

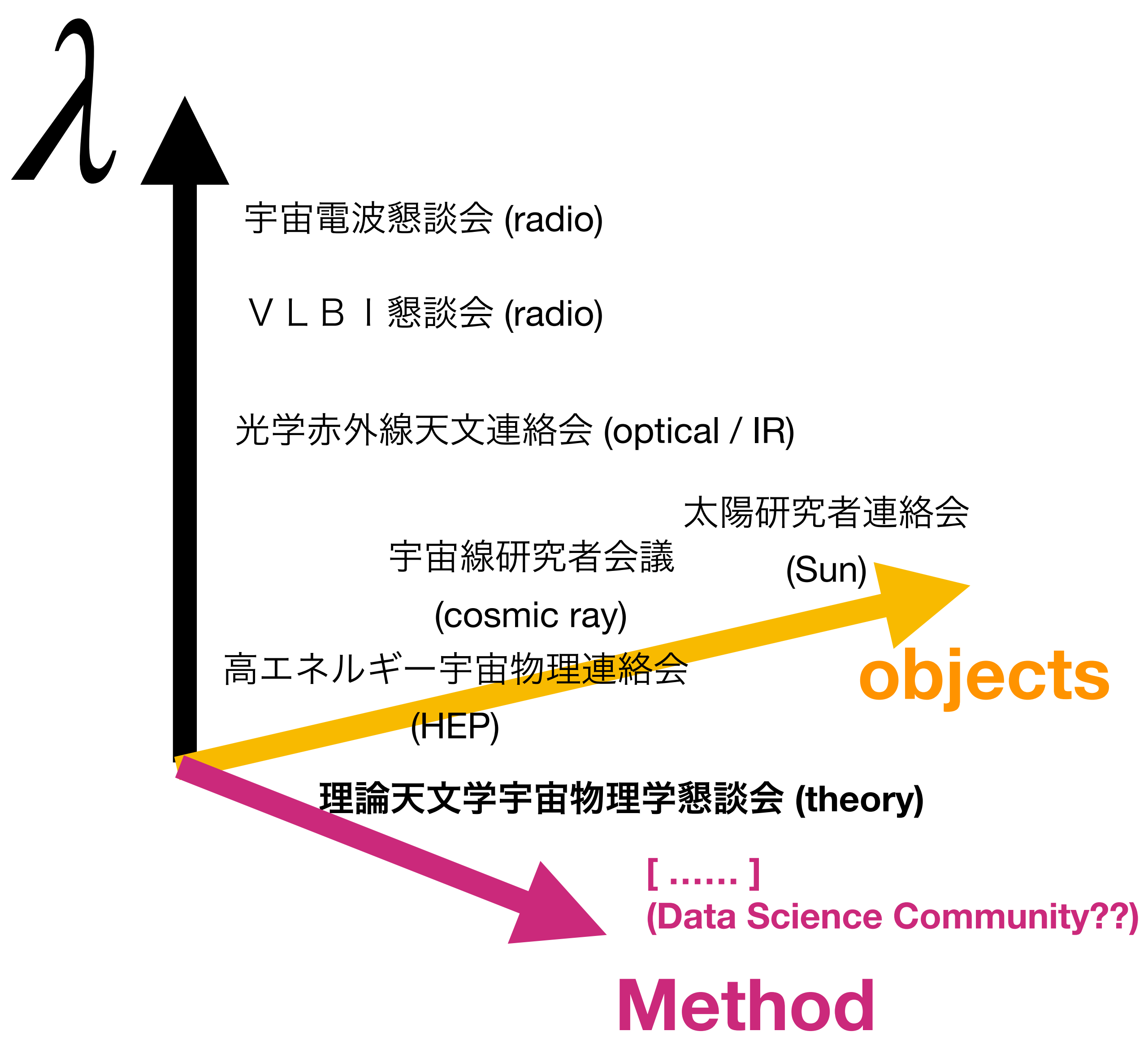
# Data Science in Astronomy

Feel free to ask questions. Comments are also welcome.

**khattori** @ism.ac.jp

**Kohei Hattori** (服部公平)

# No community of Data Science !?



2021年 春季年会

年会プログラム

於 東京工業大学 ( オンライン開催 )

2021 年 3 月 16 日 (火) ～ 3 月 19 日 (金)

Data Science Session  
(1st time in history, I guess.)

Z1. 天文データ科学

Instrument Sessions  
(long history)

V1. 観測機器 (電波)
V2. 観測機器(光赤・重)
V3. 観測機器(X線・γ線)

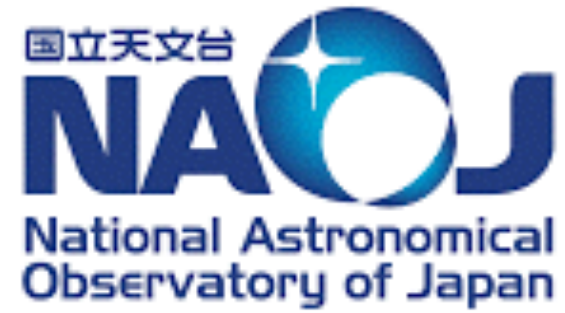
3月16日 (火)	A	Z3. 計算宇宙惑星
	B	W. コンパクト天体
	C	S. 活動銀河核
	D	V2. 観測機器(光赤・重)
	E	V3. 観測機器(X線・γ線)
	F	P2. 原始惑星系円盤
	G	Q. 星間現象
	H	
3月17日 (水)	A	Z3. 計算宇宙惑星
	B	W. コンパクト天体
	C	R. 銀河
	D	V2. 観測機器(光赤・重)
	E	V3. 観測機器(X線・γ線)
	F	P2. 原始惑/P1.星形成
	G	Q. 星間現象
	H	Y. 教育・広報・他
3月18日 (木)	A	Z1. 天文データ科学
	B	W. コンパクト天体
	C	X. 銀河形成・進化
	D	V1. 観測機器 (電波)
	E	T. 銀河団
	F	P1. 星形成
	G	M. 太陽
	H	
3月19日 (金)	A	Z2. ngVLA の天文学
	B	N. 恒星進化
	C	X. 銀河形成・進化
	D	V1. 観測機器 (電波)
	E	
	F	
	G	M. 太陽
	H	P3. 惑星系



# Institute of Statistical Mathematics (ISM = 統計数理研究所)

三鷹

立川



- Masato Shirasaki
- Kohei Hattori (myself)

We are trying to connect  
astronomers and statisticians.



ISM webpage — <https://www.ism.ac.jp>



An ideal workplace for astro data scientists.

Astronomers can use various resources.



• 共同研究スタートアップ

Data analysis consulting. (First consulting is free.)  
Any questions from astronomers are welcome!



思考院トップ > 統計思考院の事業活動 > 共同研究スタートアップ

共同研究スタートアップ

「統計的かもしれない」疑問にお答えする場を提供します。

新型コロナウイルスの感染拡大防止のため、オンラインでのご相談もお受けしています。

データ解析・統計分析に関わる問題でお悩みの方々のために「共同研究スタートアップ」プログラムを用意しています。

本プログラムの命名には、日常的な相談の中に統計学研究のテーマを見つけ出し、共同研究に発展させたいという期待が込められていますが、一般的な統計リテラシー普及の役割も担っています。統計数理研究所までお越しいただいて直接お話を伺うことを原則としておりますが、混雑時には面会の約束がかなり先になることを予めご了承ください。

助言の対象範囲には、取得済みのデータに関する解析法だけでなく、データの収集法、調査の方法、実験の計画といった事項も含まれます。



• Seminars

- 天文観測におけるビッグデータ解析と宇宙論パラメータの推定 (hosted by M. Shirasaki)
- 統計物理と統計科学のセミナー (hosted by ISM people)

• 受託研究員制度

(Need to pay. Visiting scholar / visiting PhD student)  
(I started mentoring an astro PhD student.)

Most importantly, people at ISM  
are supportive, and  
are HIGHLY interested in **ASTRONOMY** data.

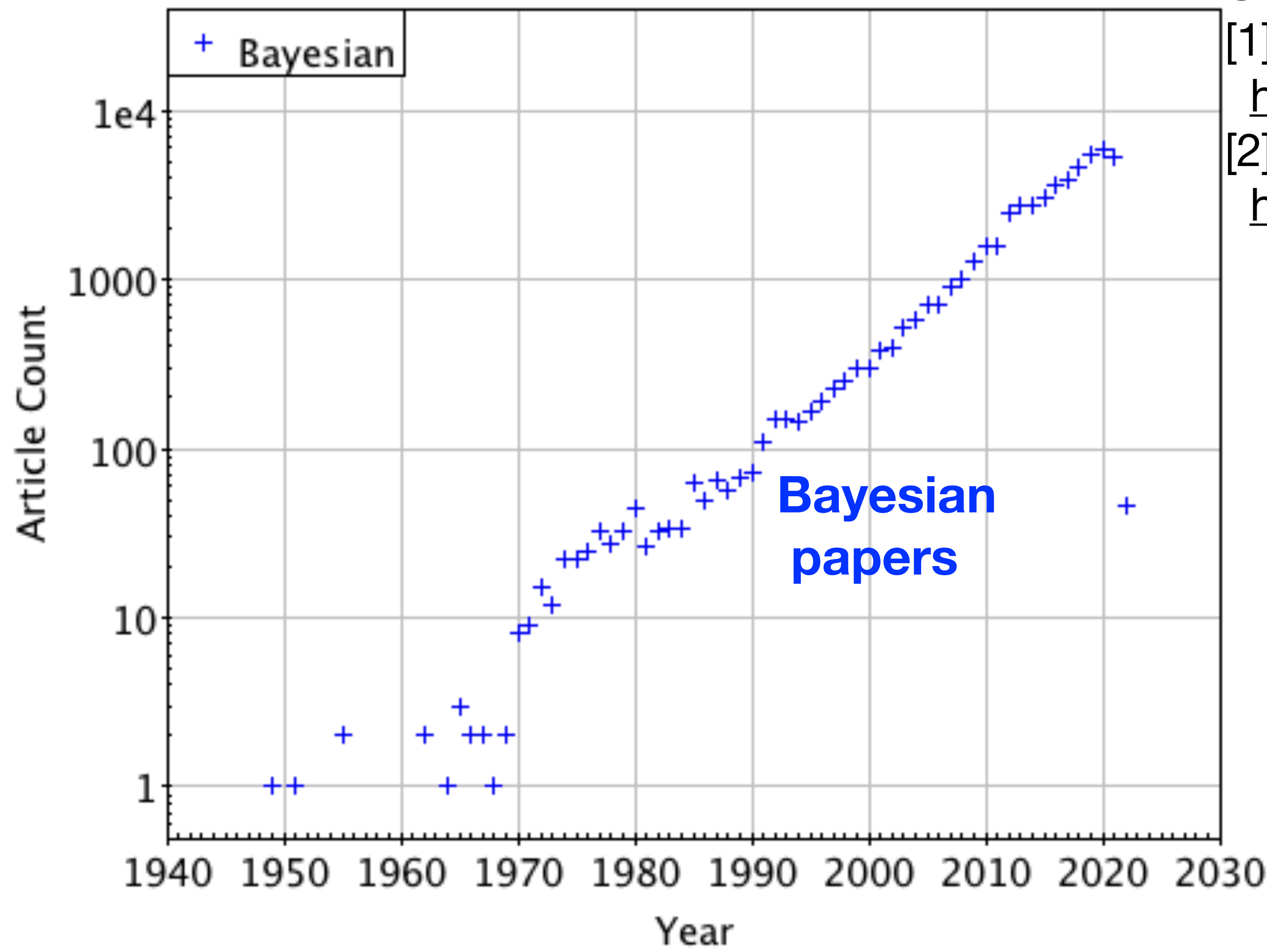
<https://www.ism.ac.jp/shikoin/startup/index.html>  
<https://www.ism.ac.jp/shikoin/overview/index.html>



# Trends in ADS papers

ADS papers with “Bayesian” in the abstract.

Exponential growth. Time scale ~7 years



Unfamiliar with Bayes? See, e.g.,

[1] Data analysis recipes: **Fitting a model to data**

<https://arxiv.org/abs/1008.4686>

[2] Data analysis recipes: Probability calculus for inference

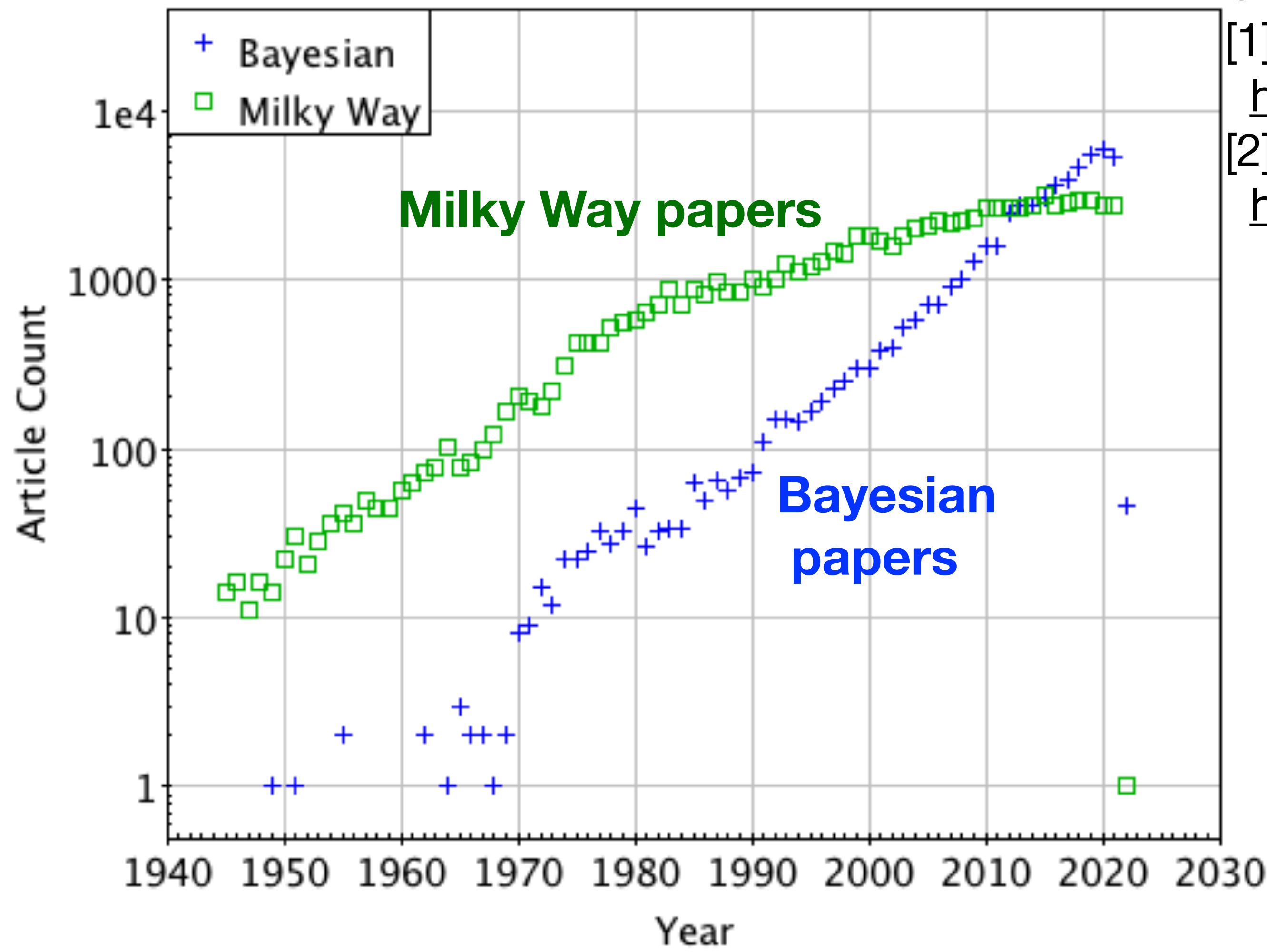
<https://arxiv.org/abs/1205.4446>



# Trends in ADS papers

ADS papers with “Bayesian” in the abstract.  
ADS papers with “Milky Way” in the abstract.

