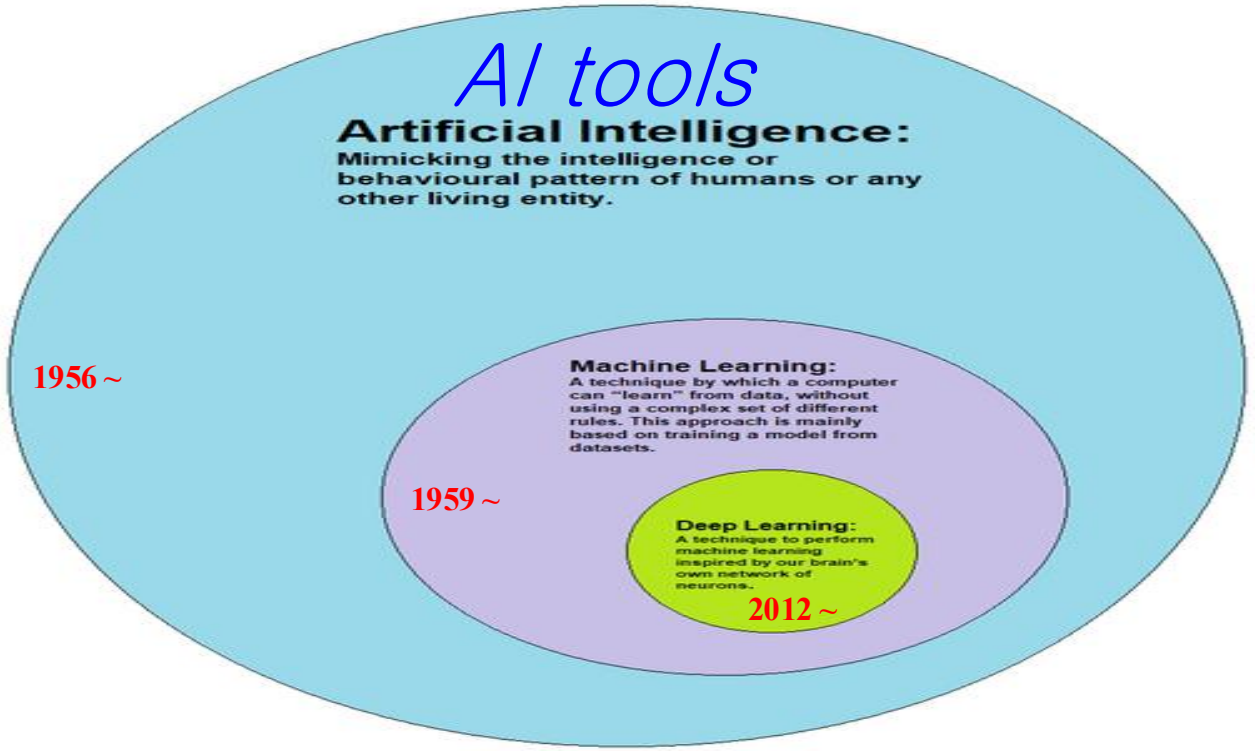
인공지능 융합형 소재/소자 설계 및 측정 가속화 기술의 현재와 미래

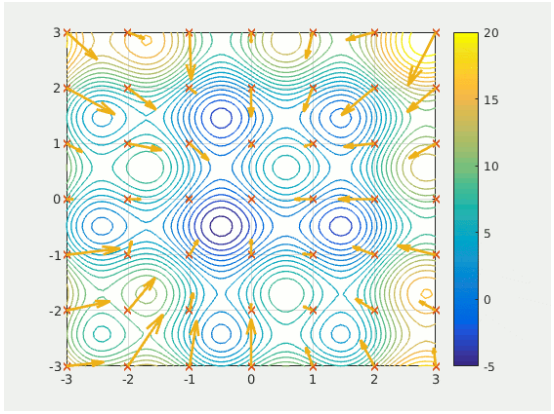
이인호
한국표준과학연구원
ihlee@kriss.re.kr

KIAS June 23, 2026

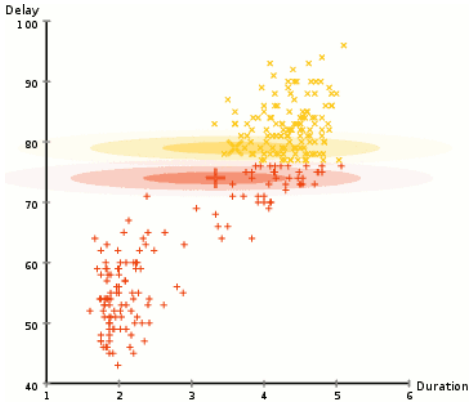
AI tools



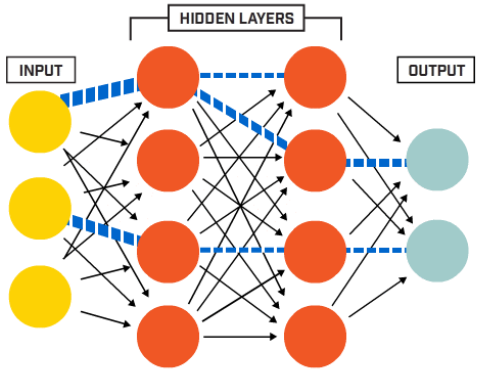
Search and optimization



Classifiers and statistical learning methods



Artificial neural networks



The overall research goal of artificial intelligence is to create technology that allows computers and machines to function in an intelligent manner.

https://en.wikipedia.org/wiki/Artificial_intelligence

KRISS

Forms of Machine Learning

Four learning types

1. Supervised learning

2. Unsupervised learning

3. Reinforcement learning

4. Evolutionary learning

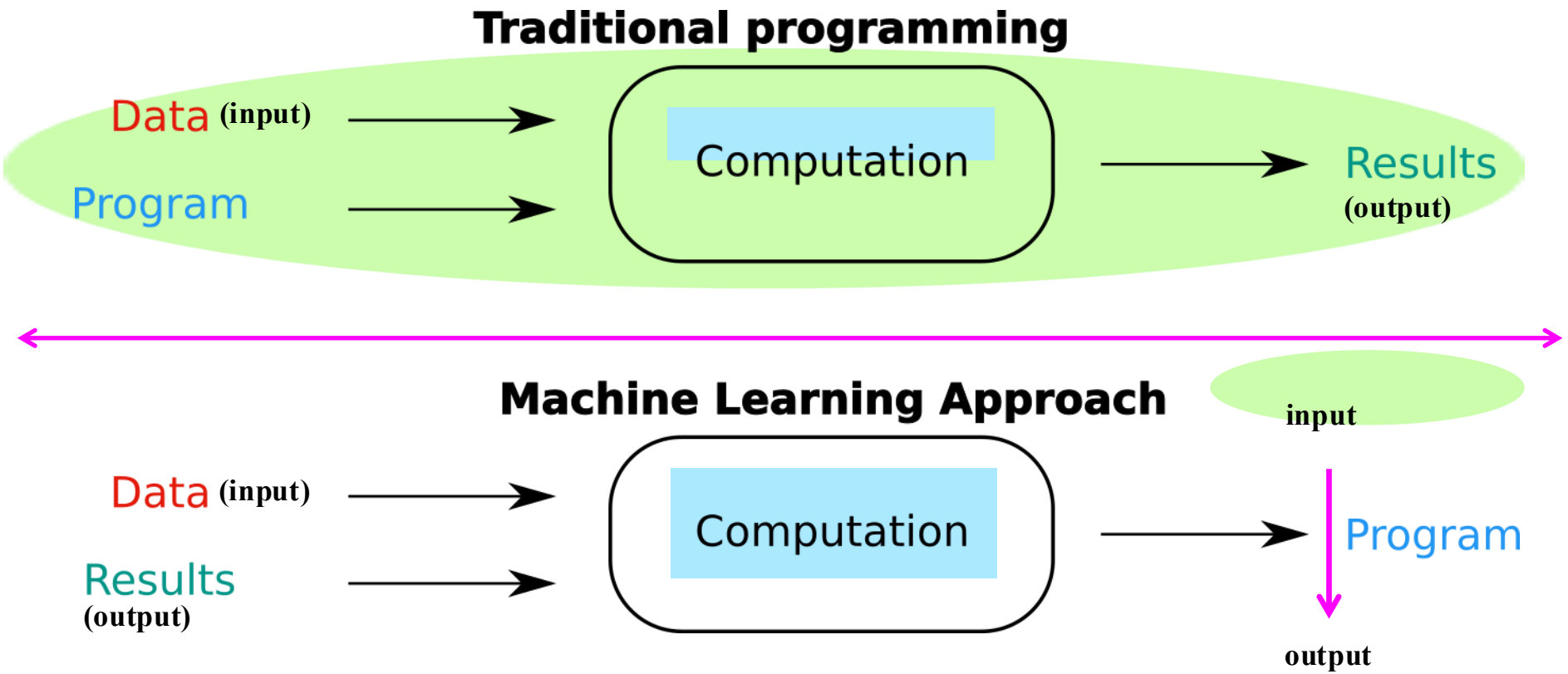
Three elements

Learning task = {1. Representation} ⊕ {2. Evaluation} ⊕ {3. Optimization}

flexible **fixed**

KRISS

ML?



learning data representations, as opposed to task-specific algorithms

KRISS

The understanding of processing-structure-properties relationships is called the materials paradigm.

Materials Project → computational
Cambridge Structural Database → experimental

in silico exploration of as-yet-unreported materials

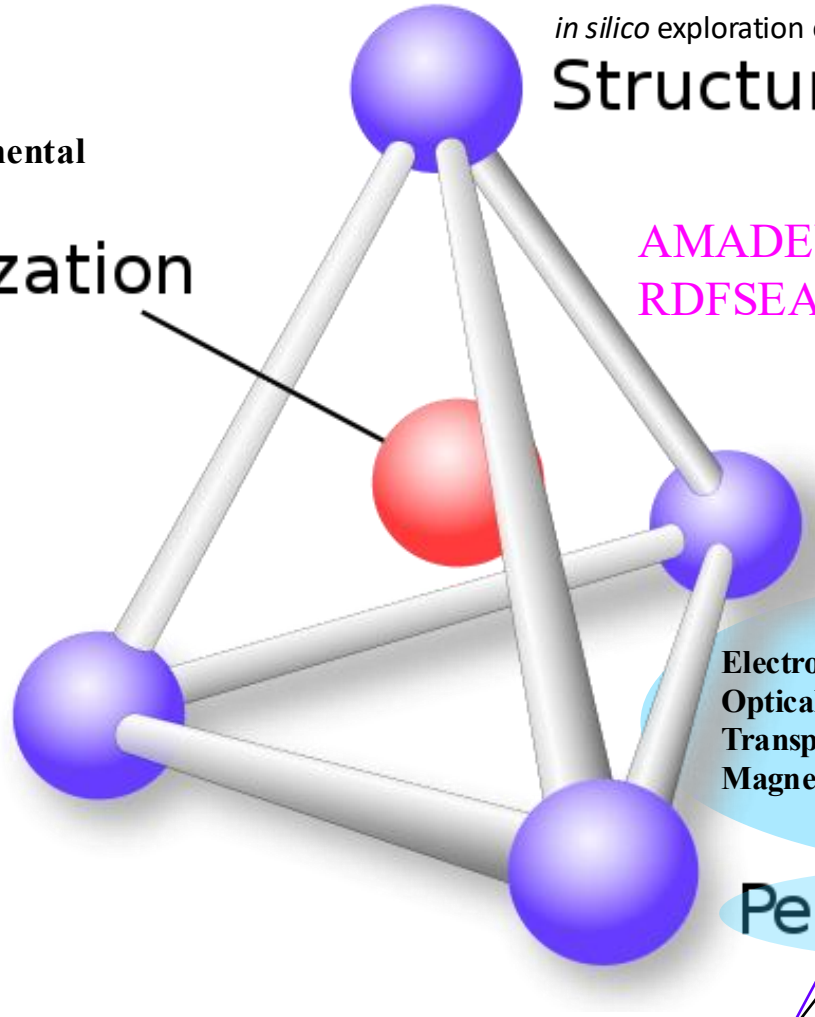
Structure — *a priori* unknown

Inverse approach

Not invertible!

AMADEUS
RDFSEARCH

Characterization



Processing

Properties

Electronic
Optical
Transport
Magnetic

Solar cell,
LED,
High mobility,
Superconductor

Performance

VESTA
VASP
Quantum Espresso
Mechanical stability
Phonopy
Wannier90
EPW
WannierTools
BerkeleyGW
BoltzTrap
PyProcar

Nature **402**, 60 (1999), Nature Rev. Chem. **2**, 0121 (2018).
https://en.wikipedia.org/wiki/Materials_science

Topological materials, Chern insulator?
https://github.com/inholeegithub/winter2022/tree/main/amadeus

KRISS

Conformational Space Annealing (CSA)

- Based on genetic algorithm(GA) → maintain a pool of conformations (bank) and new conformations are obtained by mating (crossover) and mutation (small perturbation)
- Consider only conformational space of local minima (as in MCM)
- Diversity of the bank is directly controlled by introducing the concept of *distance* between the conformations
- Narrows the search to smaller region while maintaining diversity of sampling
- Key idea : GA + annealing in conformational space

Protein structure prediction (modeling) {CASP experiments}
X-ray data → crystal structure determination
NMR → molecule structure determination
Bioinformatics
LJ clusters
Travelling salesman problem
***Ab initio* materials design (super functional materials)**
Pathway sampling (Action-CSA)
Super-functional materials/devices design
……..

