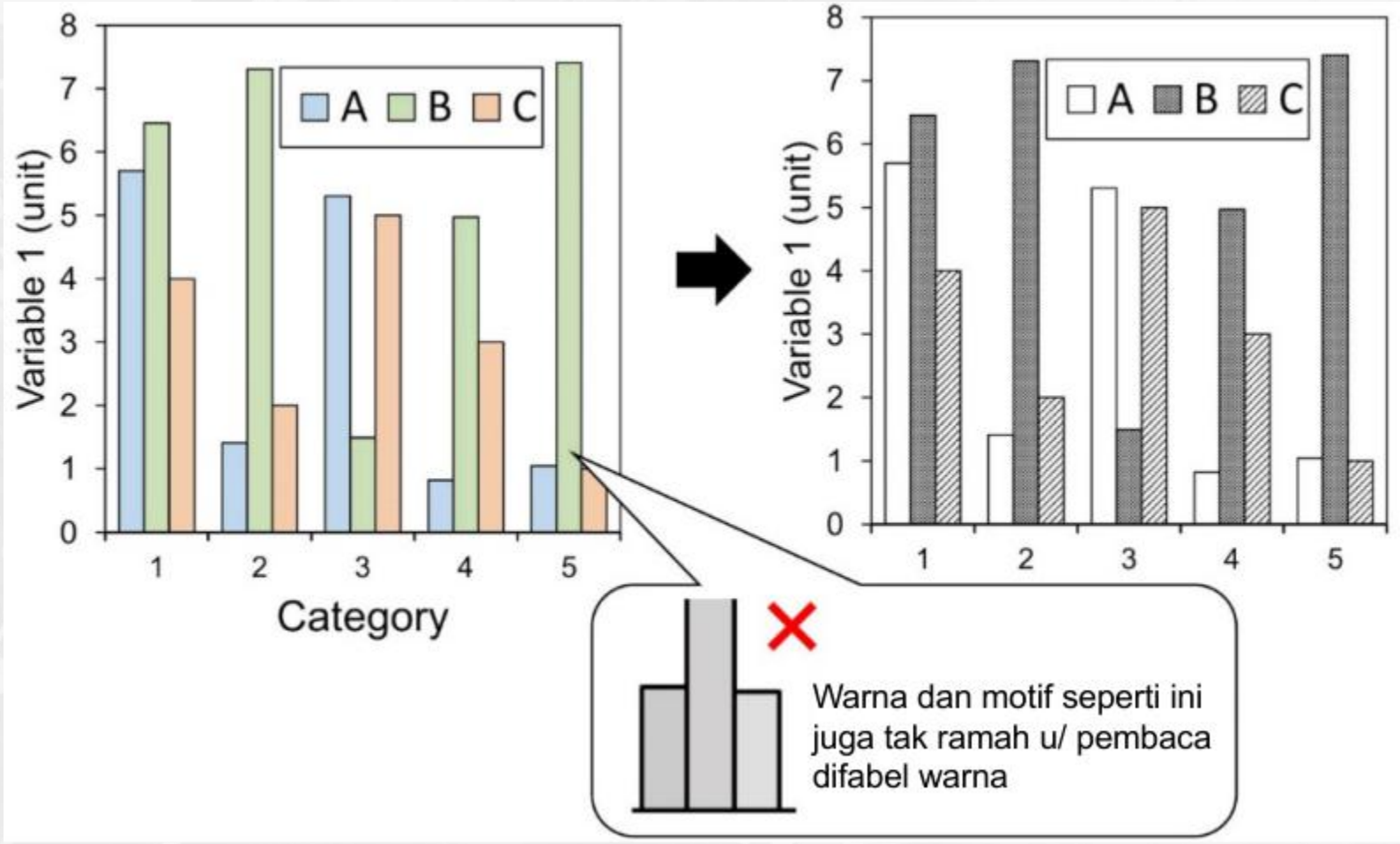
Pengaturan ruang agar tak mubazir

Buang ruang kosong



Pilihan warna & motif garis/bentuk

Ingat bahwa ketika dicetak, mayoritas penerbit akan mencetak hitam-putih



Implementasi dalam Python/Matplotlib

Python for Scientific Publications:

- https://github.com/venkatesannaveen/python-science-tutorial

Contoh realisasi dalam publikasi kami:

- https://nbviewer.org/github/artnugraha/GermaniumTellurides
- https://nbviewer.org/github/artnugraha/DiracTE
- dll.