Exponential growth. Time scale ~7 years



Unfamiliar with Bayes? See, e.g.,

[1] Data analysis recipes: **Fitting a model to data**

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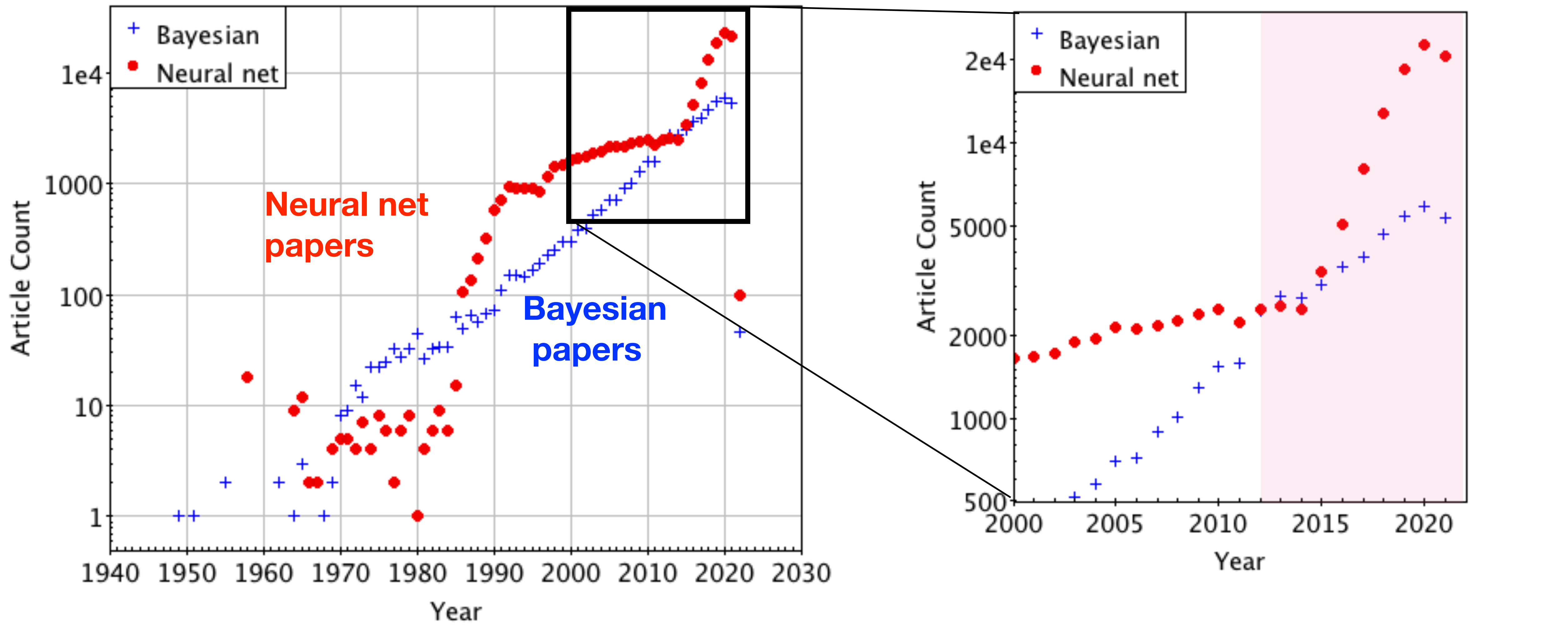
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ADS papers with “Bayesian” in the abstract.

Exponential growth. Time scale ~7 years

ADS papers with “neural net” in the abstract.

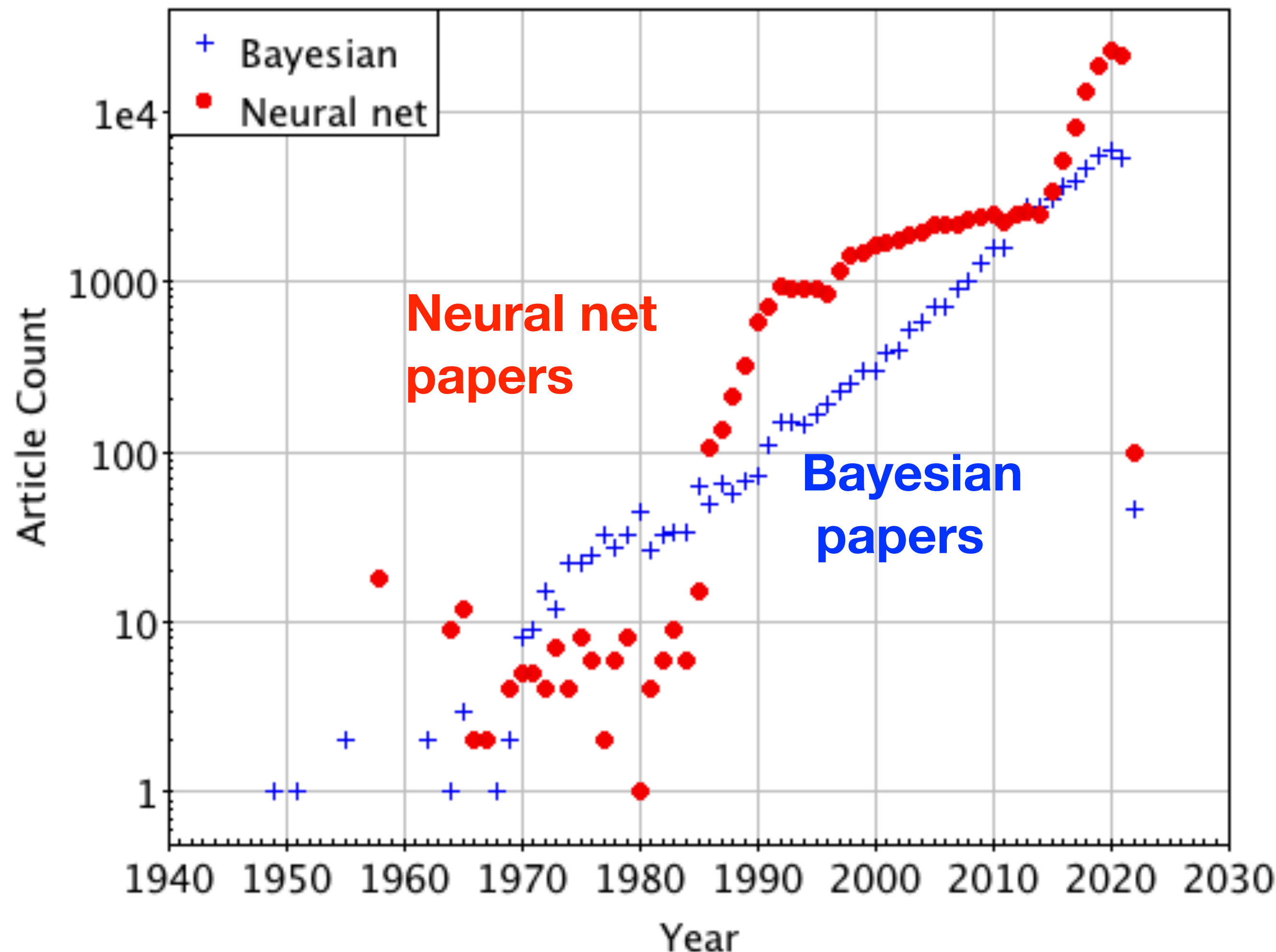
Exponential growth.  
After 2015, the time scale is ~2.5 years



# Trends in ADS papers

ADS papers with “Bayesian” in the abstract.

ADS papers with “neural net” in the abstract.



Exponential growth.

After 2015, the time scale is ~2.5 years

Inflation of ML universe.

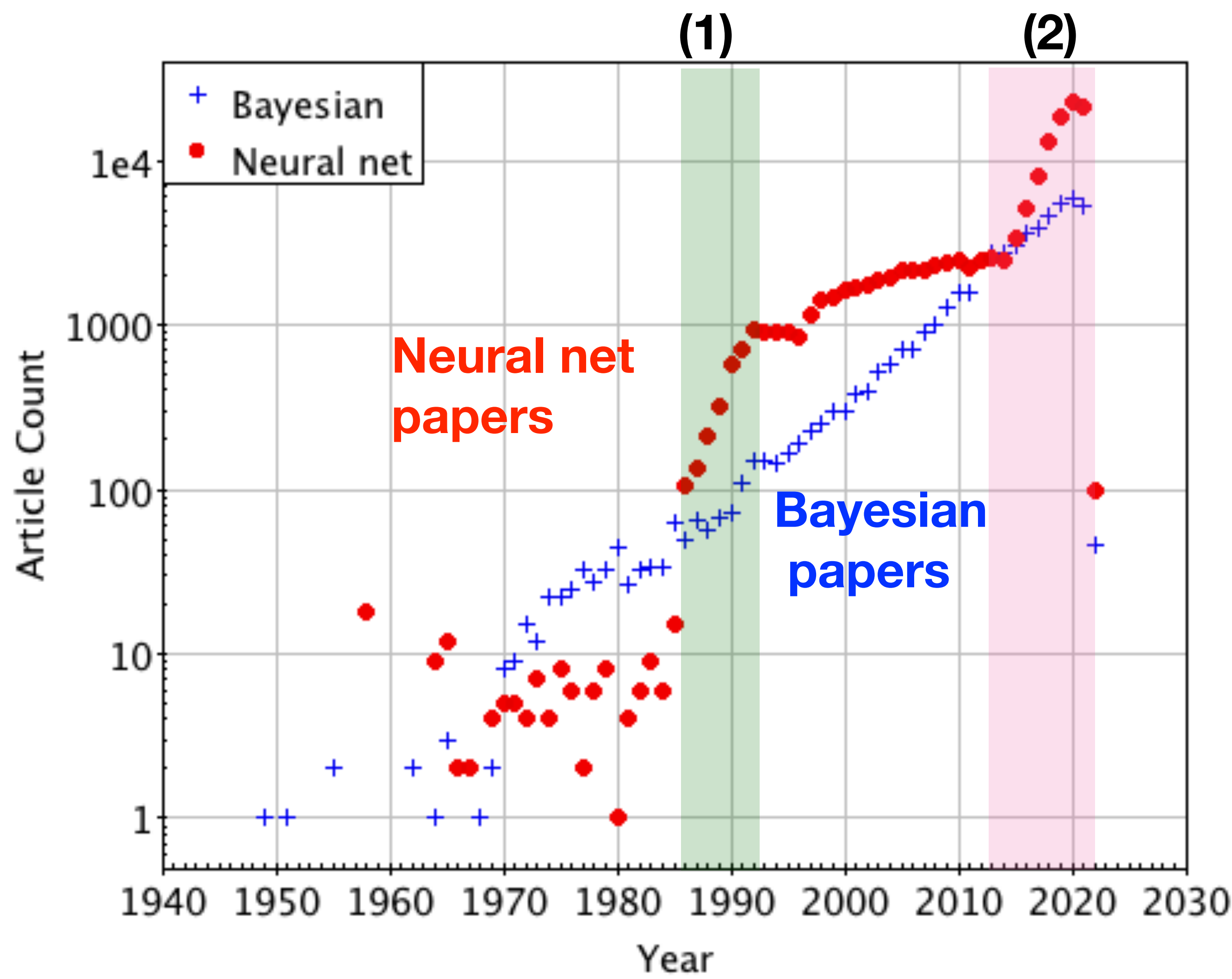
Japanese PhD course ~ 5 years  
Are we ready to train PhD student  
in this expansion of the ML world?



# Trends in ADS papers

ADS papers with “Bayesian” in the abstract.

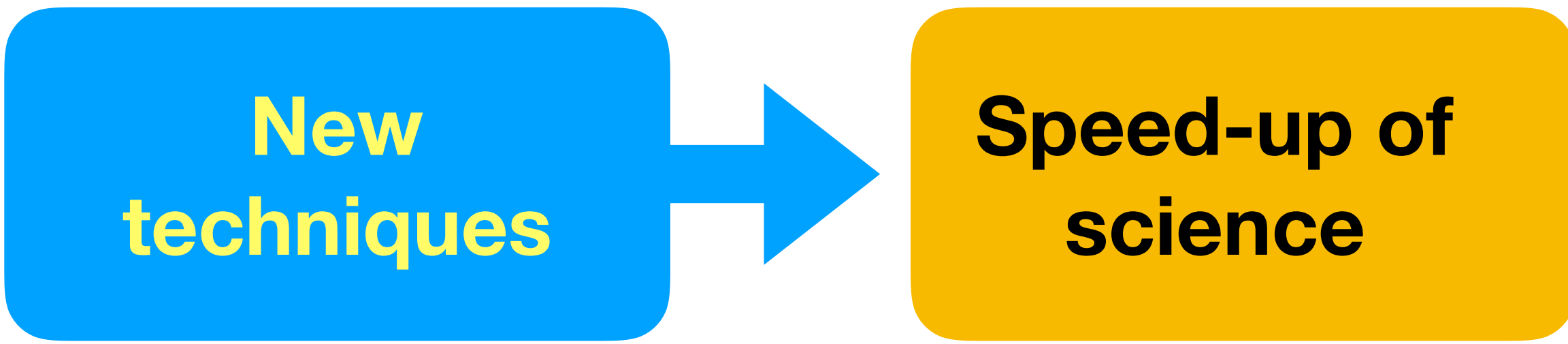
ADS papers with “neural net” in the abstract.