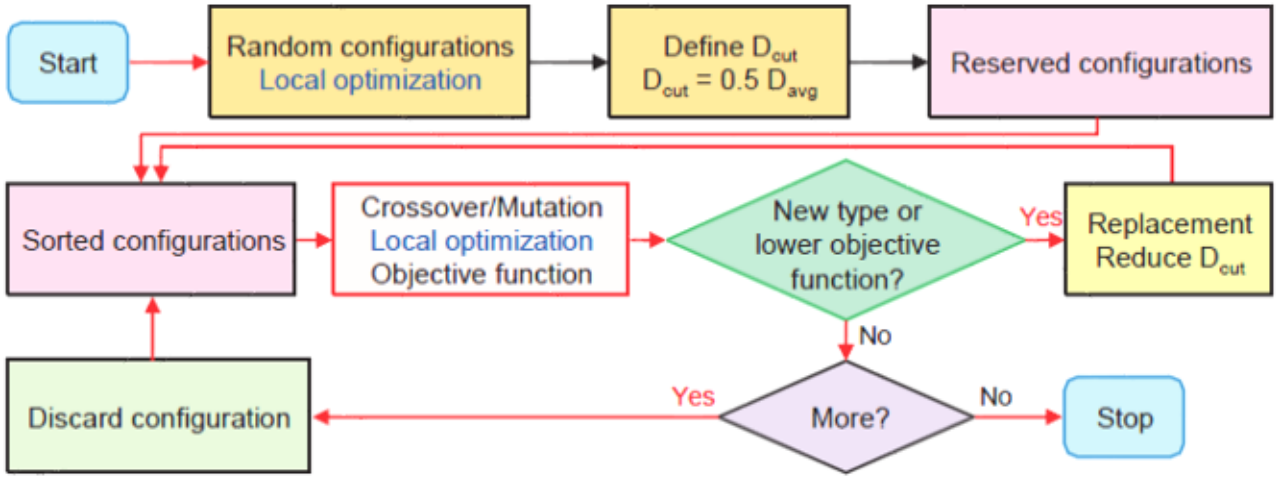
https://github.com/inholeegithub/winter2022/tree/main/amadeus

J. Comput. Chem. **18**, 1222 (1997); Phys. Rev. Lett. **91**, 080201 (2003); Comput. Phys. Commun. **203**, 110 (2016).

KRISS

Development of AMADEUS code

AMADEUS (*Ab initio* MAterials DEsign Using conformational Space annealing)



Conformational space annealing (CSA) for global optimization

with three ingredients [Phys. Rev. Lett. **91**, 080201 (2003).]

- **Genetic algorithm**
- **Simulated annealing**
- **Local minimization**

First-principles electronic structure calculations

based on density functional theory

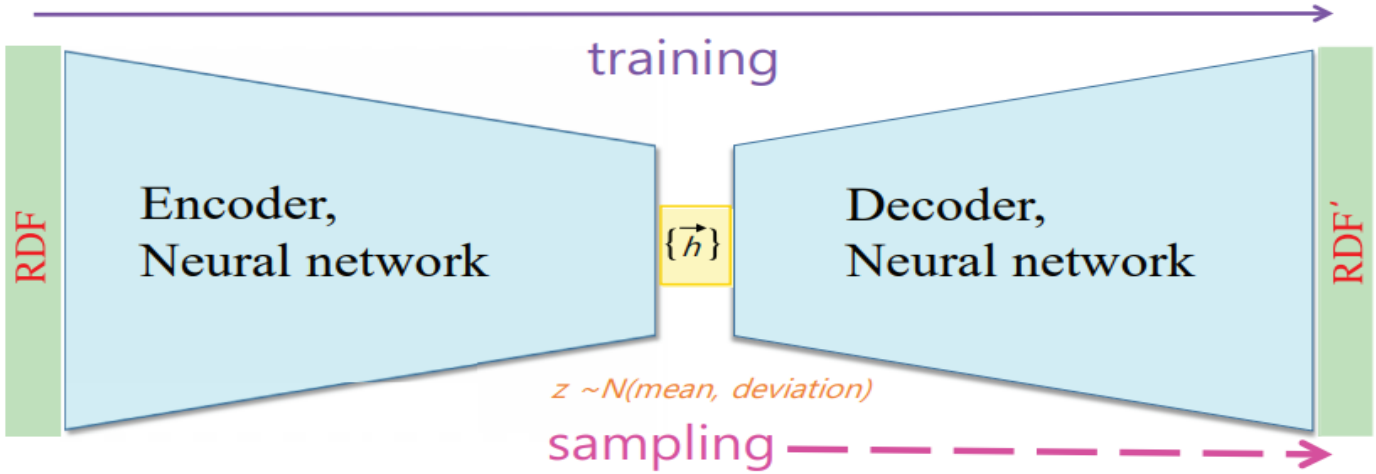
Mechanical stability
Dynamical stability
Thermal stability

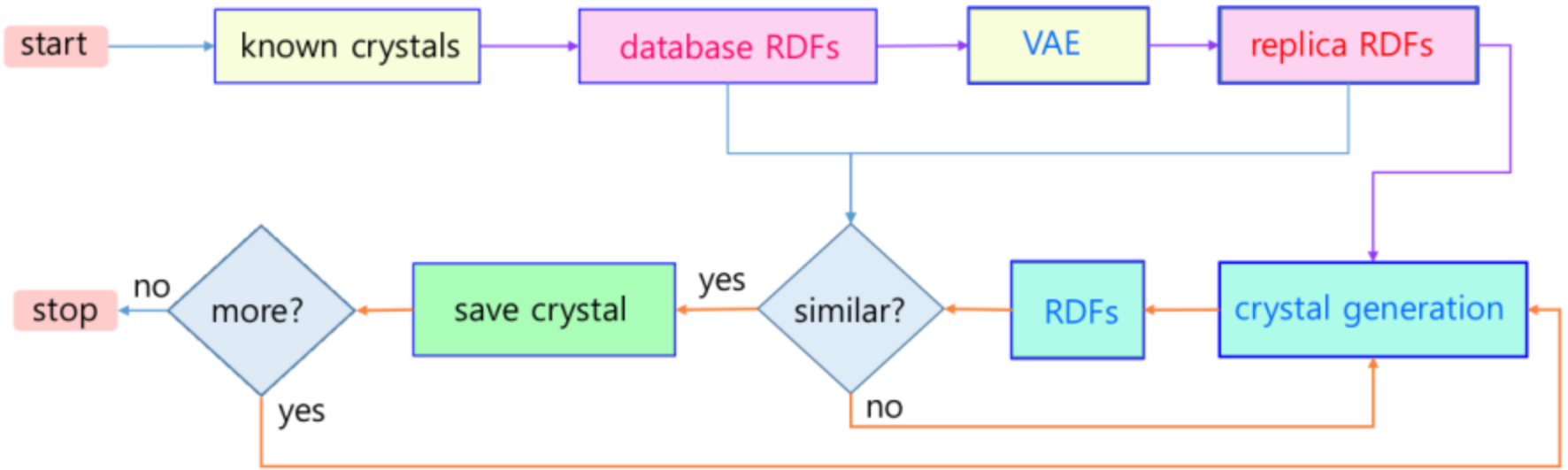
- VESTA
- VASP
- Quantum Espresso
- Mechanical stability
- Phonopy
- Wannier90
- EPW
- WannierTools
- BerkeleyGW
- BoltzTrap
- PyProcar

Comp. Phys. Commun. **203**, 110 (2016).

KRISS

Crystal structure prediction in a continuous representation space





https://github.com/inholeegithub/winter2022/tree/main/rdfsearch

Comput. Mat. Sci. **194**, 110436 (2021); Comput. Phys. Commun. **292**, 108889 (2023).

KRISS

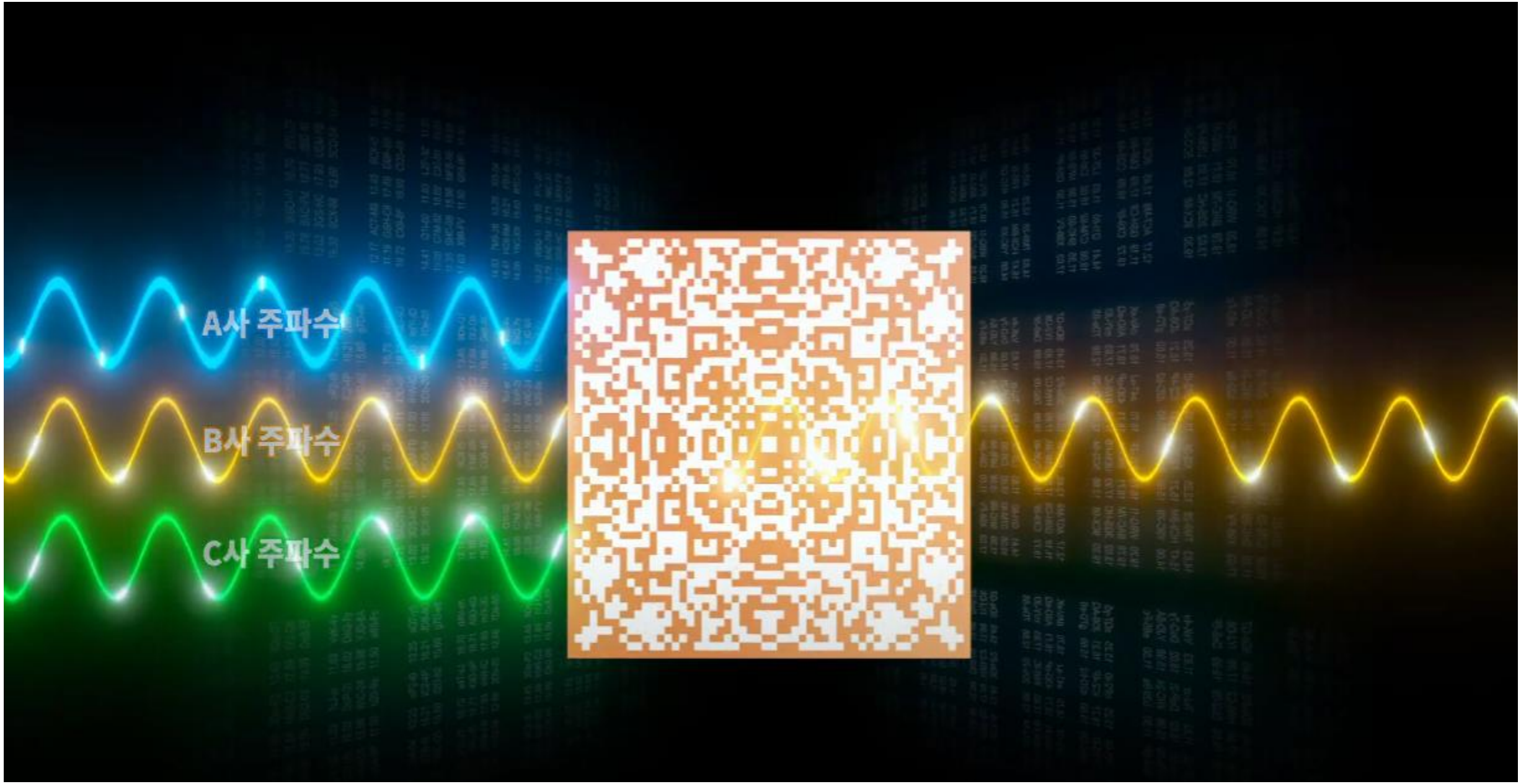
Applications

- Solar cell (Si): Phys. Rev. B **90**, 115209 (2014), Sci. Rep. **5**, 18086 (2015), Comp. Phys. Commun. **203**, 110 (2016).
- LED (C): Phys. Rev. B **93**, 085201 (2016).
- High-mobility [green phosphorus] (P): J. Phys. Chem. Lett. **8**, 4627 (2017).
- Topological materials (Si, C, $Ag_2Se_{0.5}Te_{0.5}$): J. Phys. Chem. C **123**, 1839 (2019), NPG Asia Materials **9**, e361 (2017), Nanoscale **11**, 5171 (2019).
- Structure searches (B): Sci. Rep. **7**, 7279 (2017), NPG Asia Materials **9**, e400 (2017), arXiv:1902.08390
- Superconductivity (Si): Phys. Rev. Lett. **120**, 157001 (2018).
- Topological superconductivity (Si): Phys. Rev. Mat. **5**, 104802 (2021); Phys. Rev. B **107**, 115127 (2023).
- Device design : Adv. Mat. **38**, e08332 (2026).