Exponential growth.  
After 2015, the time scale is ~2.5 years

(1) Back propagation method [誤差逆伝播法]

(2) Deep learning (AlexNet) [深層学習]





# History of science

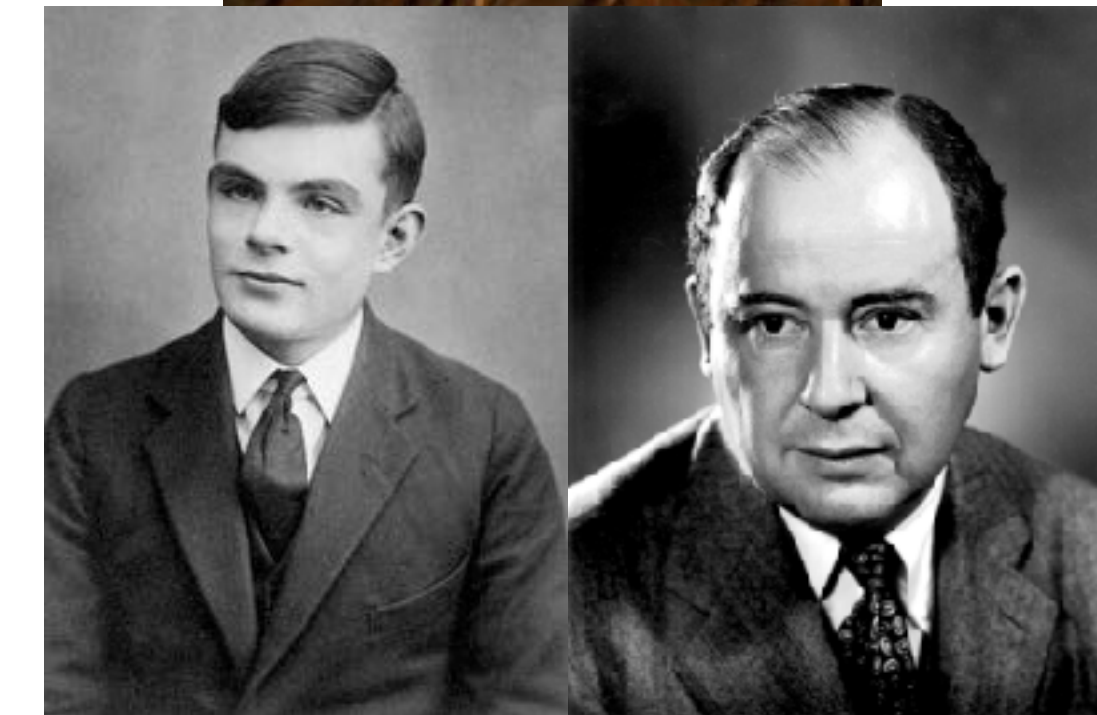
**1. Empirical science  
in the last ~1000s of years**



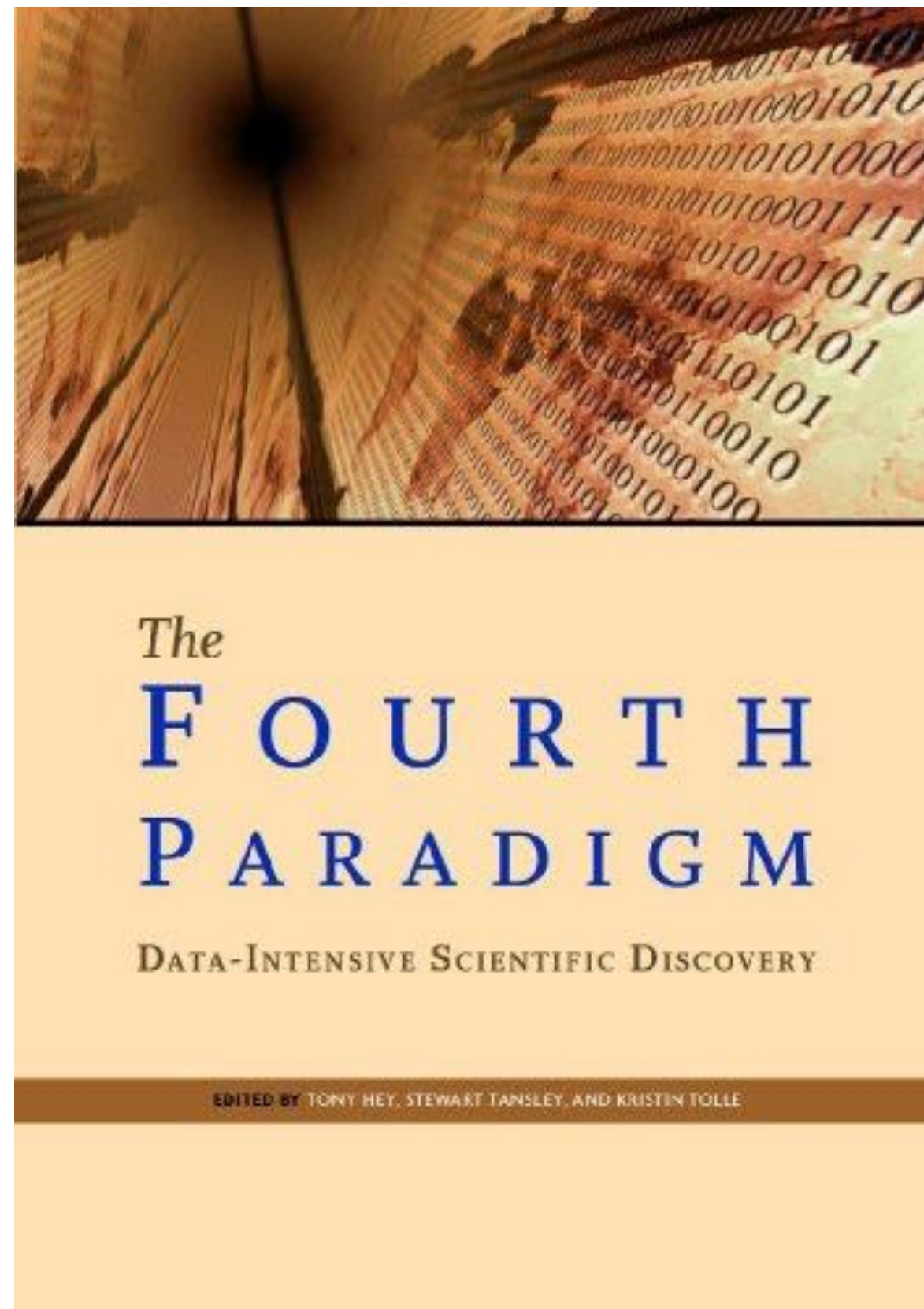
**2. Theoretical science  
in the last ~100s of years**



**3. Computational science  
in the last several decades**



**4. Data exploration  
Now**





## Today's talk

- **(1) Era of big data**
- **(2) Dimensionality reduction**
- **(3) Sparsity**
- **(4) Bayesian analysis**
- **(5) Machine learning**
- **(6) Neural network**
- **(7) Data challenge**

## Setting the stage

- **(1) Era of big data**
- **(2) Dimensionality reduction**
- **(3) Sparsity**
- **(4) Bayesian analysis**
- **(5) Machine learning**
- **(6) Neural network**
- **(7) Data challenge**



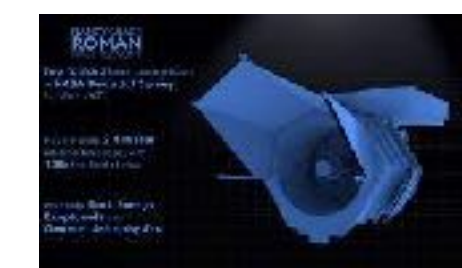
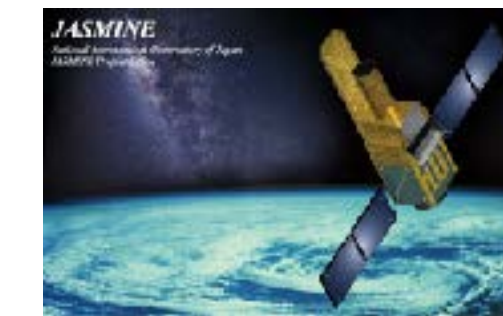
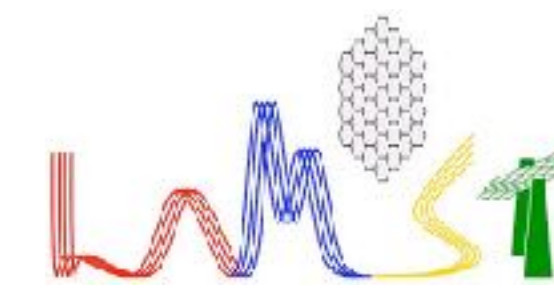
# Era of Big Data

## Keywords for astro observations

- wide-field
- deep
- high-resolution
- high-dimensional (many bands)
- time-domain
- high-precision
- large data volume (e.g., radio telescope)

Data are becoming larger / more complex.  
Most data will never be “seen” by eye.

Need to automate  
data acquisition / reduction / analysis  
... **Data science challenge**





# Main part

Trends in  
statistical mathematics

- (1) Era of big data
- **(2) Dimensionality reduction**
- **(3) Sparsity**
- **(4) Bayesian analysis**

Trends in  
machine learning

- (5) Machine learning
- (6) Neural network

Robustness / reliability  
of new methods

- (7) Data challenge

## Trends in statistical mathematics

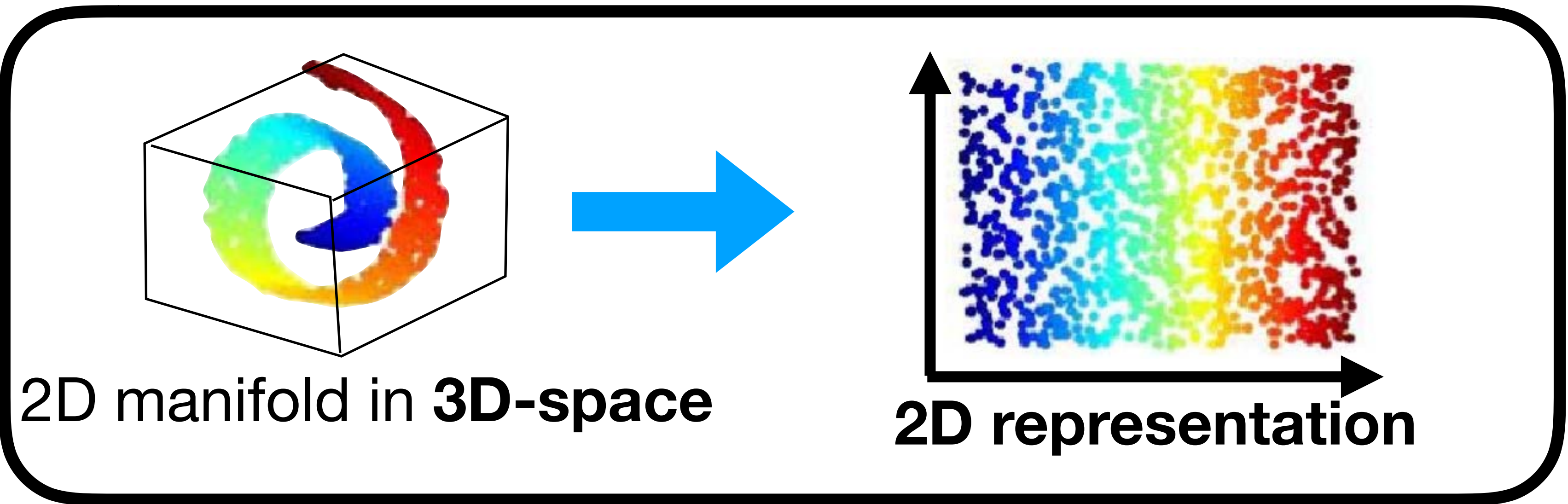
- (1) Era of big data
- **(2) Dimensionality reduction**
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- (5) Machine learning
- (6) Neural network
- (7) Data challenge



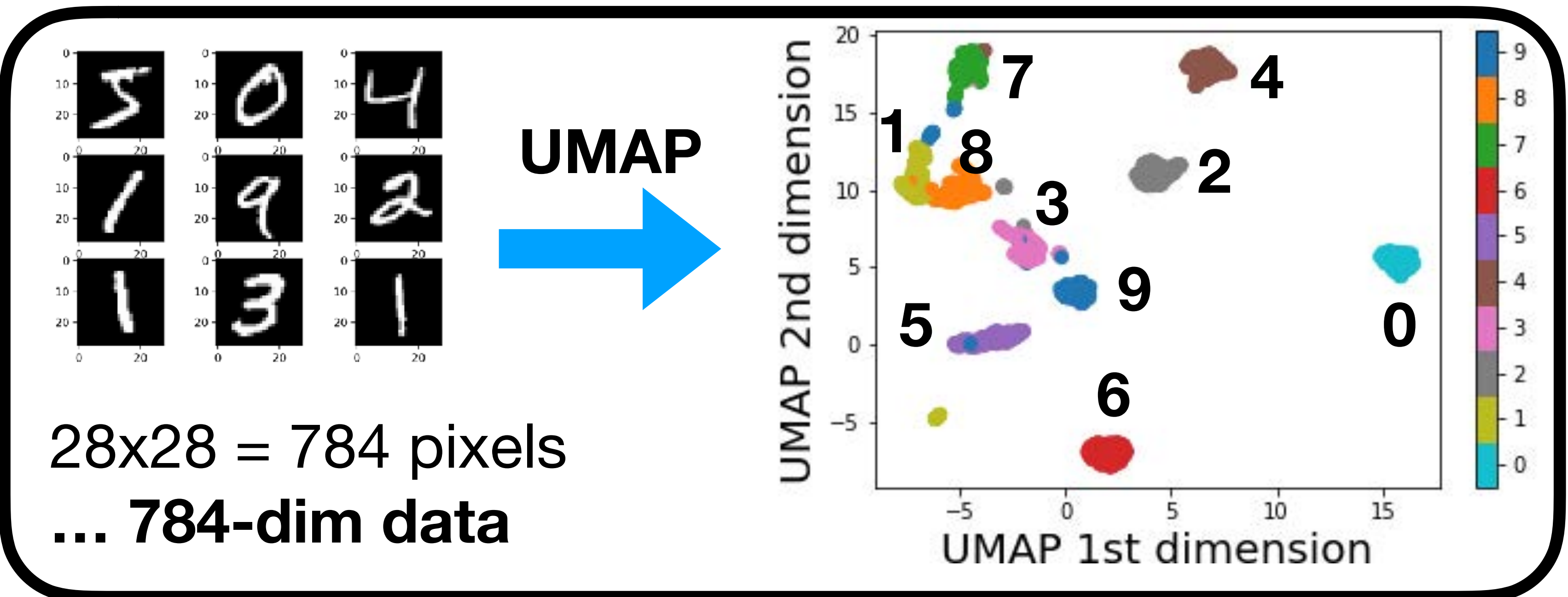
Dimensionality reduction

“特徴量”

N-dimensional “data” → low-dimensional “feature”



Simpler description  
“Manifold learning”



- Techniques
- Self-Organizing Map (SOM)
  - Isomap
  - UMAP

## Trends in statistical mathematics

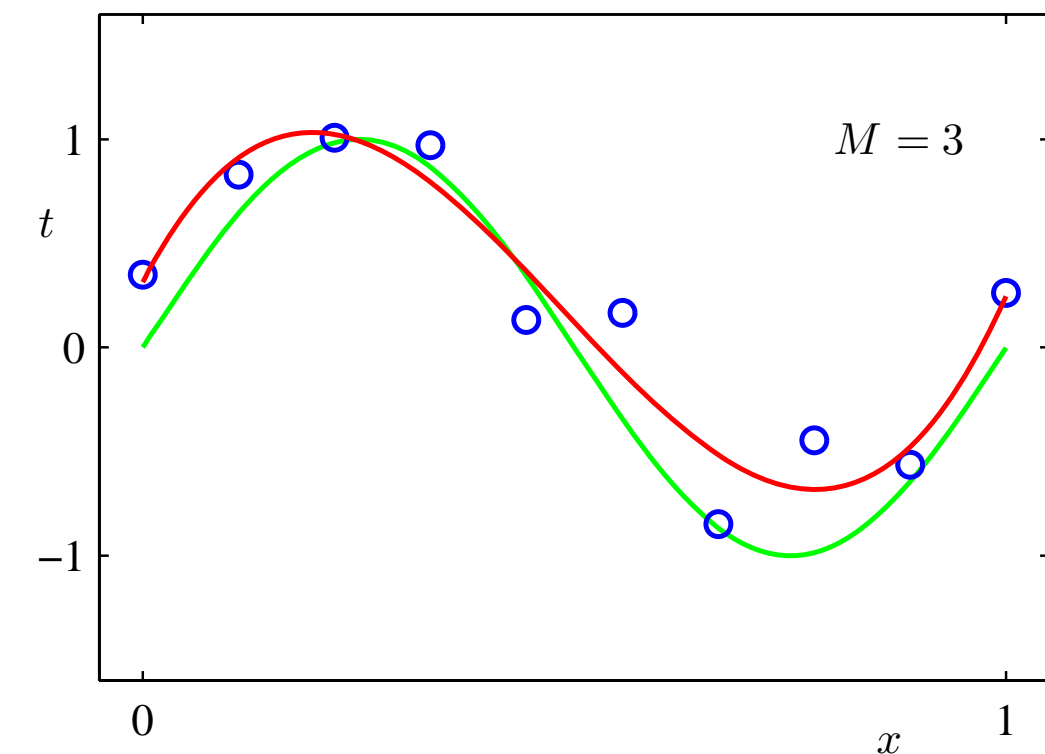
- (1) Era of big data
- (2) Dimensionality reduction
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# Sparse Modeling