https://github.com/inholeegithub/InAsSb_atomic_structures

https://github.com/inholeegithub/winter2022/tree/main/amadeus

KRISS



https://www.youtube.com/watch?v=4vw6wVP81No&list=PLTIv6N2kNYZamqDqPdGSBDN1Gc6rW-KET&index=11

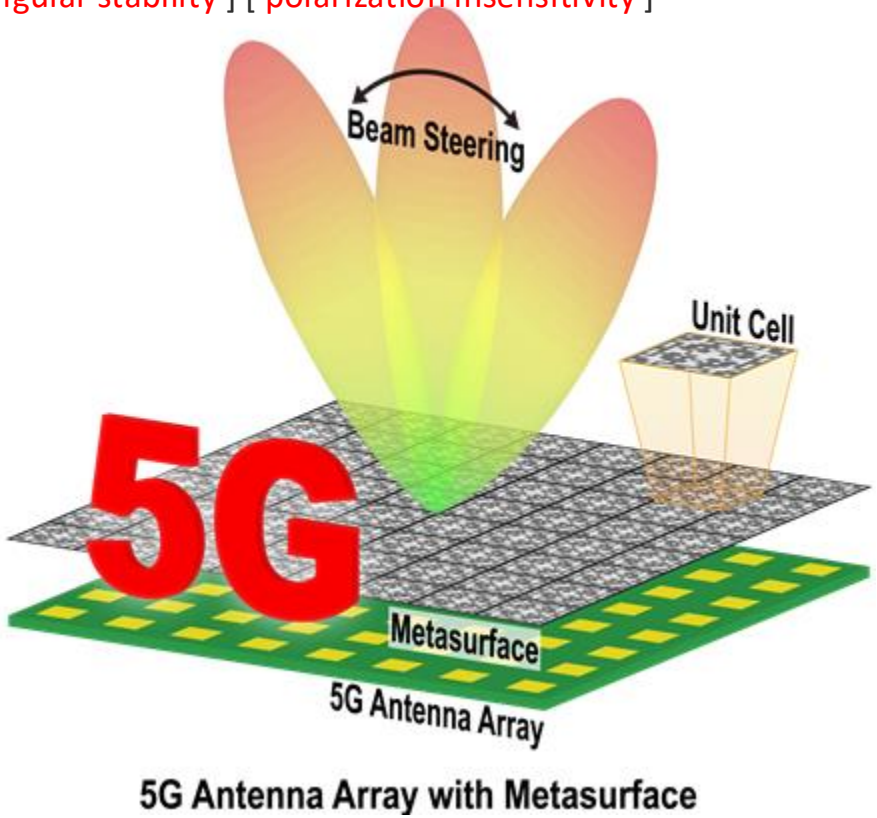
Design of single-layer metasurface filter by CSA for 5G mm-wave communications

It is anticipated that 28 GHz and 38 GHz mmWave bands will play a key role in 5G deployments and beyond-5G systems.
[pre-assigned frequency response characteristic functions required in the 5G frequency band]
[low in-band loss and high out-of-band suppression] [the widest bandwidth]
[angular stability] [polarization insensitivity]

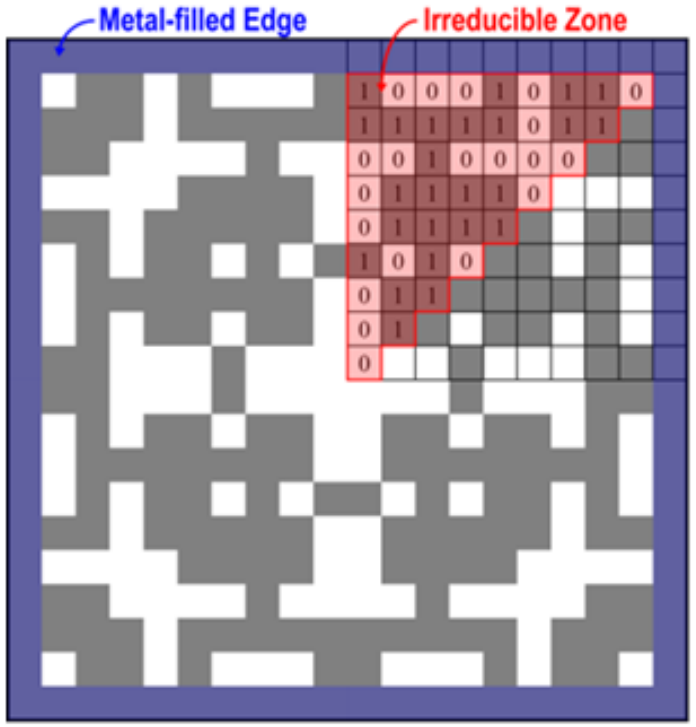
The more pixels the better.

Objective function

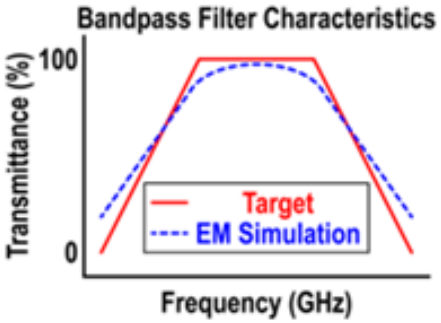
$$f(\vec{x}) = \sum_{k=1}^{N} | T_{target}(\nu_k) - T_{EM}(\nu_k;\vec{x}) | .$$



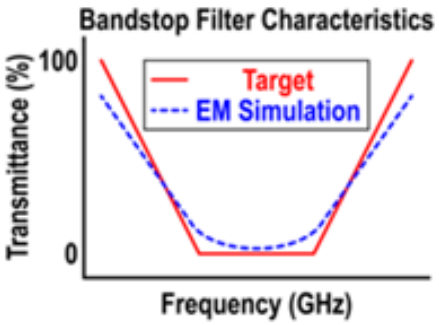
5G Antenna Array with Metasurface



(a)



(b)



(c)

Coexistence of 5G With Fixed Satellite Service at 28 GHz

50 μm thick flexible polyethylene terephthalate film
6 μm thick copper foil

IEEE Access **9**, 29764 (2021); Appl. Phys. Lett. **119**, 174101 (2021); IEEE Ant. Wir. Prop. Lett. **23**, 1536 (2024); J. Appl. Phys. **137**, 213108 (2025). License-out

KRISS

PSSFSS

- https://github.com/simonp0420/PSSFSS.jl
- Analysis of polarization and frequency selective surfaces in Julia

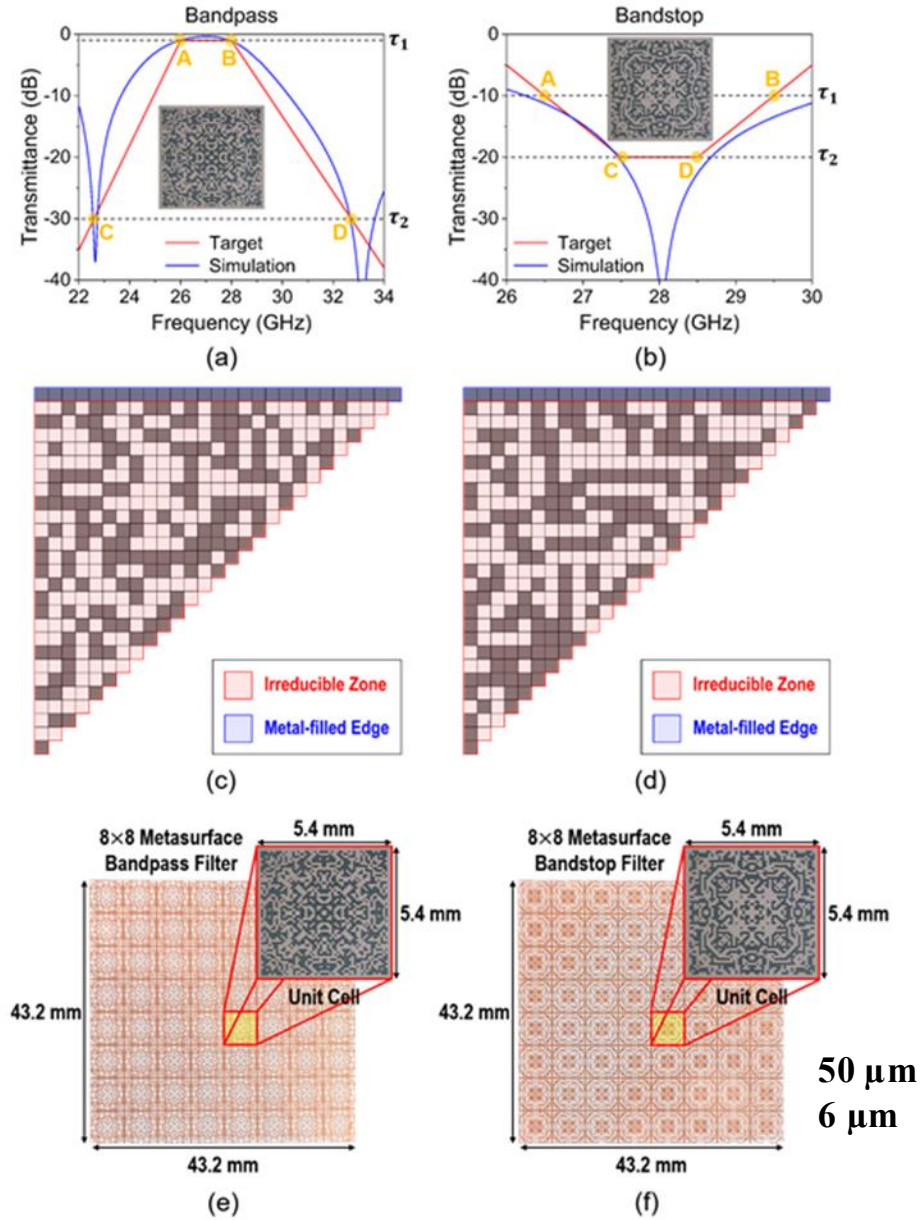
•주파수를 **낮추고 싶으면?** ℓ을 키워야 함, 금속 패턴을 **길게** 연결하거나 꼬불꼬불하게 만듦.
•주파수를 **높이고 싶으면**? ℓ을 줄여야 함, 금속 패턴을 **짧고 굵게** 만듦.

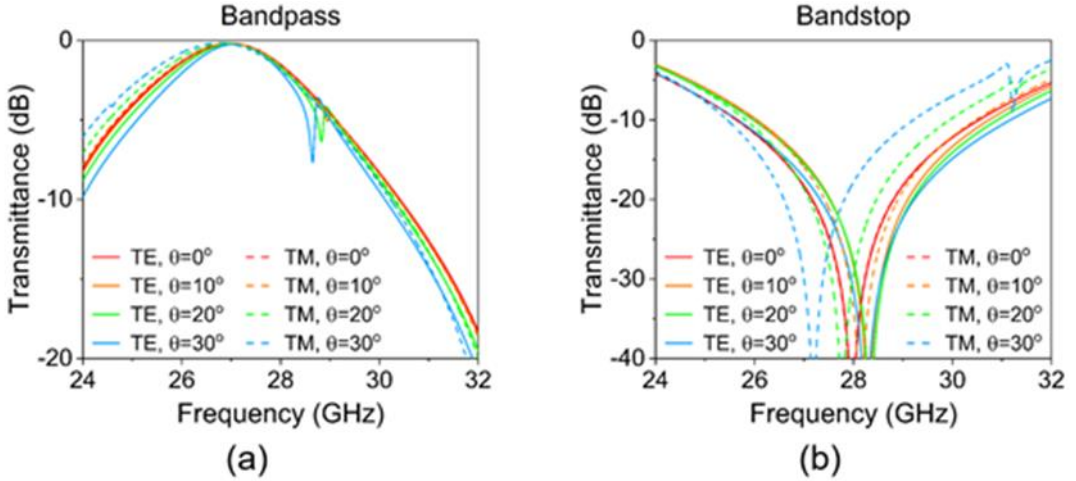
ACES JOURNAL **39**, 139 February (2024). https://journals.riverpublishers.com/index.php/ACES/article/view/22443

KRISS

googol= 10^{100}

2^{351} = 4586997231980143023221641790604173881593129978336562247475177678773845752176969616140037106220251373109248
$\sim 4.5 \times 10^{105}$





The emerging 5G systems will need to coexist with a number of incumbent systems in these bands.