**Easy case:**

**(# of model params)  $\leq$  (# of data points)**

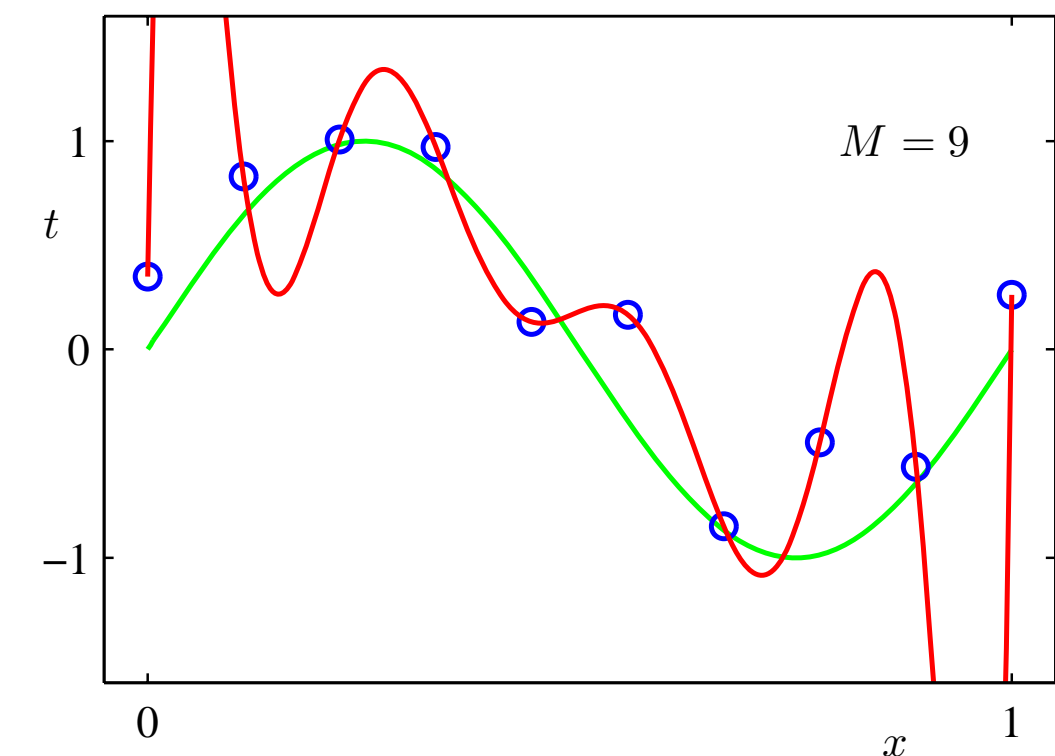
$$N \leq M$$



**What if ...**

**(# of model params)  $>$  (# of data points)**

$$N > M$$



**In general, it fails (degenerate params).**

**But there is a hope, if the model is **sparse**.**

**Tibshirani (1996)**

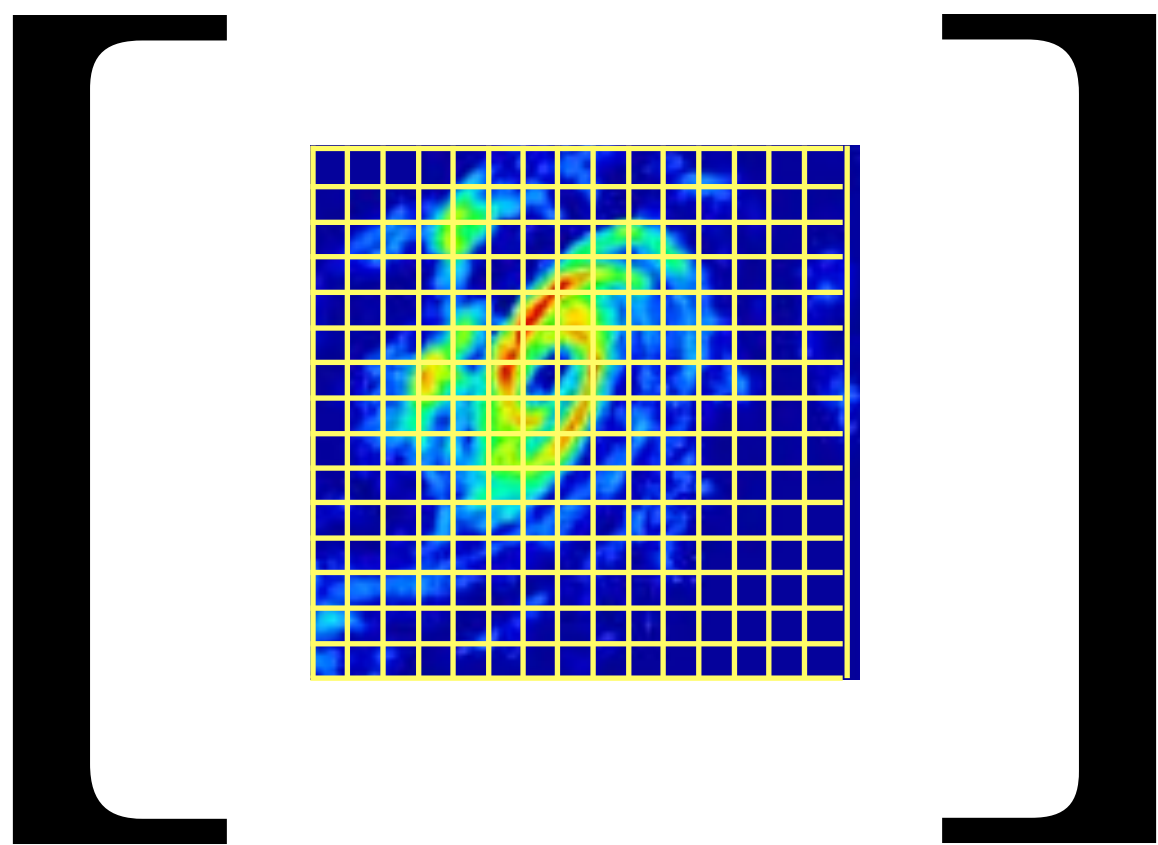


# Sparse Modeling for image data

Visibility

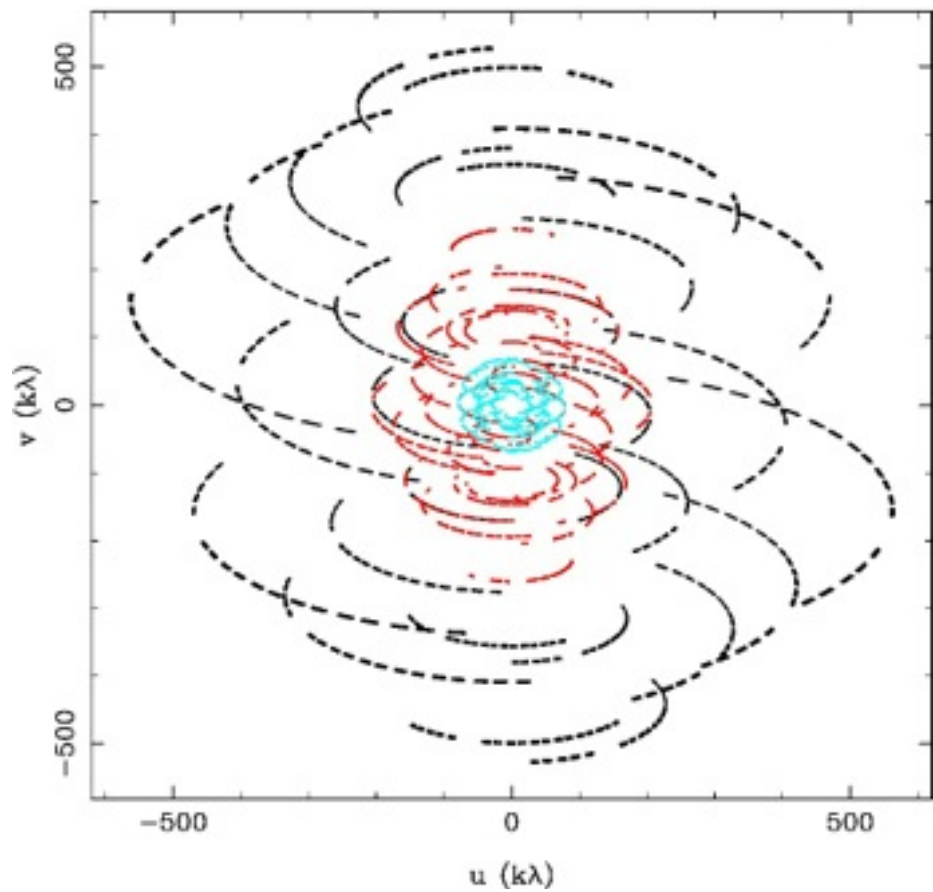
$$v(U, V) = \mathcal{F}$$

Fourier transformation of a radio image



Model **brightness ( $\beta$ )**  
has N pixels.

incomplete sampling




**M** data points for  
the observed  $v(U,V)$

$$\begin{bmatrix} v_1 \\ \vdots \\ v_M \end{bmatrix} = \mathcal{F} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_N \end{bmatrix}$$

Often, we have  $M < N$ .  
No unique solution for  $\beta$ .

## Sparse Modeling

$$\begin{bmatrix} v_1 \\ \vdots \\ v_M \end{bmatrix} = \mathcal{F} \begin{bmatrix} \beta_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \beta_N \end{bmatrix}$$


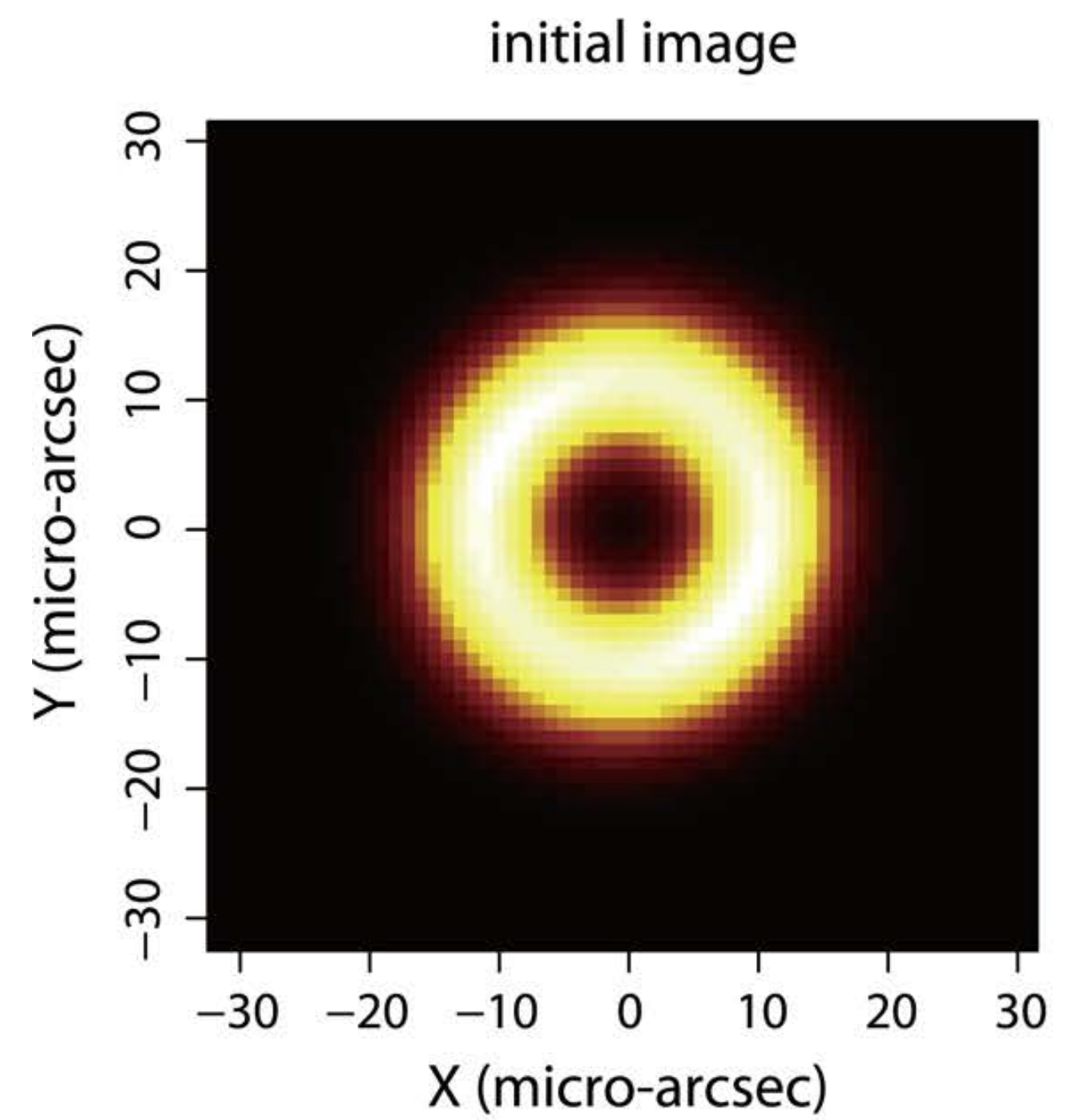
➡ If we **assume** that the image is sparse (many zeros in beta), we can obtain a **LASSO** solution:

$$\hat{\beta} = \arg \min \left[ \frac{1}{2} \overset{\text{residual}}{\|\mathbf{v} - F\beta\|_2^2} + \lambda \overset{\text{penalty}}{\sum_i |\beta_i|} \right]$$