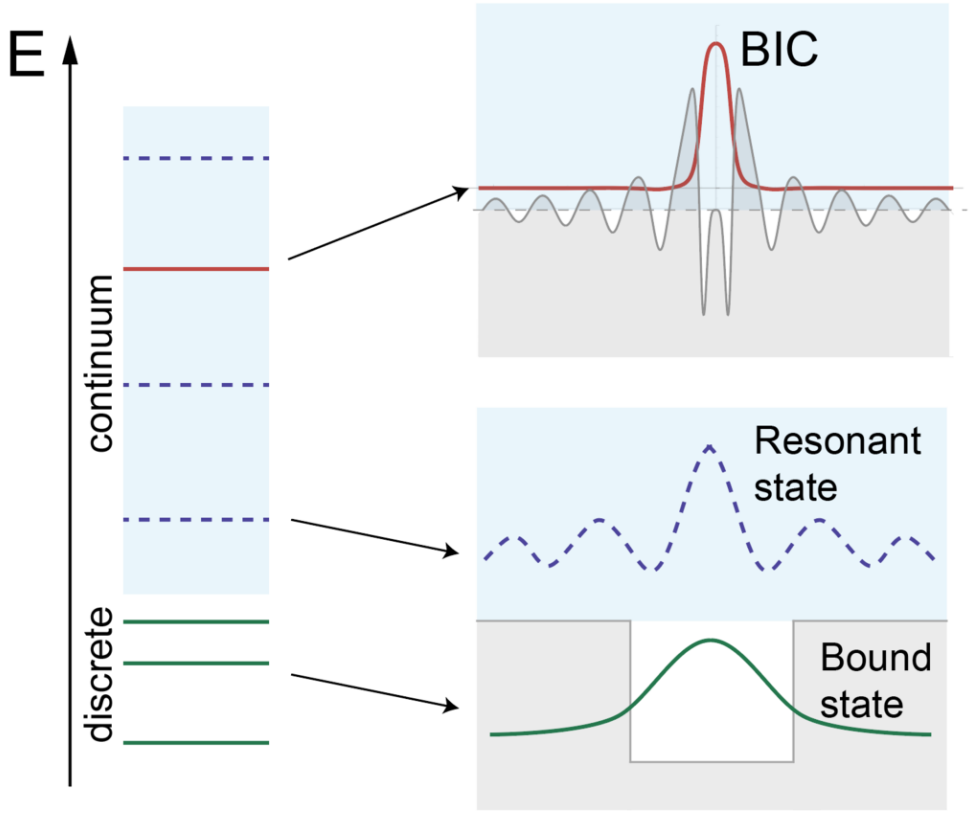
co-channel coexistence of 5G in two critical mmW bands,
27.5-28.35 GHz (28 GHz) and 71-76 GHz (70 GHz) bands

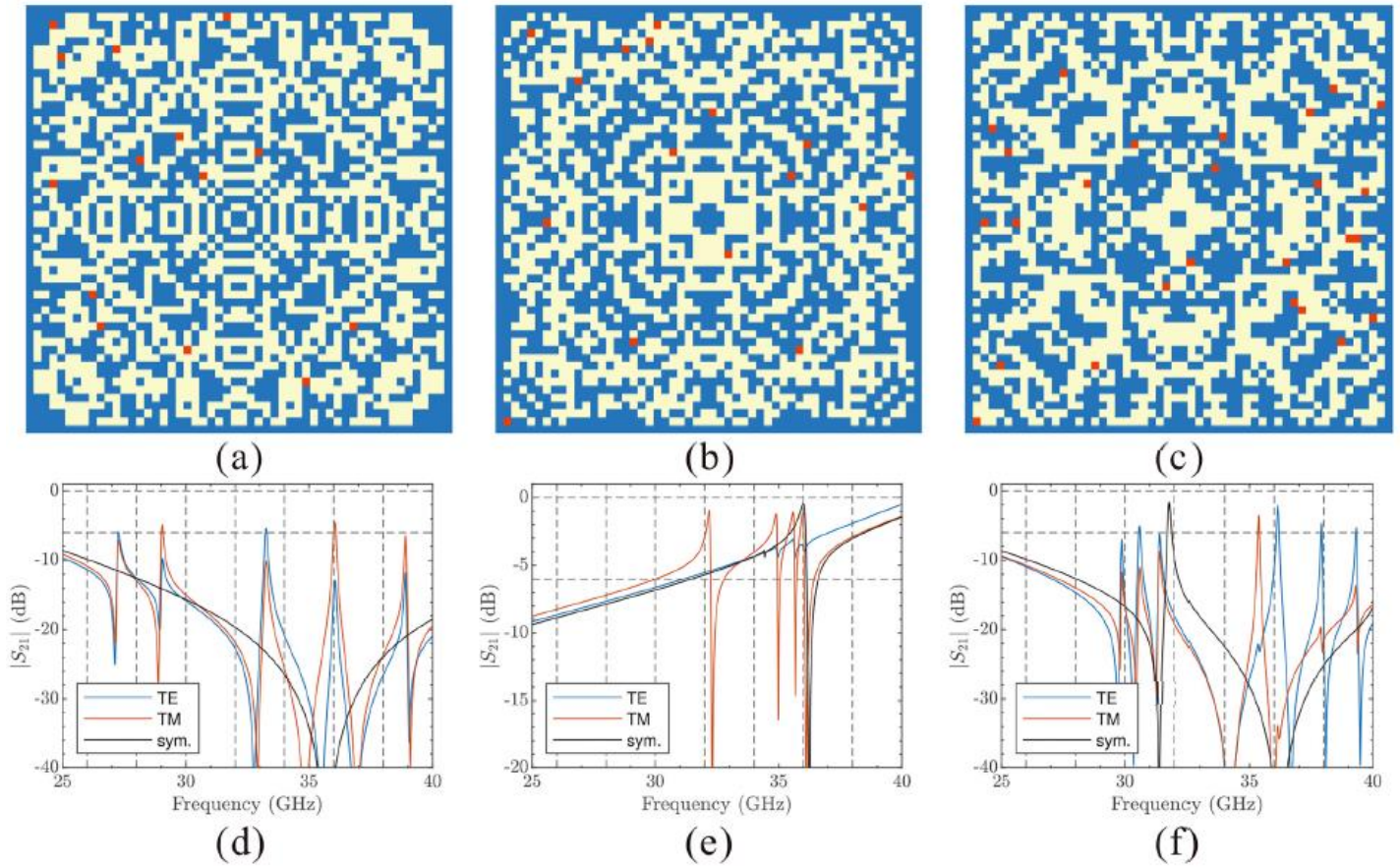
fixed satellite service and fixed service, such as wireless backhaul

IEEE Access **9**, 29764 (2021); Appl. Phys. Lett. **119**, 174101 (2021); IEEE Ant. Wir. Prop. Lett. **23**, 1536 (2024); J. Appl. Phys. **137**, 213108 (2025). License-out

KRISS

High quality-factor resonances in an asymmetric pixelated metasurface

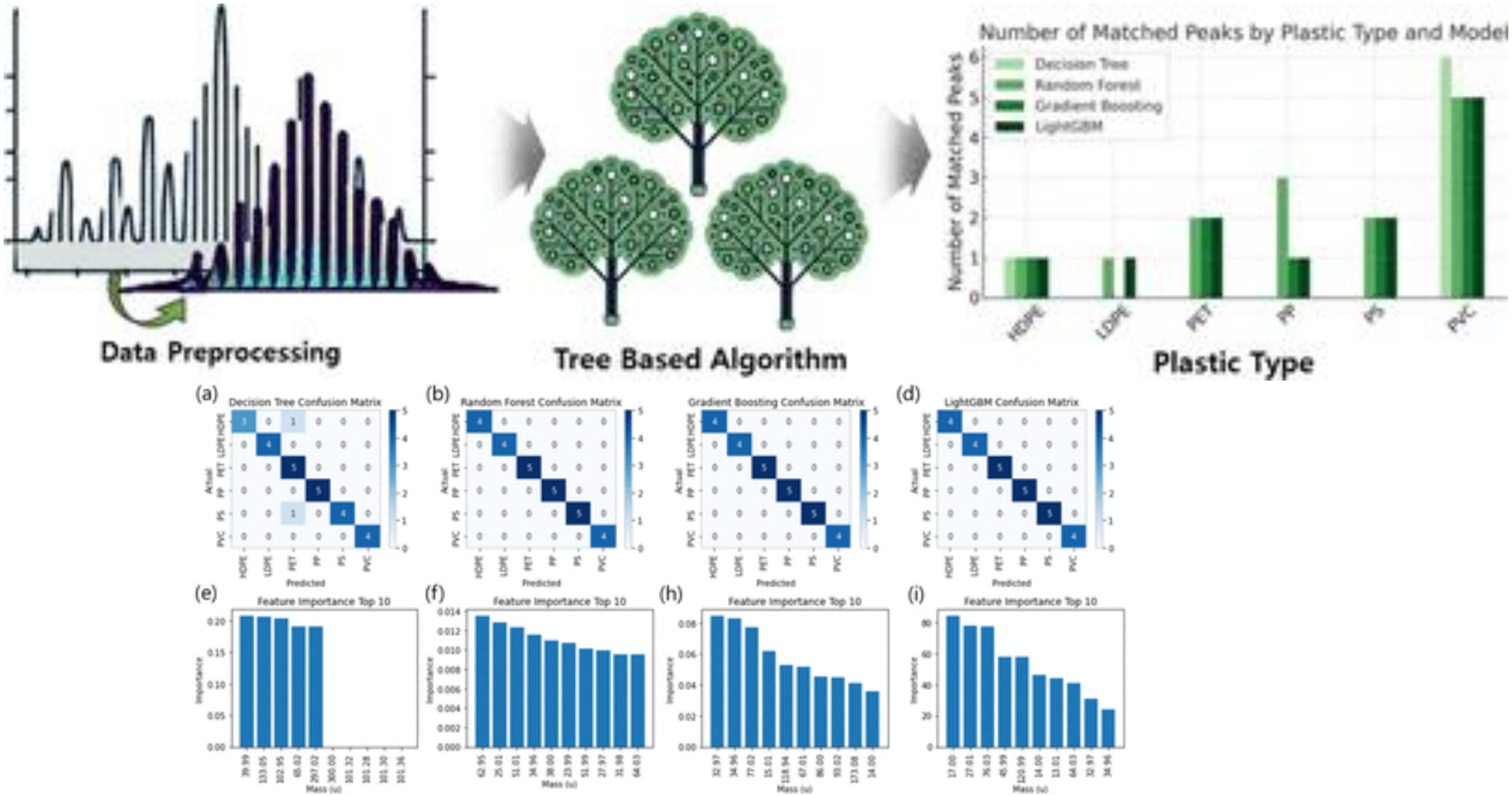




In fact, Fano resonance is closely associated with the physics of bound states in the continuum (BICs).
It is known that symmetry protected BICs cannot be excited if the symmetry is not broken.

https://en.wikipedia.org/wiki/Bound_state_in_the_continuum
J. Appl. Phys. **137**, 213108 (2025).

Applications of machine-learning methods

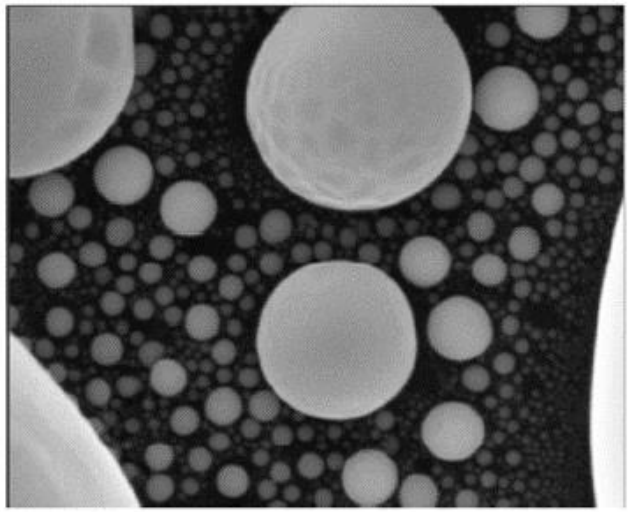


Peak-based machine learning for plastic type classification in time-of-flight secondary ion mass spectrometry

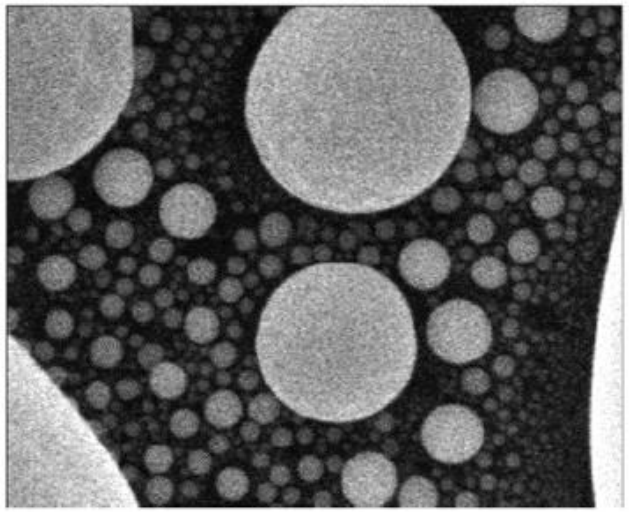
J. Am. Soc. Mass Spectrom. **35**, 3107 (2024).