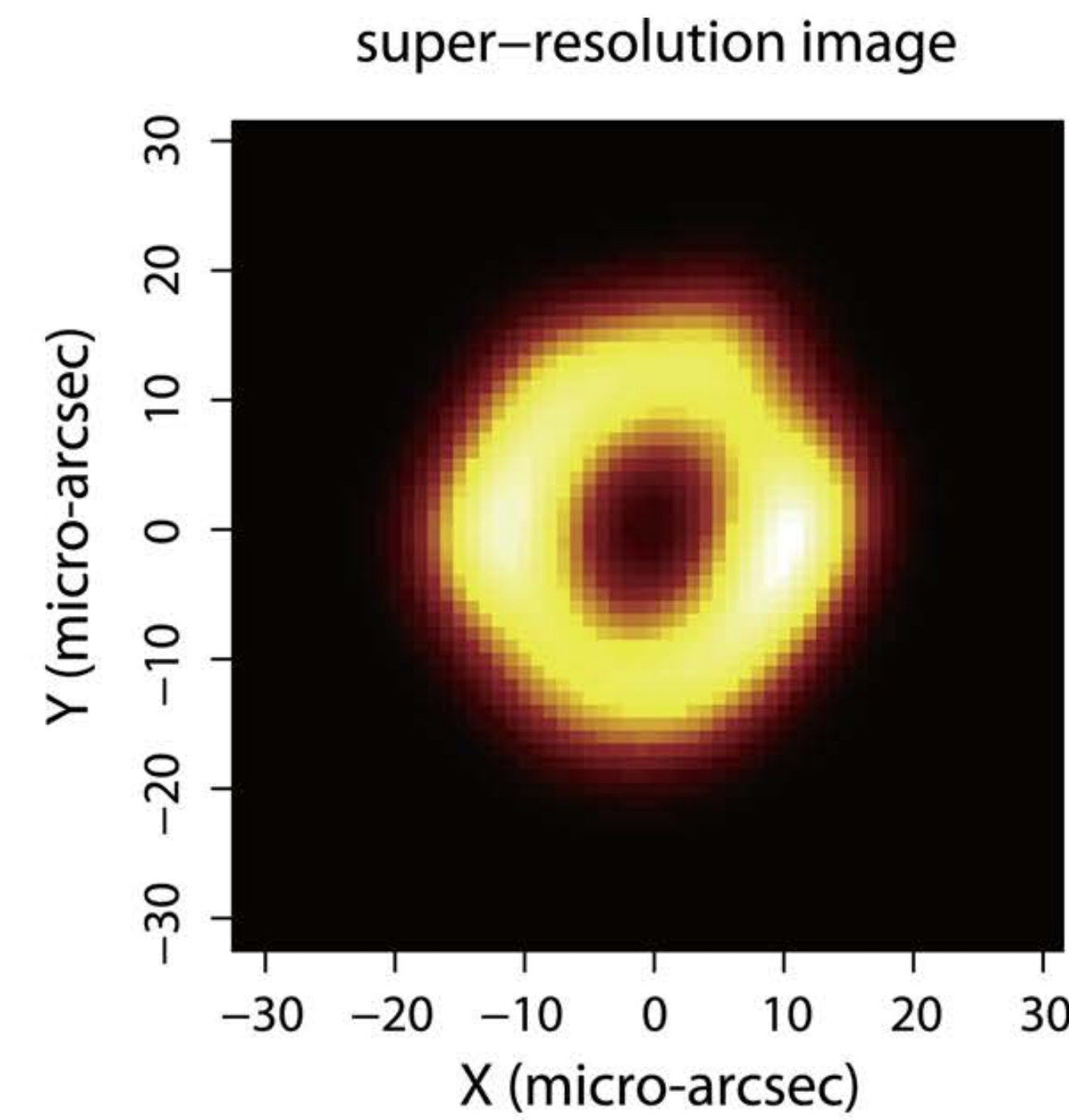
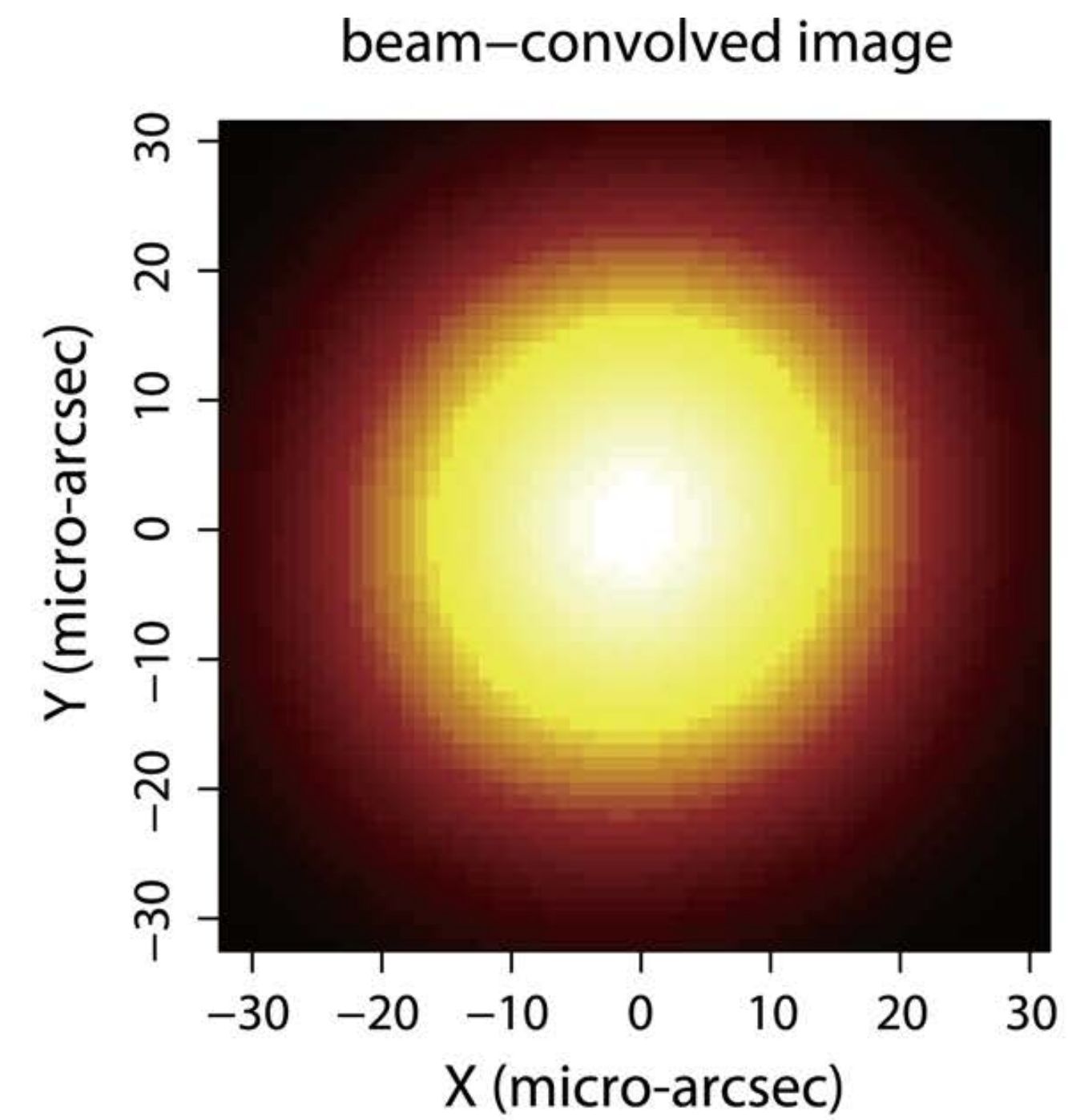
➡ **By adopting a large lambda, we obtain a sparse solution.**  
(Adequate lambda depends on the science case. Need cross-validation.)

# Sparse Modeling

## Ground truth



## LASSO



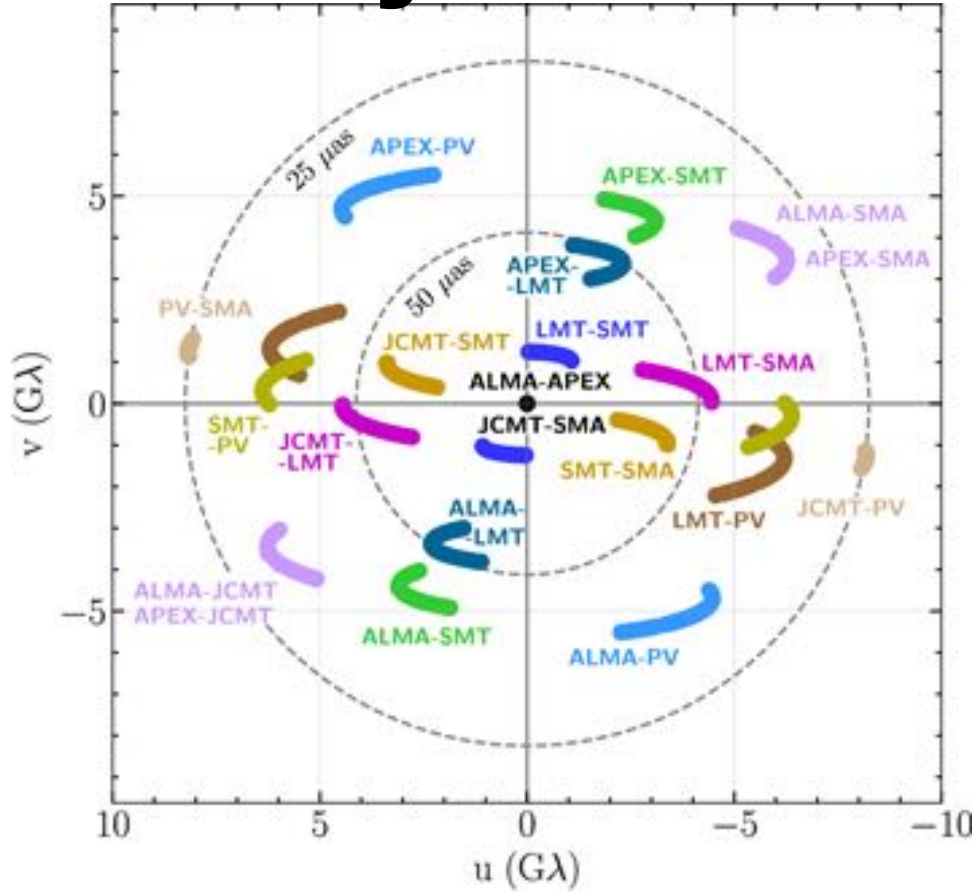


Sparse Modeling

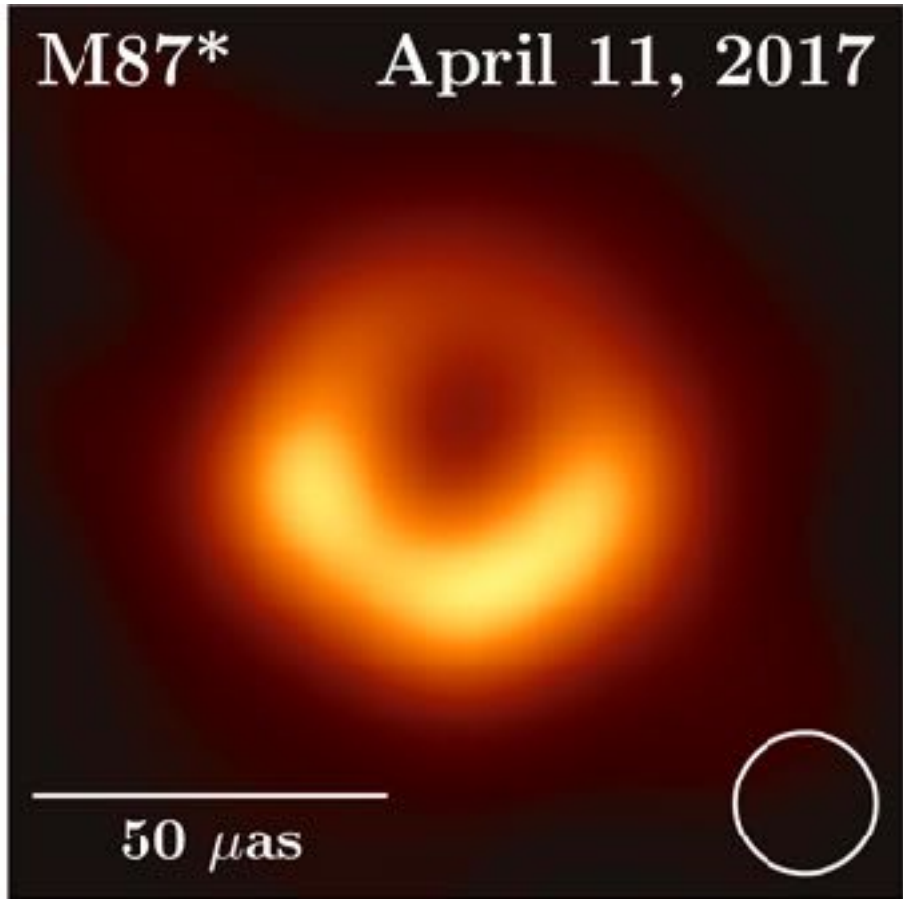
To believe or not to believe; *blind test* is important.