KRISS

Applications of deep learning-based denoising methods



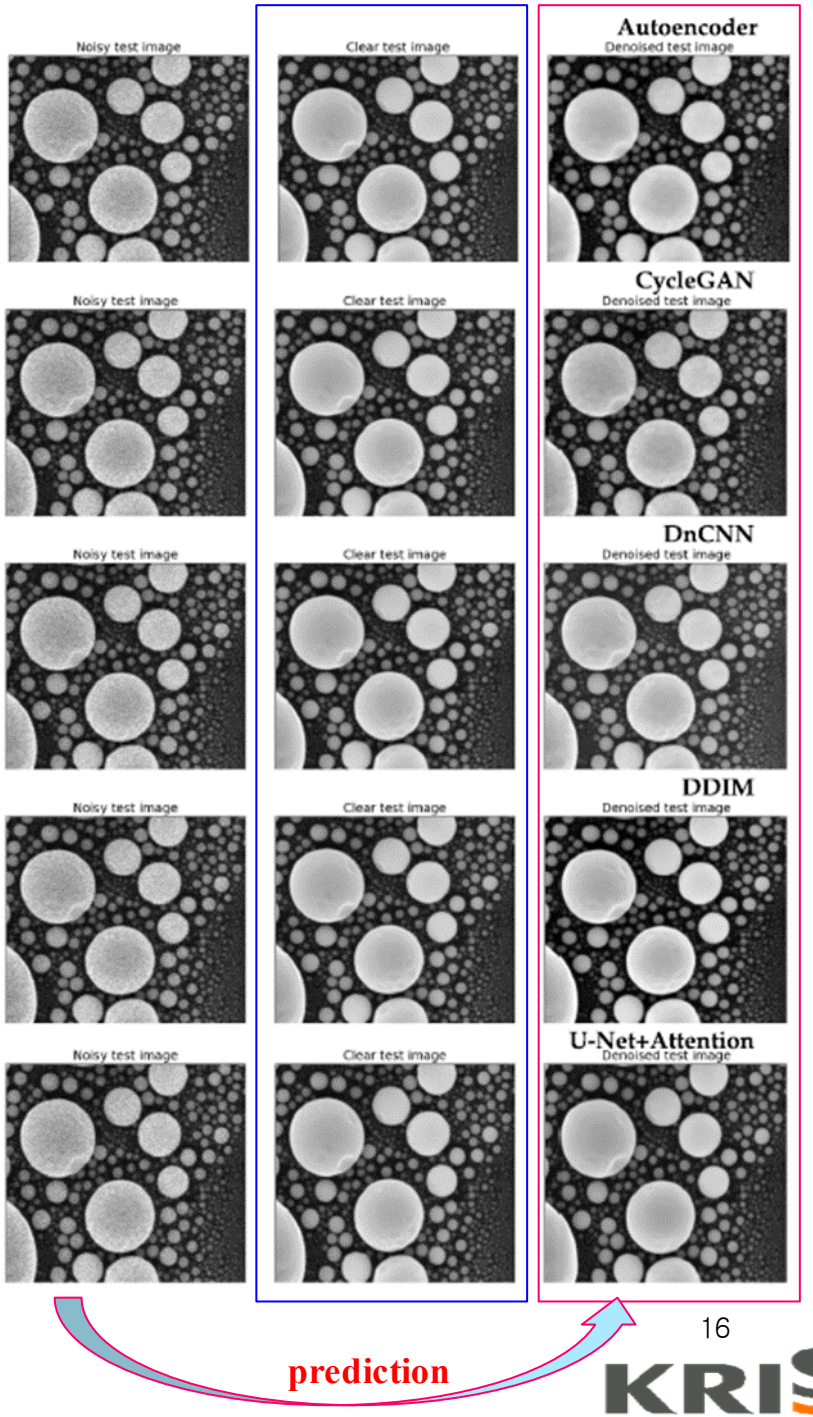
(a) Clear image taken with the pixel dwell time of 30 μs.



(b) Noisy image taken with the pixel dwell time of 100 ns.

Low Dose → High Dose

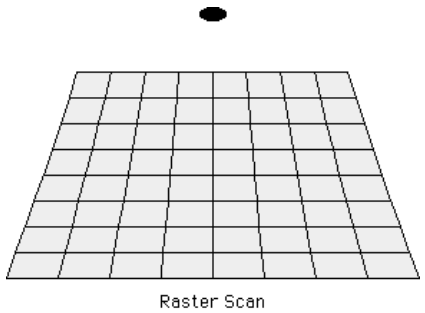
Medical, materials science, measurement, and more

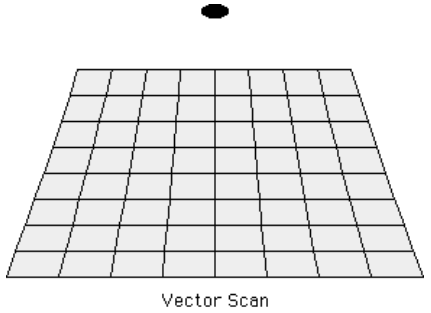


Autoencoder, CycleGAN, DnCNN, DDIM, U-net + Attentio

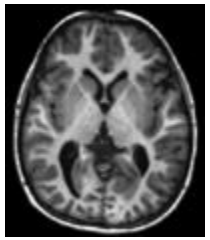
Measurement Science and Technology **36**, 015406 (2025). https://github.com/seoleuns/SEMdenoising

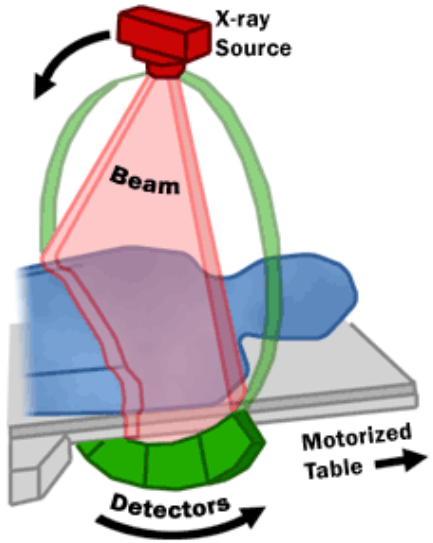
Applications of Bayesian inference methods for fast and accurate scan





- Laser printer
- SEM(scanning electron microscopy)
- AFM/STM/STS
- CT
- MRI
- Quantum gates(e.g., single electron transport)





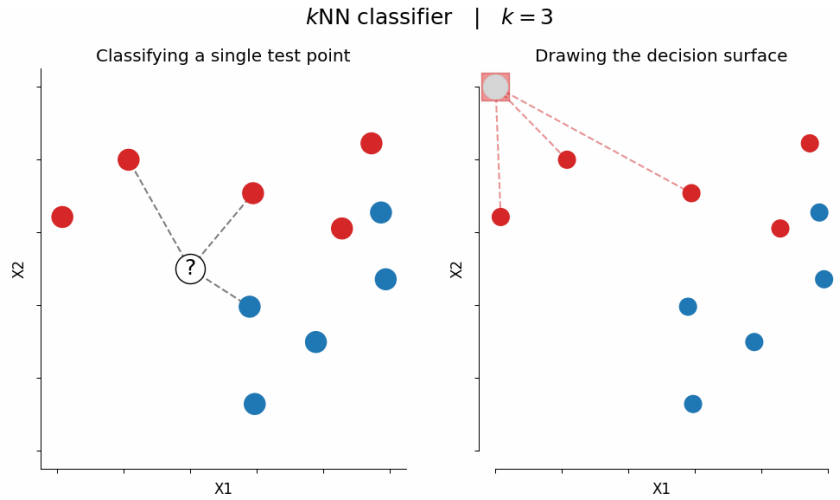
ionizing radiation

computed tomography scan (CT scan)

https://web.cecs.pdx.edu/~jeske/litho/scanning.html
https://en.wikipedia.org/wiki/CT_scan
https://en.wikipedia.org/wiki/Magnetic_resonance_imaging

KRISS

k-nearest neighbors(KNN) regressors: *O(n)*



Many KNN regressors
→ Bayesian inference
→ mean and variance

Gaussian process(GP): *O(n³)*

$$p(\vec{f} \mid \vec{x}) \sim \mathcal{N}(\vec{f} \mid \vec{\mu}, K) \text{ (normal distribution, mean : } \vec{\mu}, \text{covaraiance : } K).$$

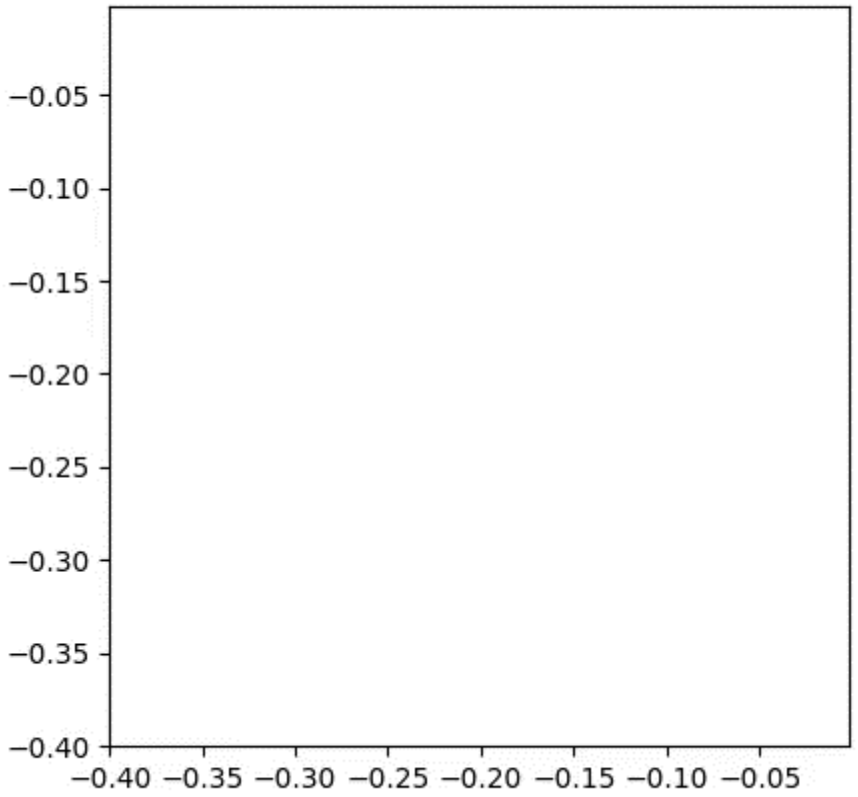
$$p(\vec{f}_* \mid \vec{X}_*, \vec{X}, \vec{f}) \sim \mathcal{N}(\vec{f}_* \mid \vec{\mu}_*, K_*) \text{ (normal distribution, mean : } \vec{\mu}_*, \text{covaraiance : } K_*),$$