M87's black hole shadow

Visibility data



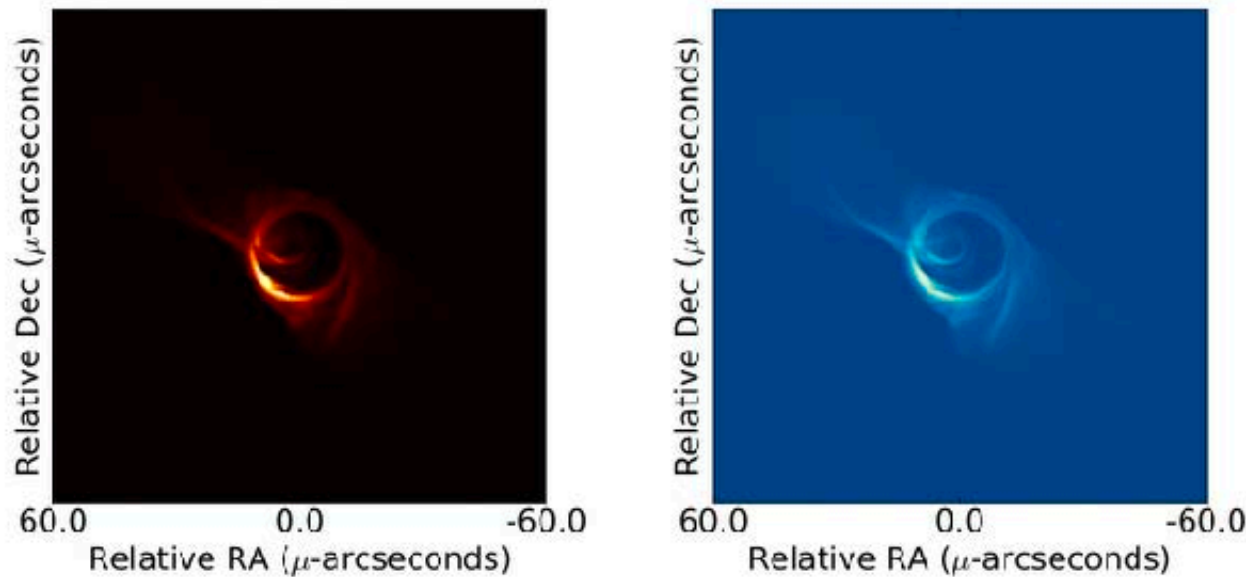
Reconstructed image



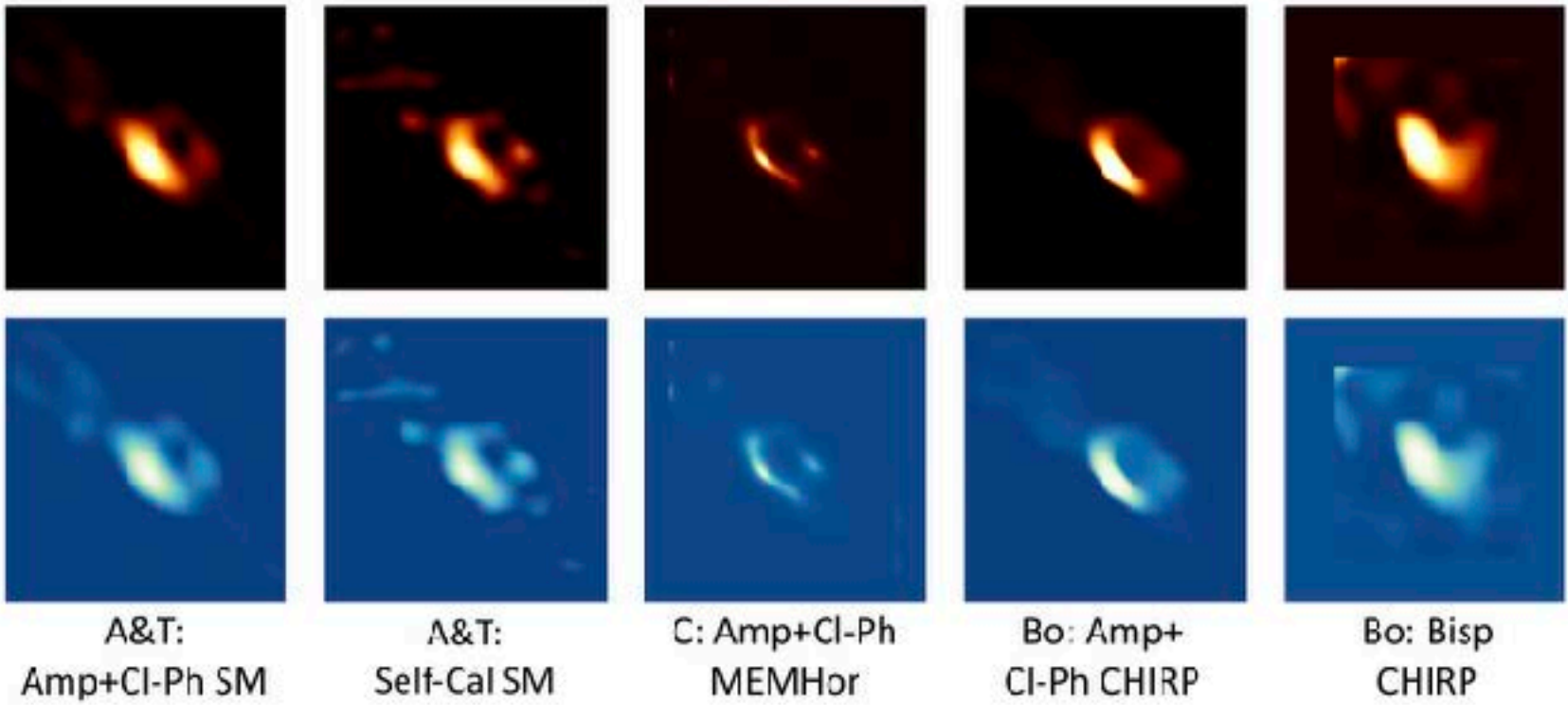
EHT Collaboration, Akiyama et al. (2019)

Data challenge (Mock analysis)

Ground truth



Reconstructed image



Katherine L. Bouman PhD thesis (2017)

Radio telescopes opened a new window into SMBHs and possibly IMBHs (ALMA, SKA, ngVLA).

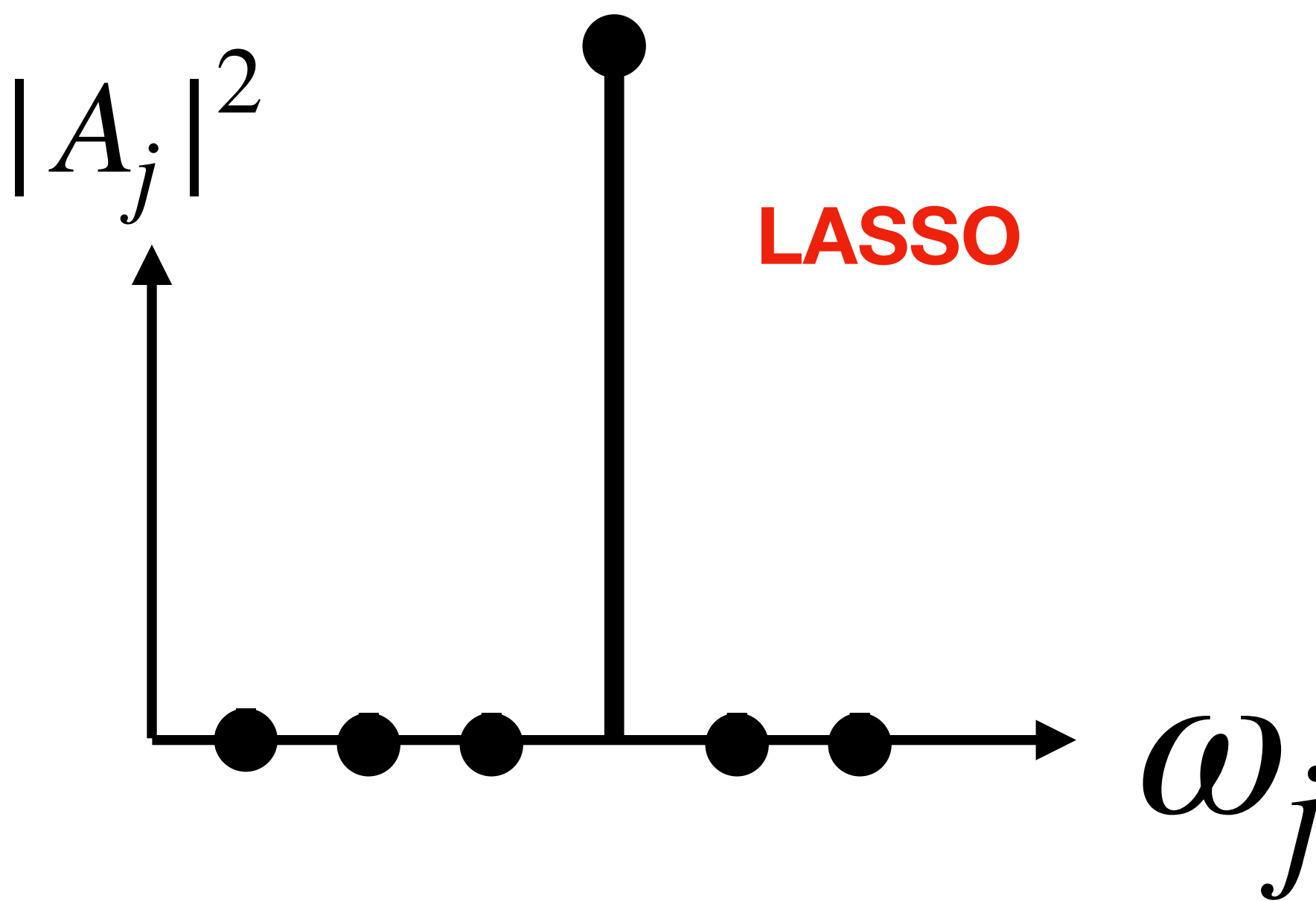
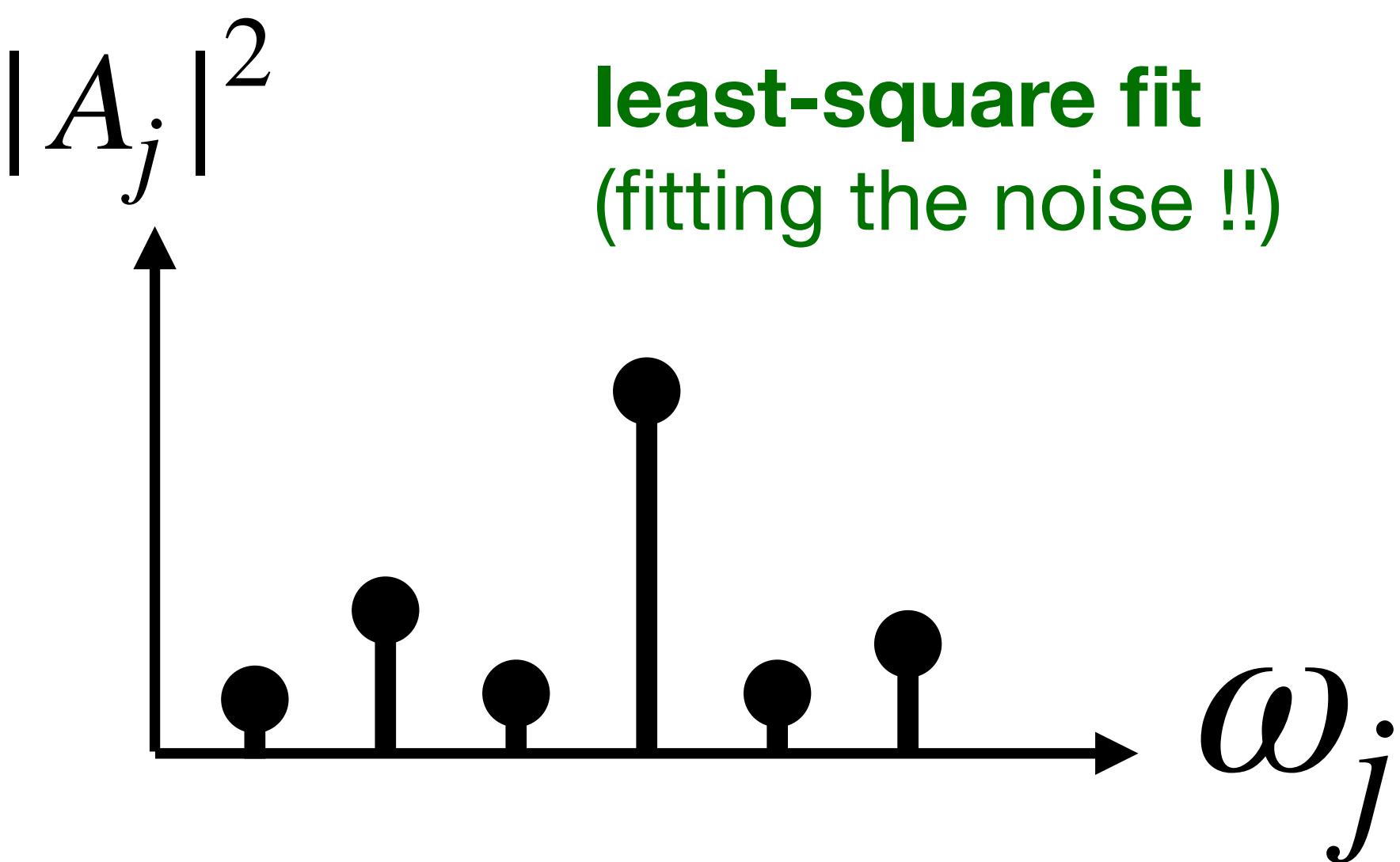
**Sparse Modeling** for **time-series data**

**flux:**  $y(t) = \sum_j A_j \exp(i\omega_j t)$

Kato & Uemura (2012)\*

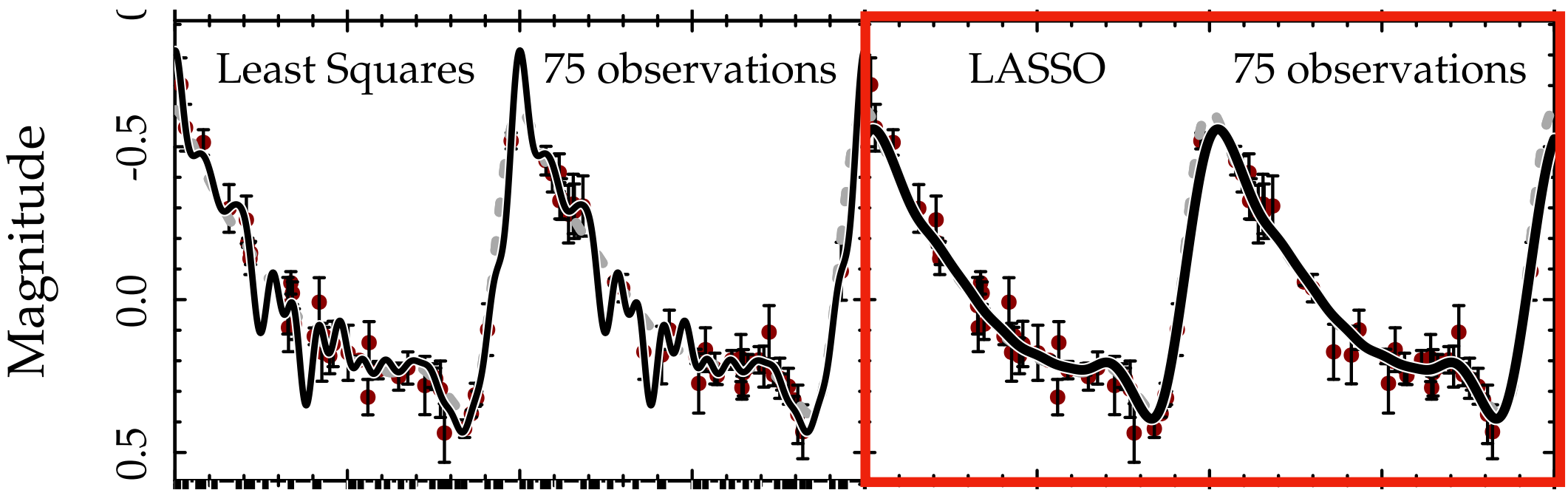
**Regular variable stars (e.g., Cepheids, RR Lyrae)**  
have only few frequencies with non-zero amplitude.

**LASSO in power-spectrum space.**  
>> **Simplest representation** of the light curve.



Bellinger, Wysocki, Kanbur (2016)

**Successful LASSO for RR Lyrae**



\* Data taken from **VSNET**.