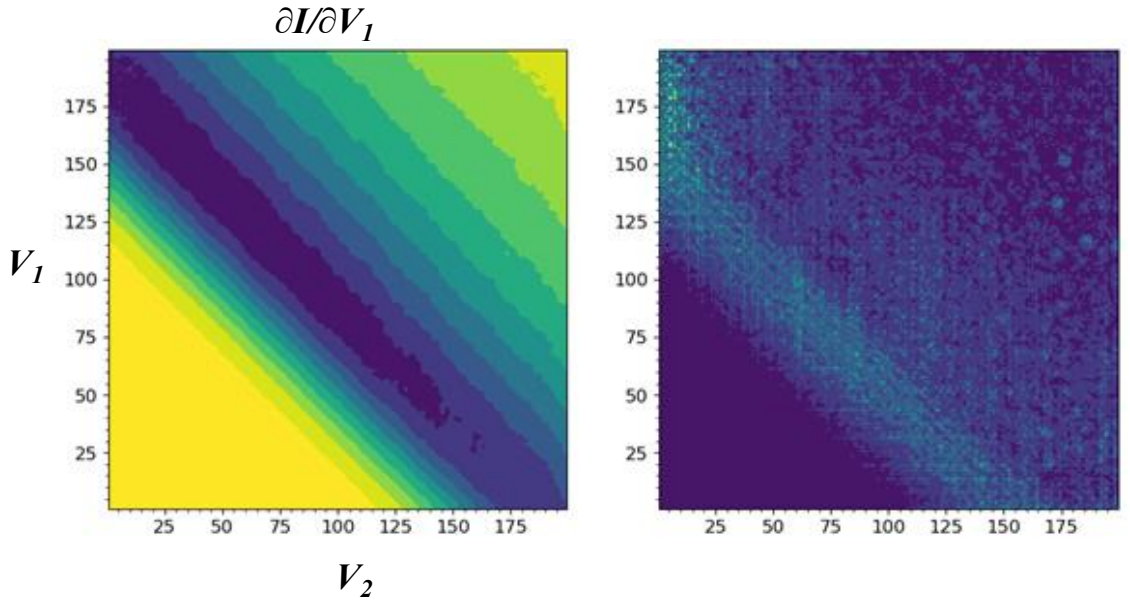
$$\vec{\mu}_* = K_*^T K^{-1} \vec{f},$$

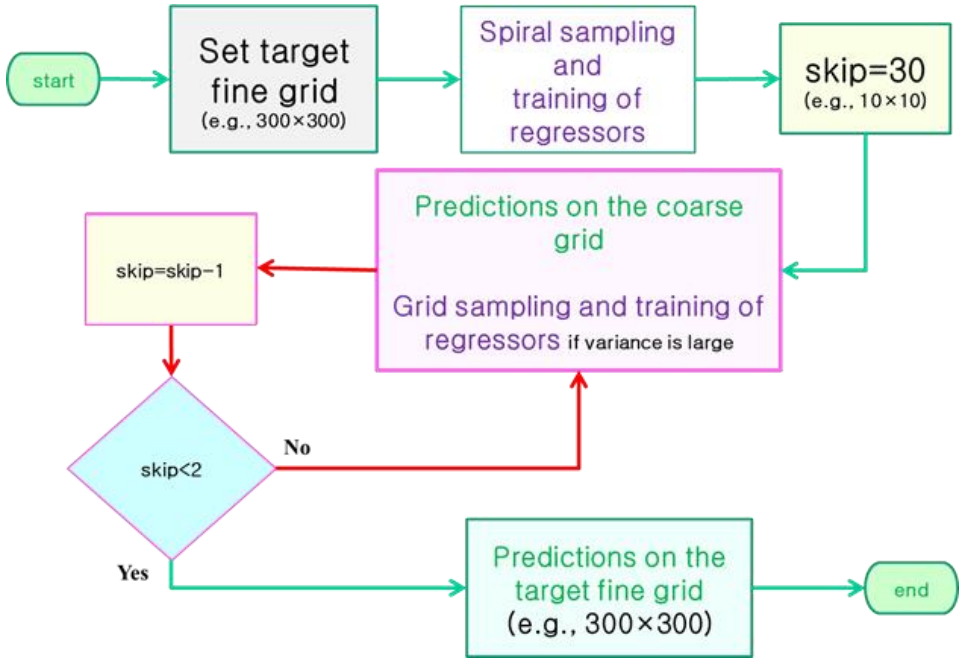
$$K_* = K_{**} - K_*^T K^{-1} K_*,$$

https://en.wikipedia.org/wiki/Gaussian_process
https://en.wikipedia.org/wiki/K-nearest_neighbors_algorithm#/media/File:KNN_decision_surface_animation.gif

Example

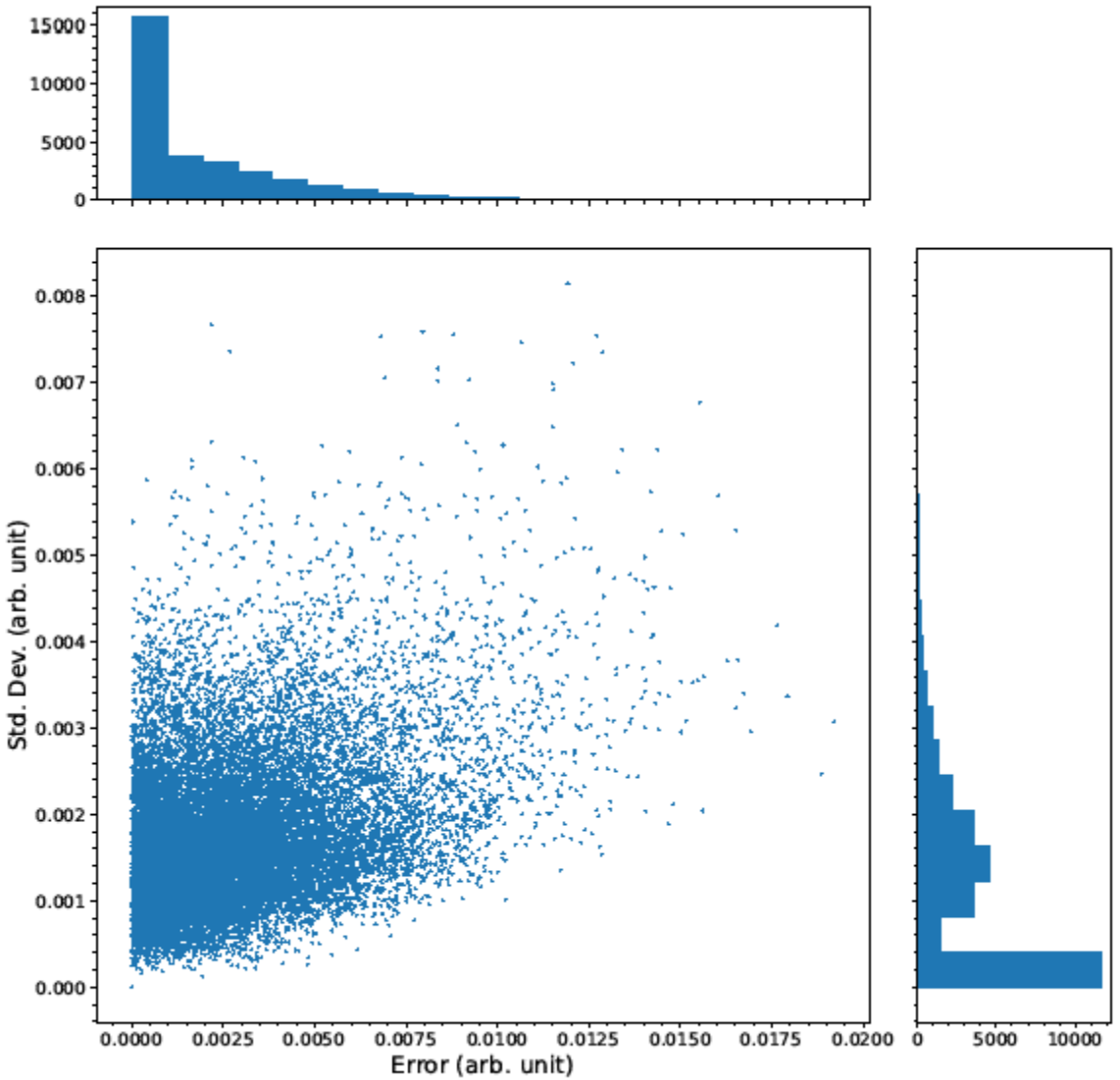






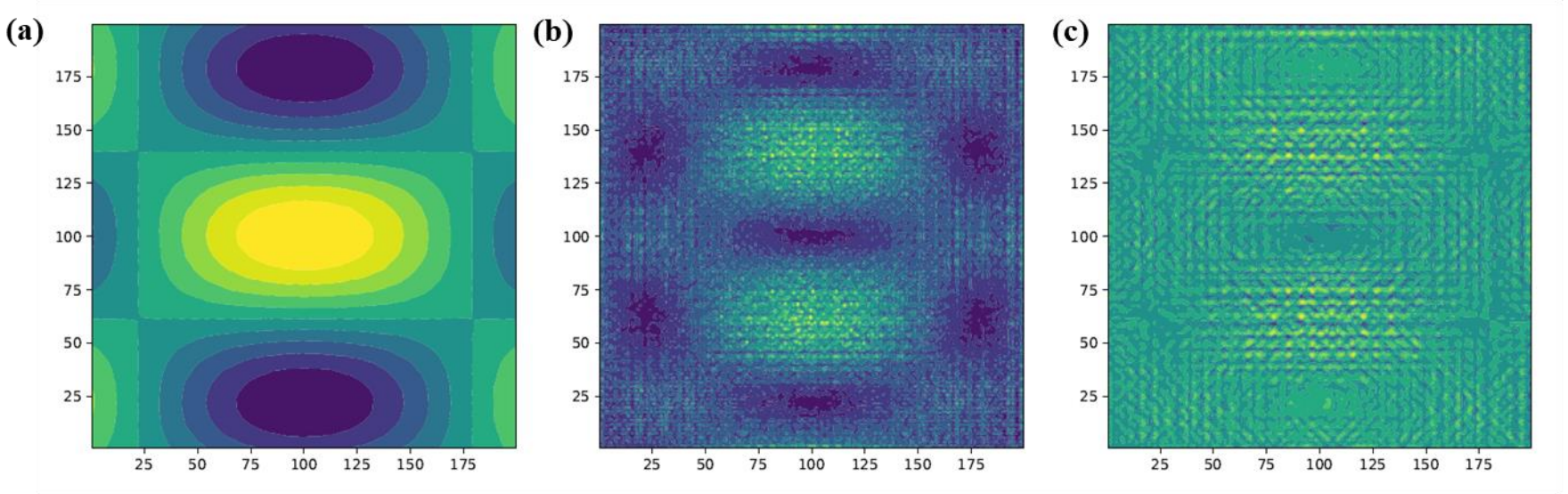
unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

KRISS

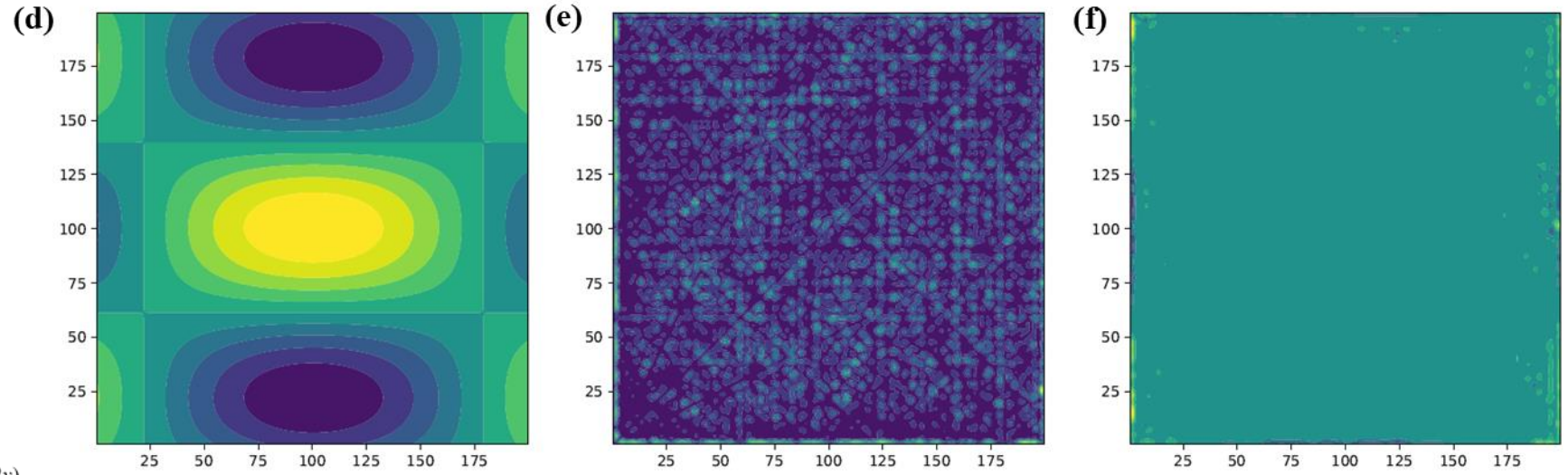


unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

KNN



GP



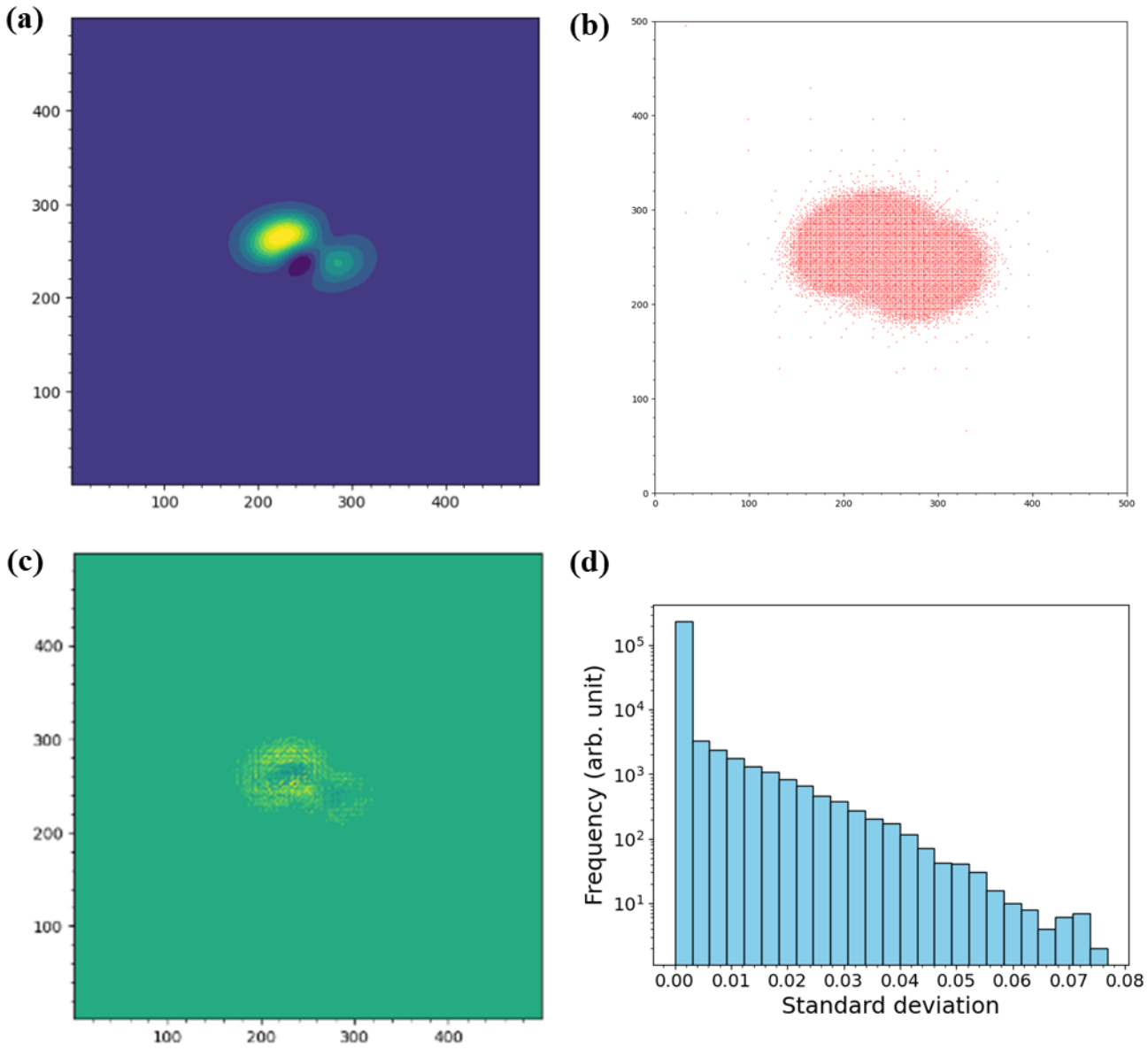
$$f(x, y) = \cos(0.1x)\cos(0.2y).$$

$$\Delta_{ML} = max\{|\, f_{ML}(x, y) - f(x, y)\,|\}\,/max\{|\, f(x, y)\,|\}\,.$$

unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

KNN

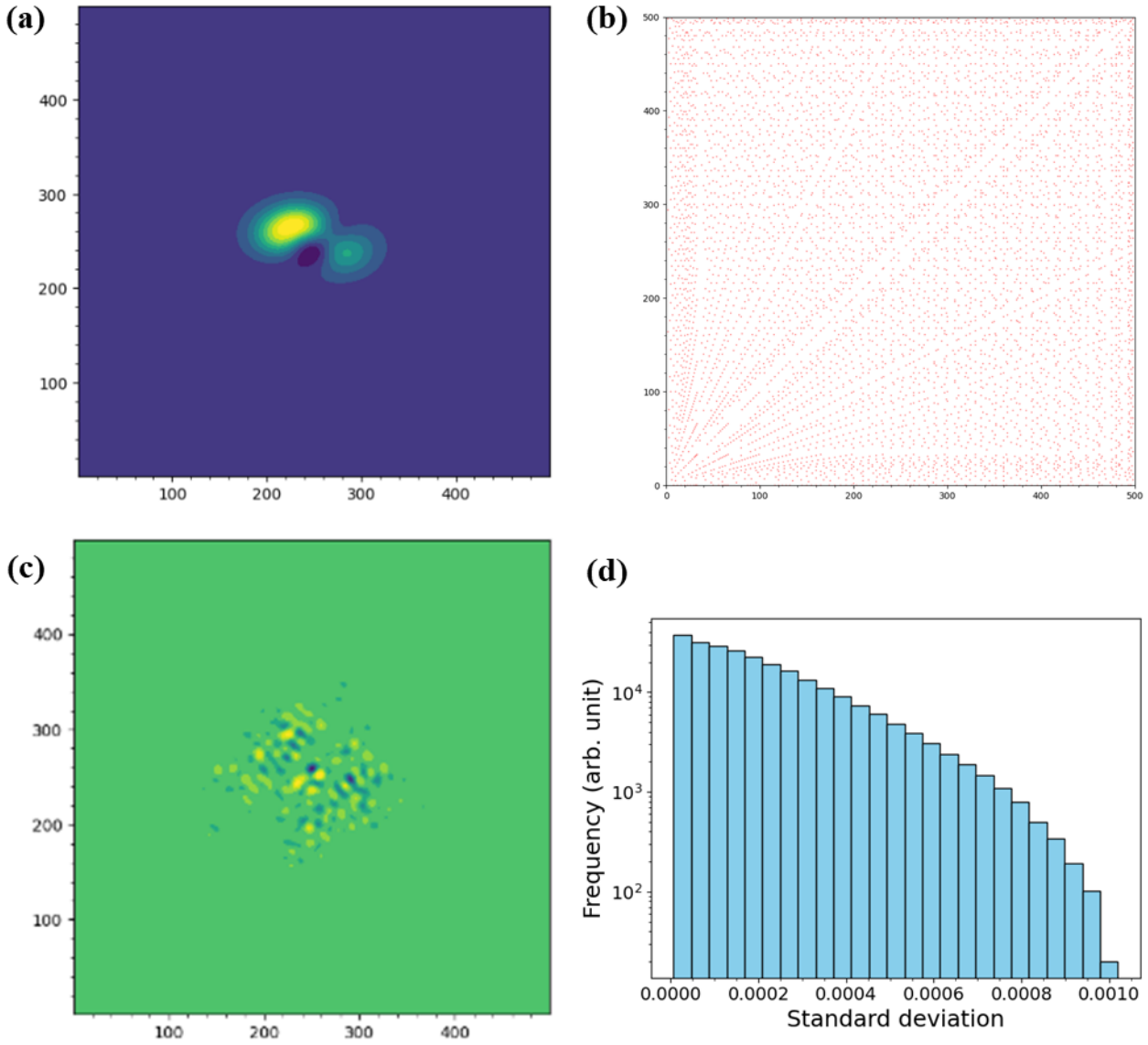
Complexity: *O(n)*



unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

GP

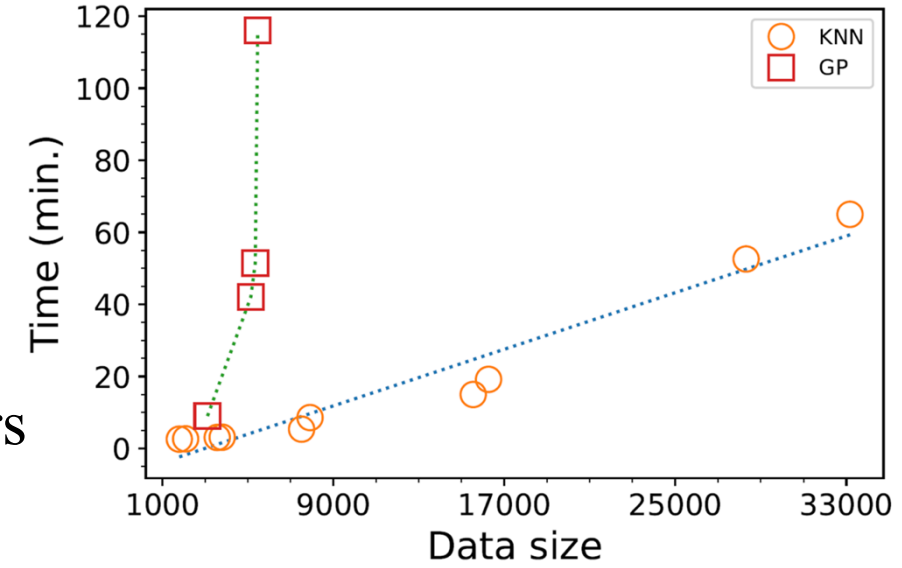
Complexity: $O(n^3)$

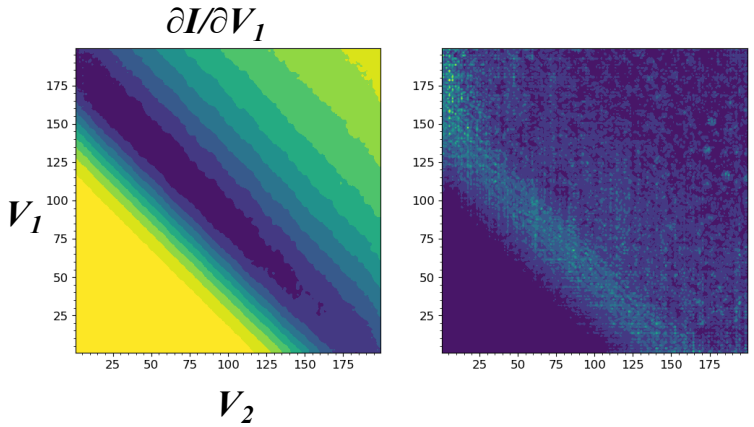


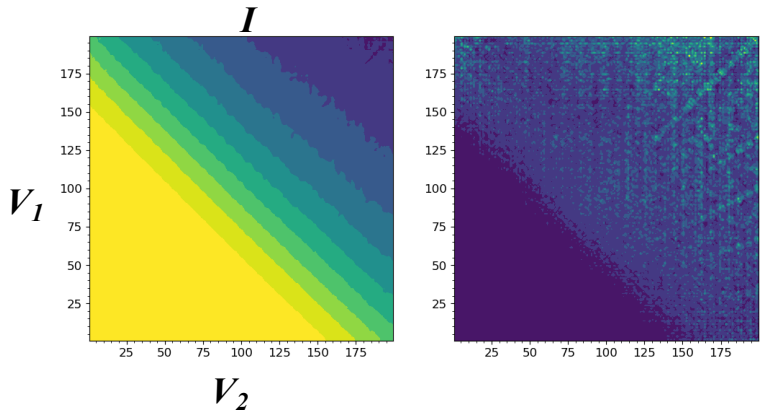
unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

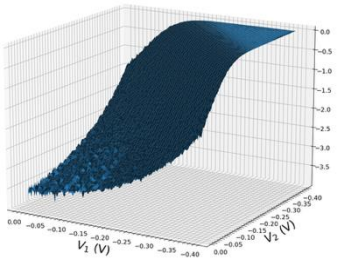
Variance and *O(n)*

Raster scan applications(SEM, AFM, STM/STS, CT, MRI, ….)
Bayesian inference : mean, variance
Gaussian process(GP), *k*-nearest neighbors(KNN) regressors
O(n) complexity *vs* $O(n^3)$, Large data sizes ($n > 5000$)