# Sparse Modeling



森田耕一郎 教授  
(1954 - 2012)



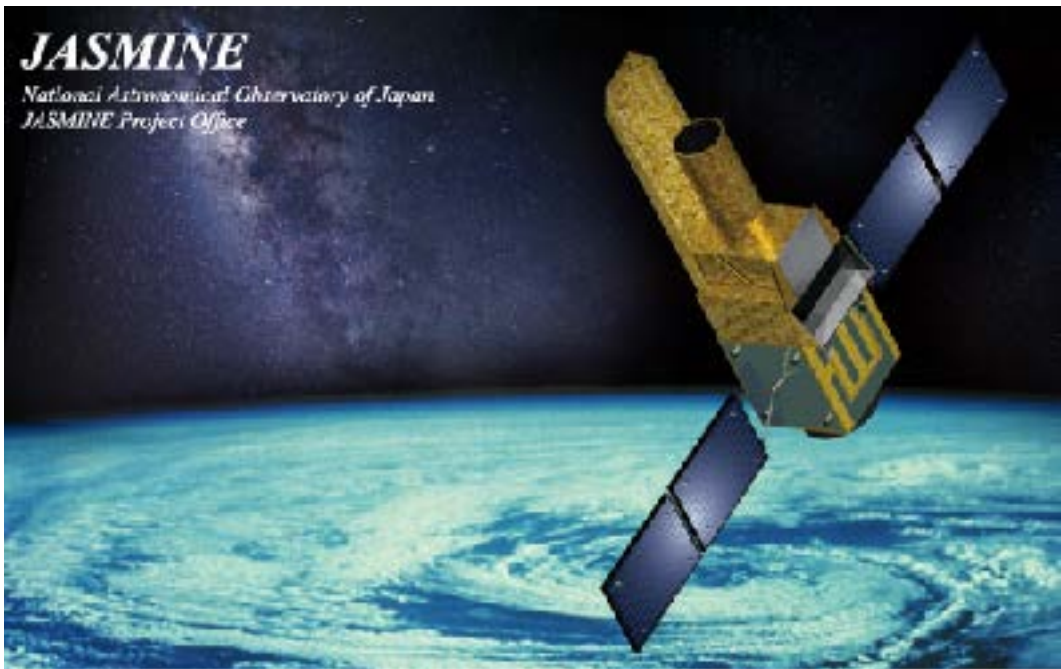
One of the first persons in astronomy who envisioned the importance of **sparse modeling** in radio interferometry.

# Sparse matrix ... Tough example

JASMINE will **stare at** the MW center region.

JASMINE will

- observe 1e5 stars
- take photo for 80 x 2000 times for each star (**Paparazzi !**)
- measure N=1e7 params (including satellite attitude)



If we are to make the most of JASMINE,  
we need to solve a huge matrix inversion problem

$$\begin{array}{c} \updownarrow 10^{10} \\ \begin{pmatrix} o_1 \\ \vdots \\ o_\ell \\ \vdots \\ o_L \end{pmatrix} \simeq \begin{pmatrix} \hat{o}_1 \\ \vdots \\ \hat{o}_\ell \\ \vdots \\ \hat{o}_L \end{pmatrix} + \underbrace{\begin{pmatrix} \frac{\partial}{\partial p_1} f_1^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\lambda} f_1^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\Lambda} f_1^{\mathcal{P}} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \frac{\partial}{\partial p_\ell} f_\ell^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\lambda} f_\ell^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\Lambda} f_\ell^{\mathcal{P}} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \frac{\partial}{\partial p_L} f_L^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\lambda} f_L^{\mathcal{P}} & \cdots & \frac{\partial}{\partial p_\Lambda} f_L^{\mathcal{P}} \end{pmatrix}}_{D^{\mathcal{P}}} \begin{pmatrix} p_1 - \hat{p}_1 \\ \vdots \\ p_\lambda - \hat{p}_\lambda \\ \vdots \\ p_\Lambda - \hat{p}_\Lambda \end{pmatrix} \\ \downarrow 10^7 \end{array}$$

$\overleftarrow{10^{10} \times 10^7 \text{ matrix}}$

$\mathbf{o} \simeq \hat{\mathbf{o}} + D^{\mathcal{P}} \Delta \hat{\mathbf{p}}$

Although the **design matrix** is **sparse**, it will be tough to solve it quickly.  
>> Need a Parallel Computing LSQR (Least Squares with QR-factorization) method?



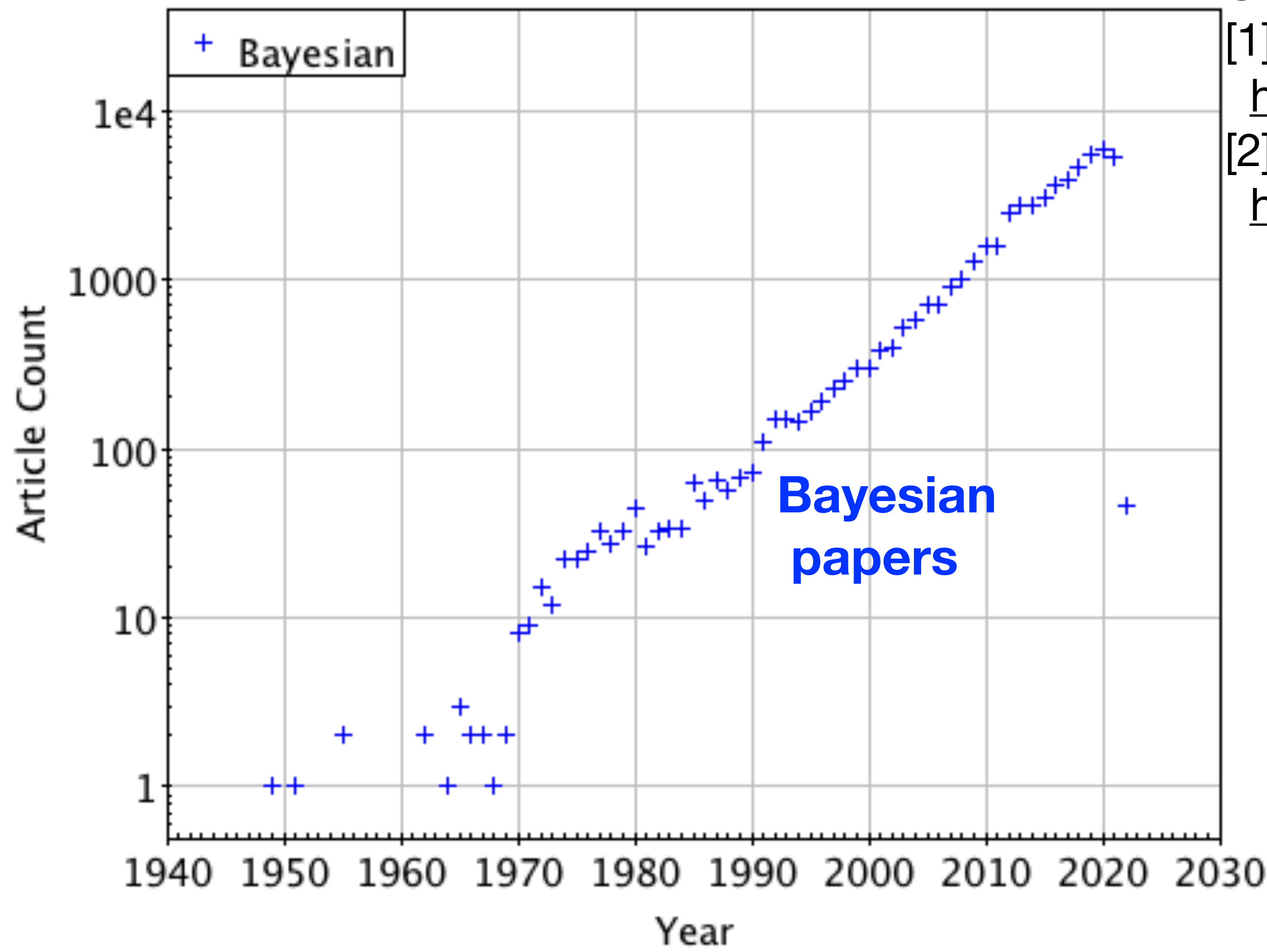
## Trends in statistical mathematics

- (1) Era of big data
- (2) Dimensionality reduction
- (3) Sparsity
- **(4) Bayesian analysis**
- (5) Machine learning
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- (7) Data challenge

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Exponential growth. Time scale ~7 years



Unfamiliar with Bayes? See, e.g.,

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[2] Data analysis recipes: Probability calculus for inference

<https://arxiv.org/abs/1205.4446>





# Bayesian analysis

**Only 3 topics (to save time):**

- (1) MCMC in high-dimensional space is tricky, especially if the posterior distribution is multi-modal.**
  - >> Try *nested sampling* (Skilling 2004). [e.g., Hikage et al. 2019]**
- (2) Bottleneck in MCMC is the computational cost in the likelihood.**
  - >> Simplify the likelihood function (e.g., interpolation) [e.g., Nishimichi et al. 2019]**
  - >> Reduce the *effective* data size [e.g., Hattori et al. 2021]**
- (3) “Likelihood” is sometimes hard to define (e.g., likelihood of **N-body** model?)**
  - >> Try ABC “*Approximate Bayesian Computation*”**  
**= MCMC-like analysis for the summary statistics**

## **Trends in machine learning**

- **(1) Era of big data**
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# Machine learning

**Machine learning is the science of getting computers to act  
without being explicitly programmed.**

**— Andrew Ng**

**A set of methods that can automatically detect patterns in data,  
and then use the uncovered patterns to predict future data,  
or to perform other kinds of decision making under uncertainty.**

**— Kevin P. Murphy**

**Machine learning is the study of computer algorithms that can  
improve automatically through experience and by the use of data.**

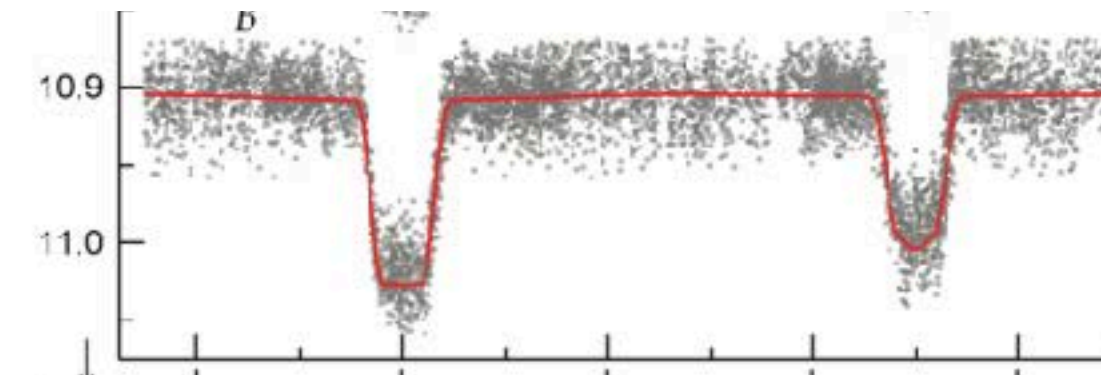
**— Wikipedia**



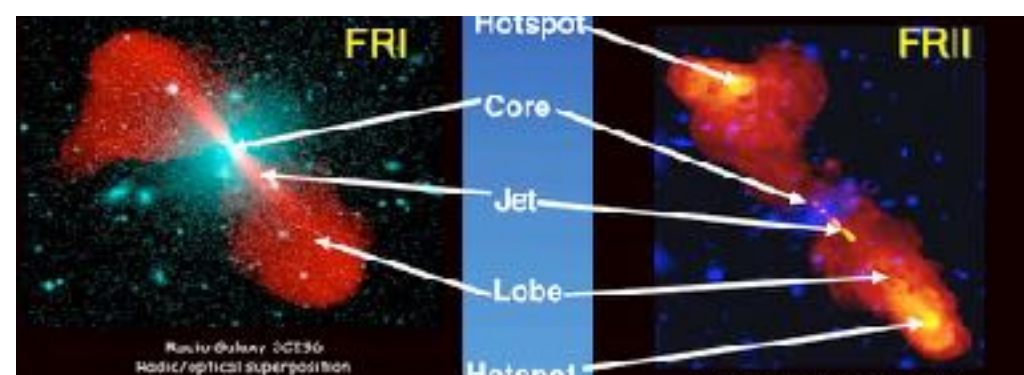
# Machine learning

**Supervised learning:** Based on the “input-output” pairs (test data), find the function that maps input to output.

## Classification



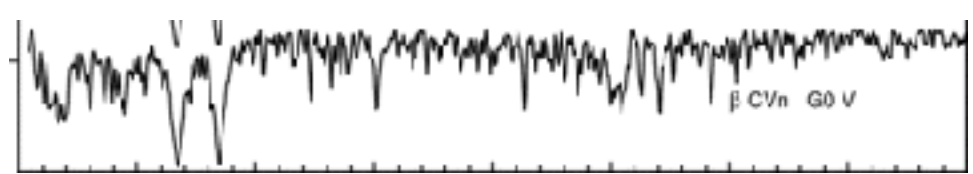
Transients / Variables /  
Flares / Micro-lensing / SNe



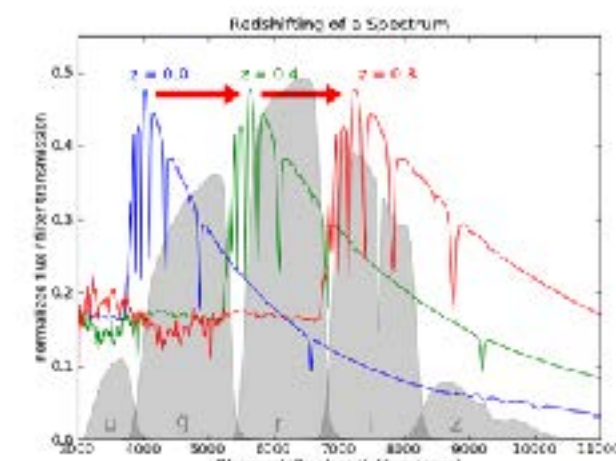
Radio galaxy types

PLASTiCC challenge

## Parameter inference



Spectral analysis  
(Subaru PFS / GA)



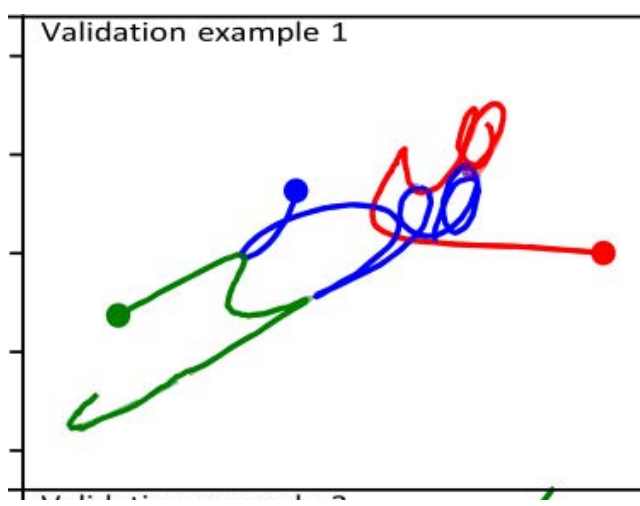
Photometric redshift

## Identification



Find strong  
lensing images

## Model generation



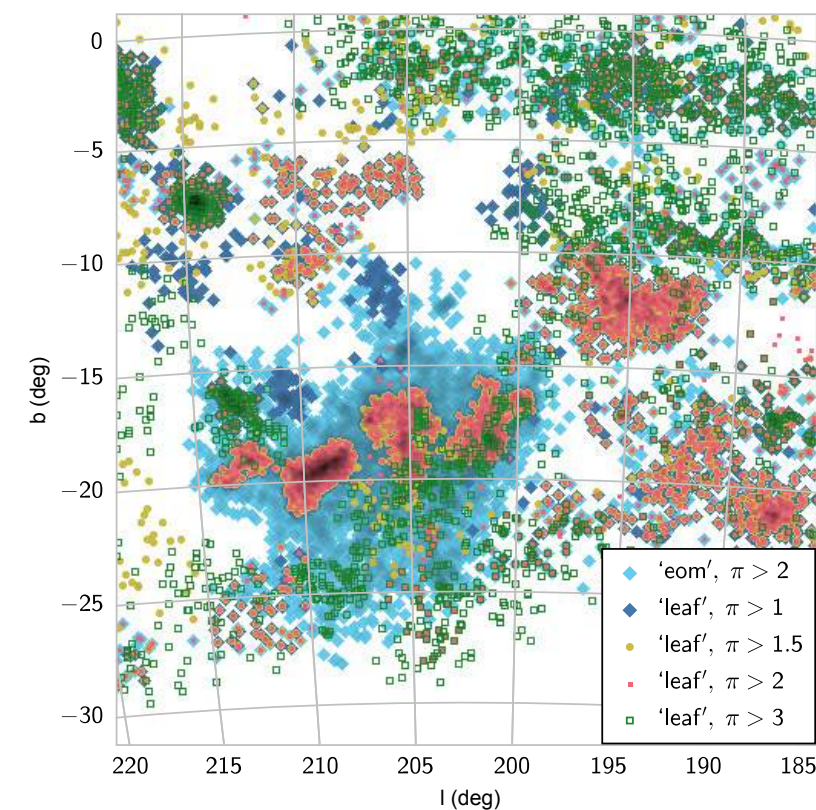
Chaotic  
3-body model

... etc.