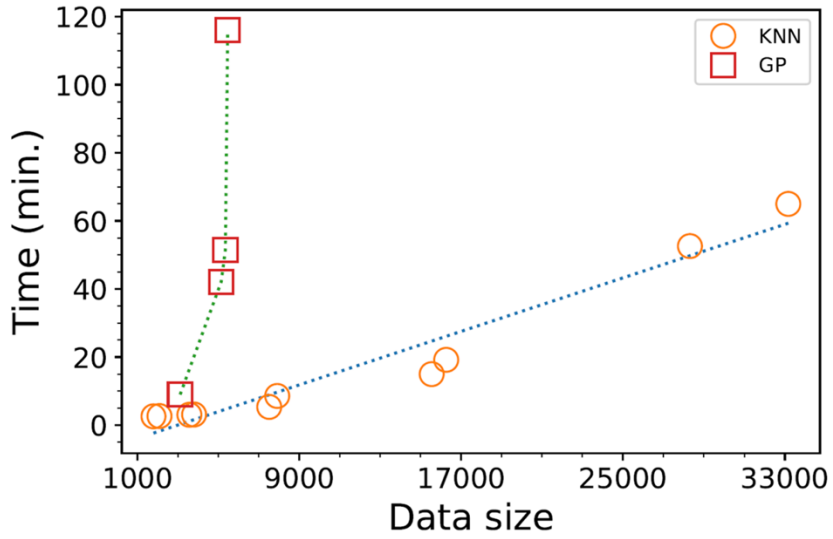


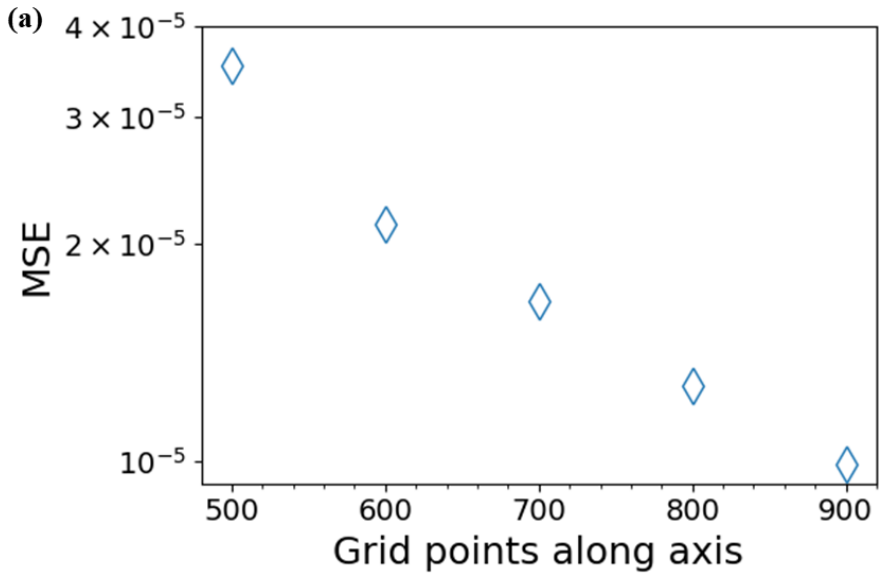


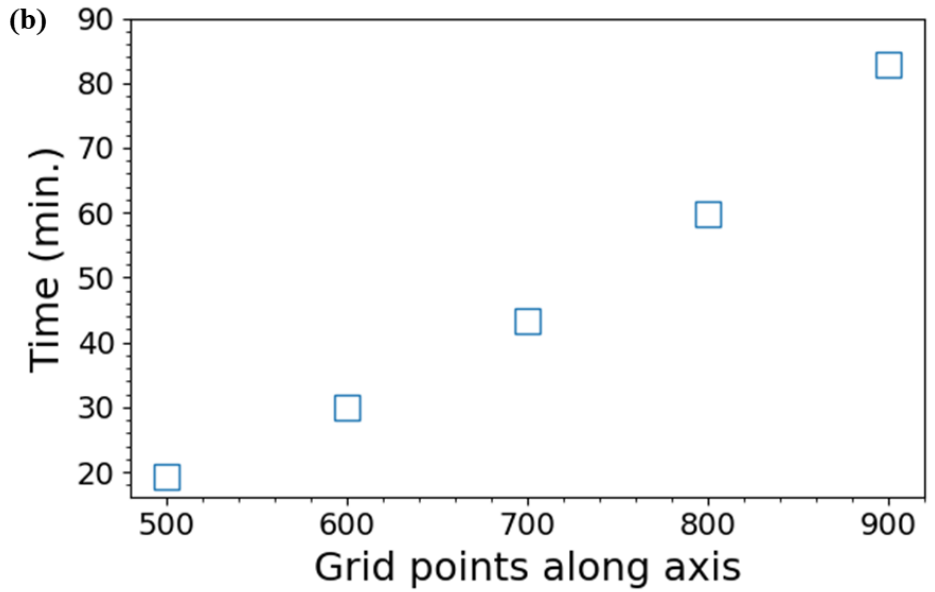




unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference

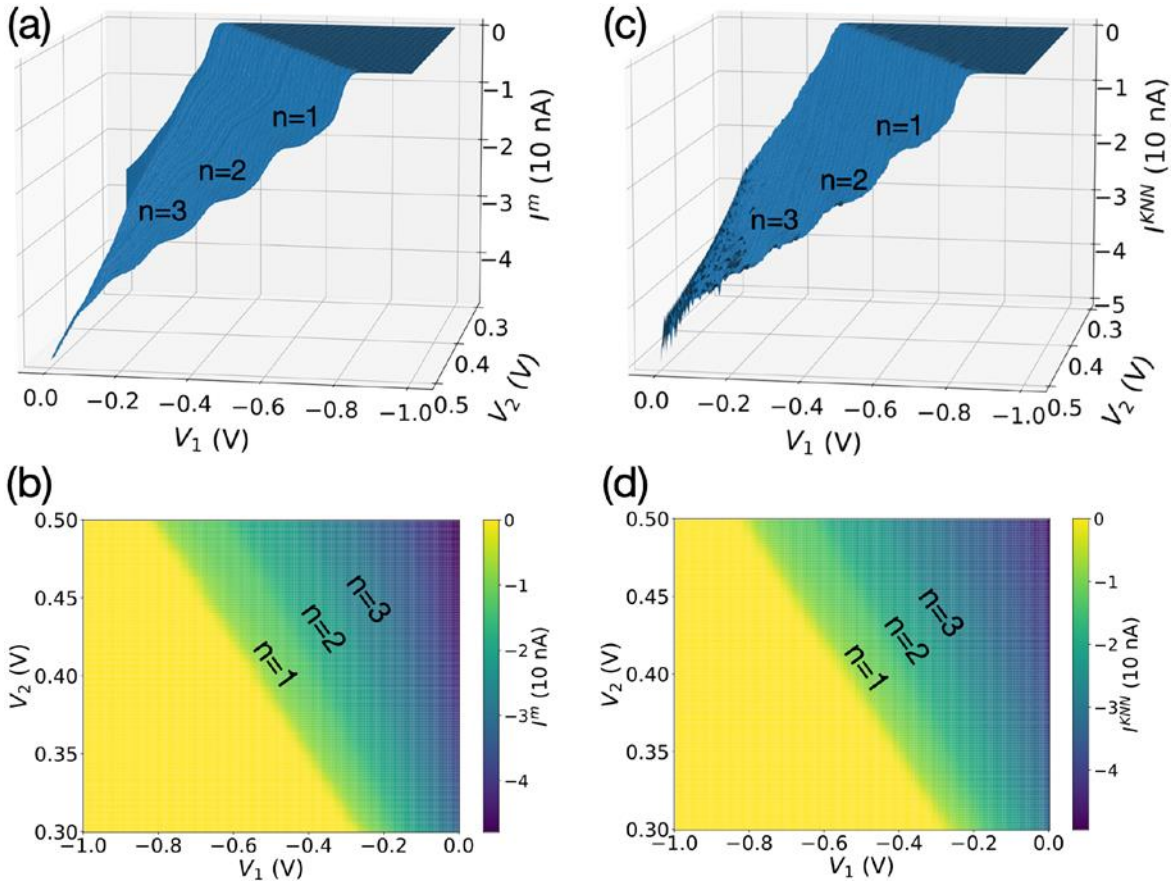


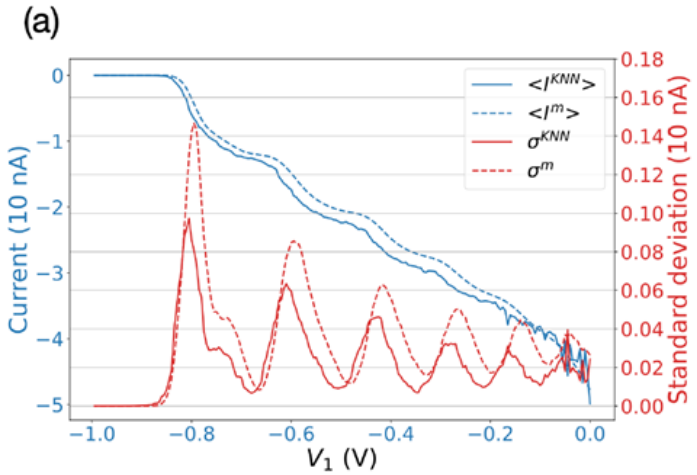


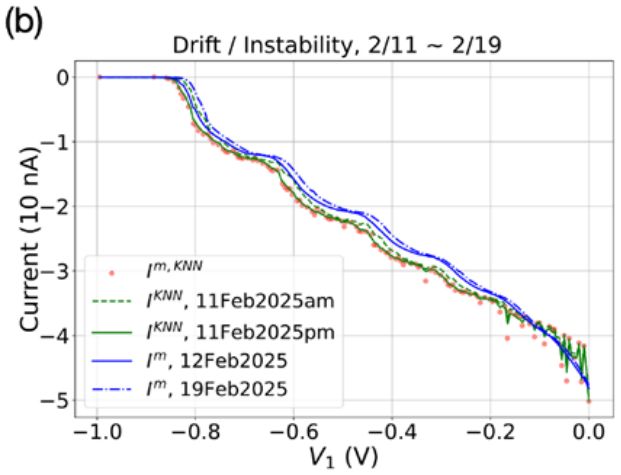


Measurement Science and Technology, *submitted* (2025). https://github.com/inholeegithub/Bayesian_Inference

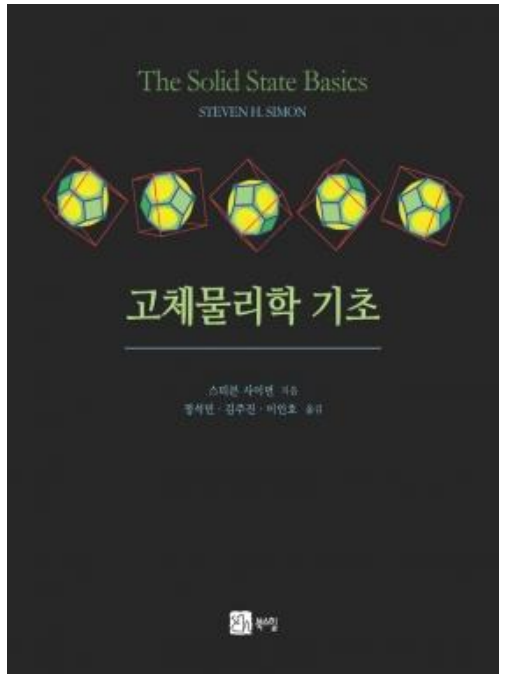
Applications of Bayesian inference methods for single-electron transport experiments

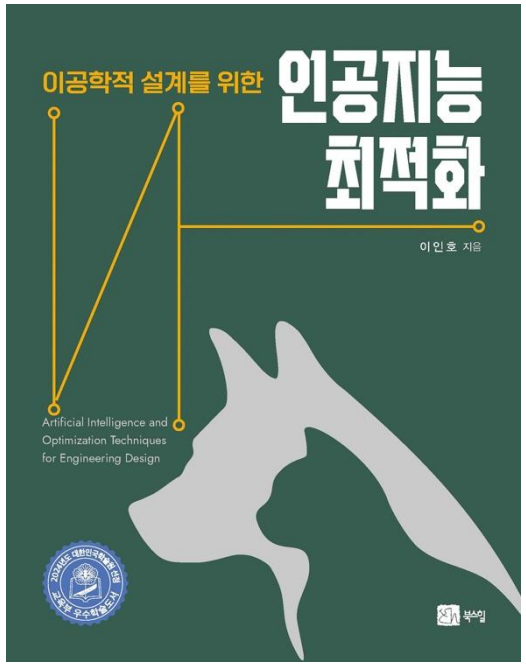


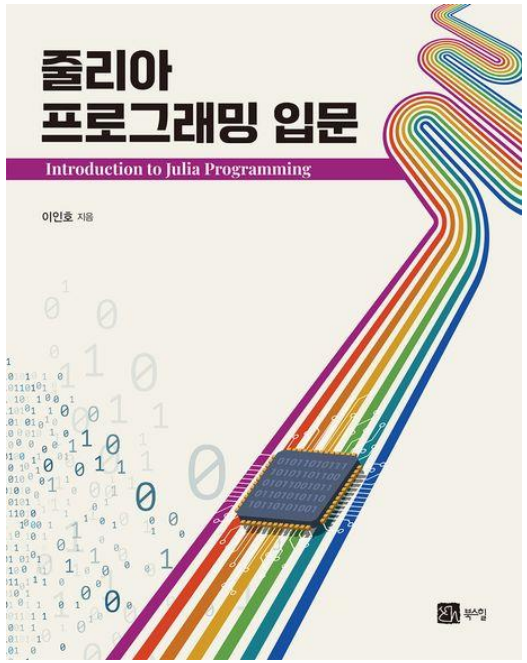


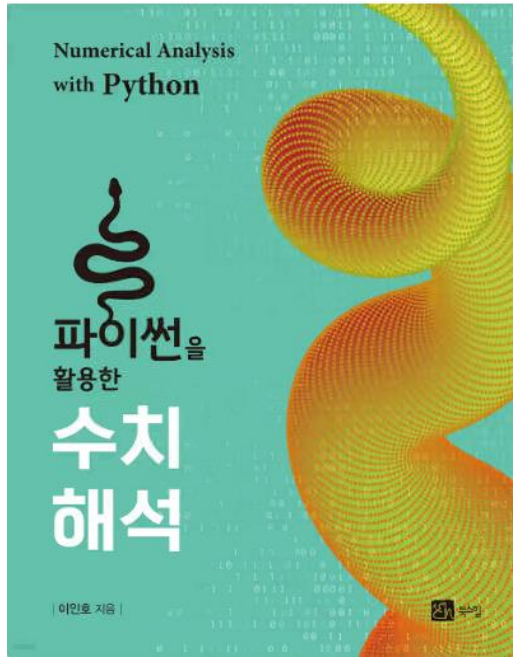


unpublished (2025). https://github.com/inholeegithub/Bayesian_Inference









2024년 대한민국학술원 우수학술도서

정리

- 다양한 공학적 최적화 작업이 가능함(소재/소자 설계 최적화)
- 매우 다양한 응용이 가능함(다양한 과학적 측정 및 분석이 필요)
- 측정방법에 AI 적용이 가능함
- 효율적이고 정확한 측정(1d, 2d, 3d,…)
- pyVISA 사용 [아나콘다 설치를 회피할 수 있음][LabVIEW,MATLAB]
- 초기능성 소재/소자[위상초전도체/고이동도 소재/주파수 선택표면…]
- 자신의 데이터 + 관련 논문
- AI응용 그 자체는 문제가 아님, 자신의 데이터/장비 제어, 연구 내용이 문제가 됨.
- ….