# Machine learning

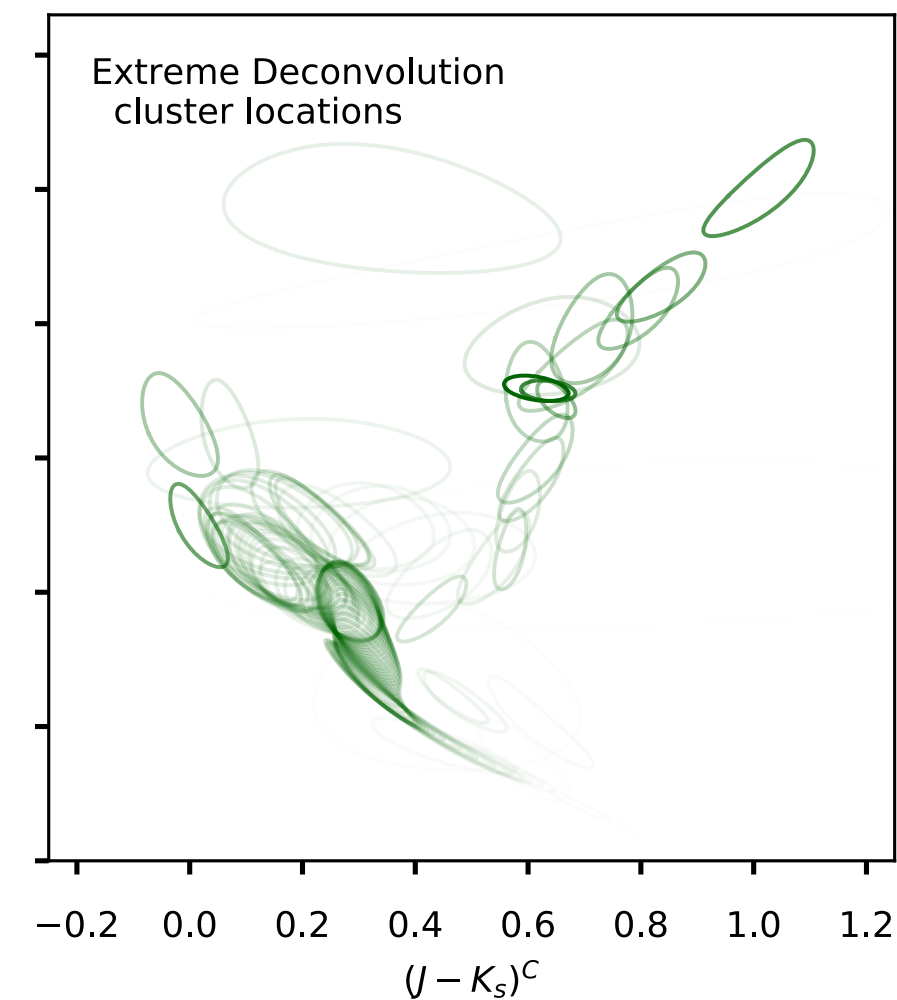
**Unsupervised learning:** Find the pattern in the data without external information.

## Clustering



Find open clusters /  
Over-density of galaxies

## Density estimation



Deriving precise CMD /  
Deriving 3D dust map

## Anomaly detection



Pair-instability SNe /  
Hypervelocity stars /  
Gravitational lensing

... etc.



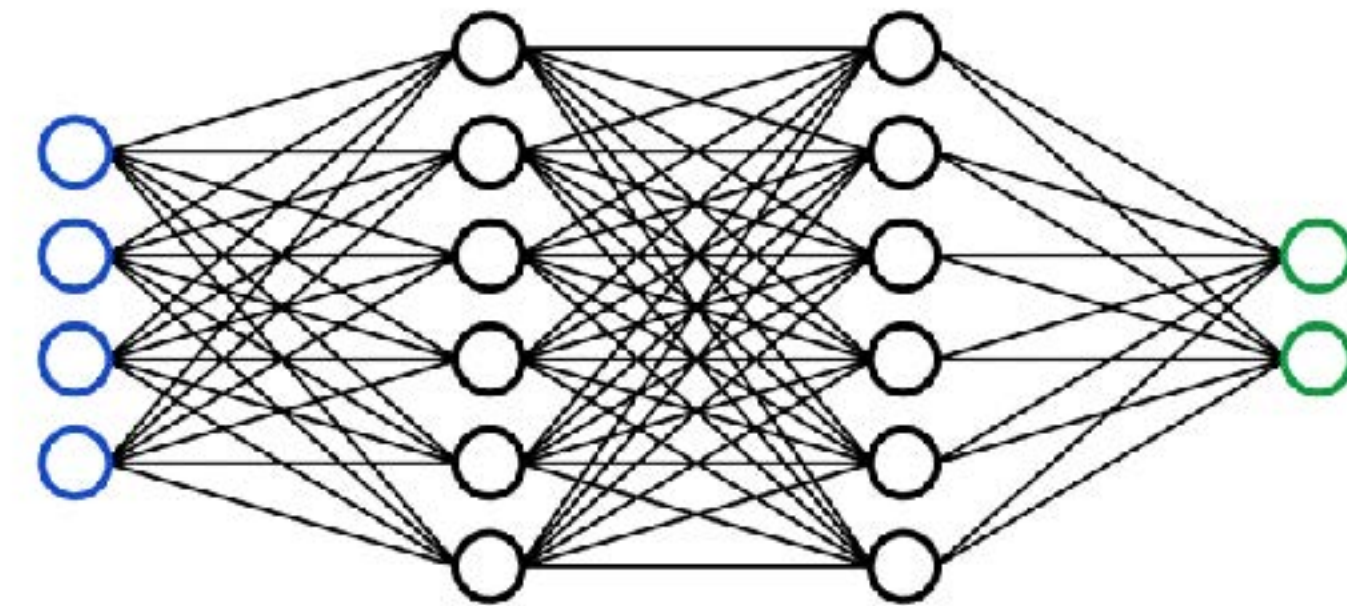
# Machine learning

## Classical methods

**K-means**  
**Support Vector Machine (SVM)**  
**Random Forest**  
**Gaussian Mixture Model (GMM)**



## Neural network

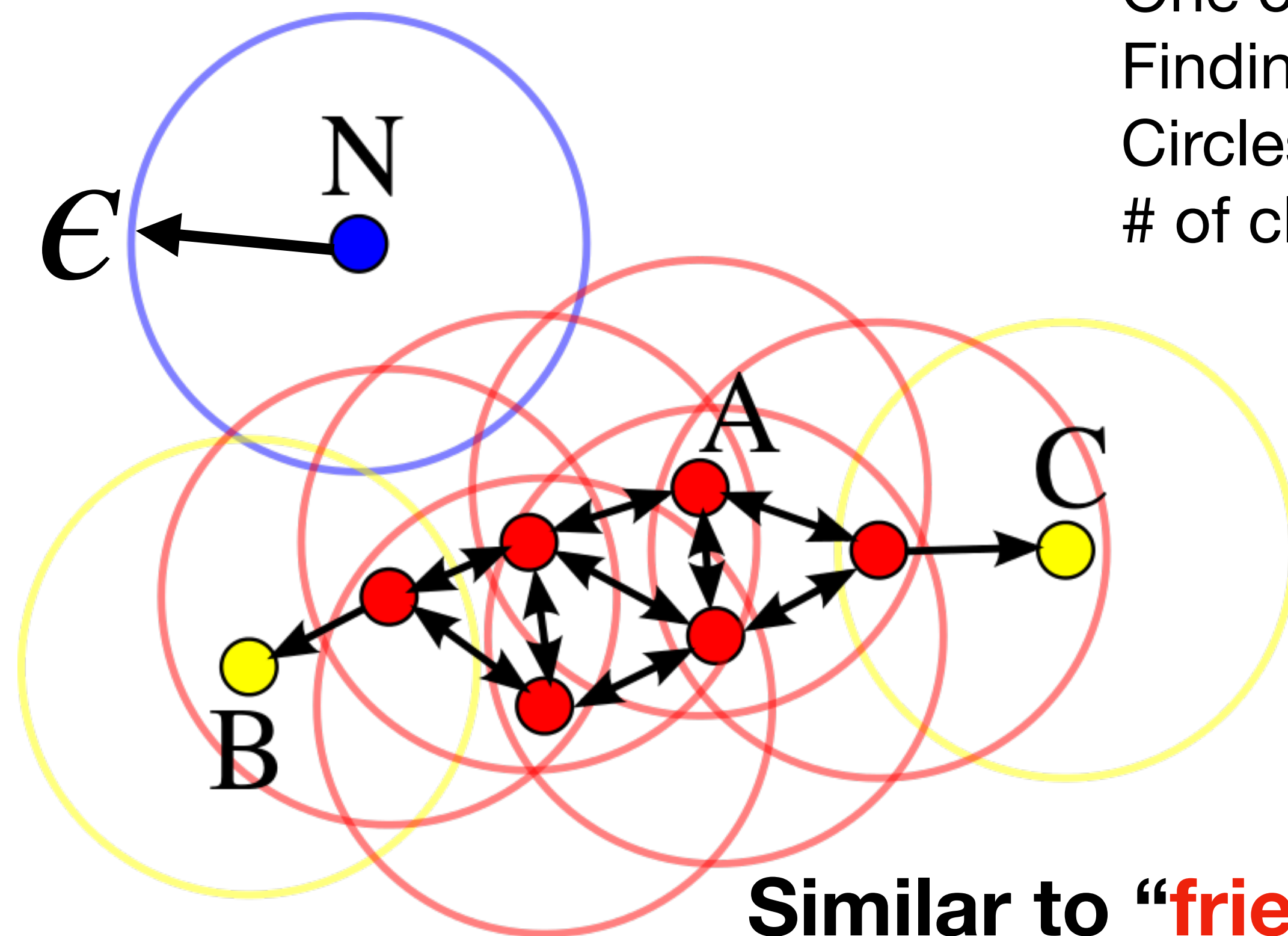




One of the fast / successful / easy-to-implement methods:

**DBSCAN** (Density-based spatial **clustering** of applications with noise)

One of the most widely used clustering method.  
Finding data points within a given radius  $\epsilon$ .  
Circles which encloses less than  $N_{\min}$  are ignored.  
# of clusters is automatically determined.



**$N_{\min} = 4$ .**  
**Only red circles form the cluster.**

Similar to “**friend-of-friend**” method in **N-body** simulation.



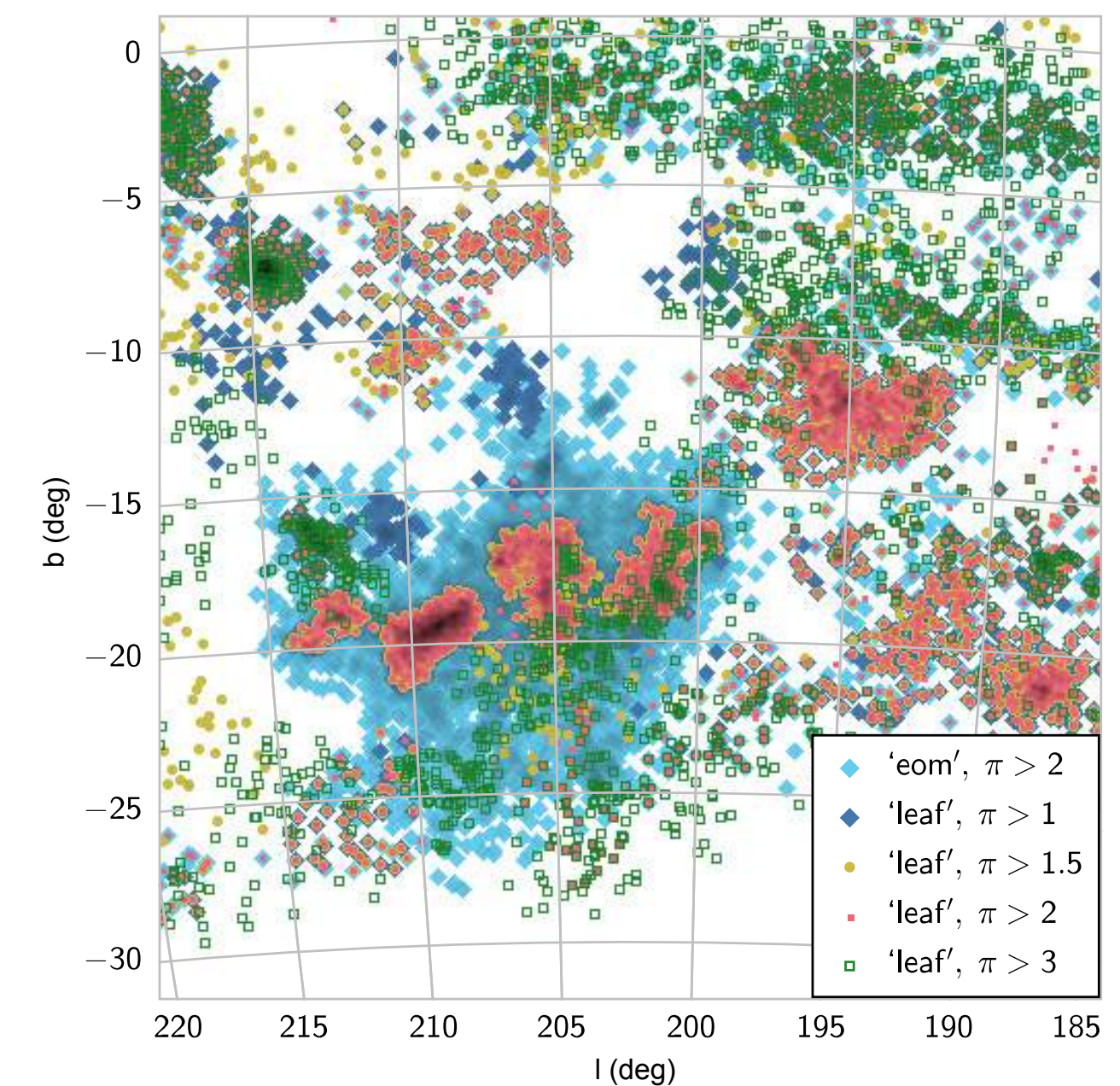
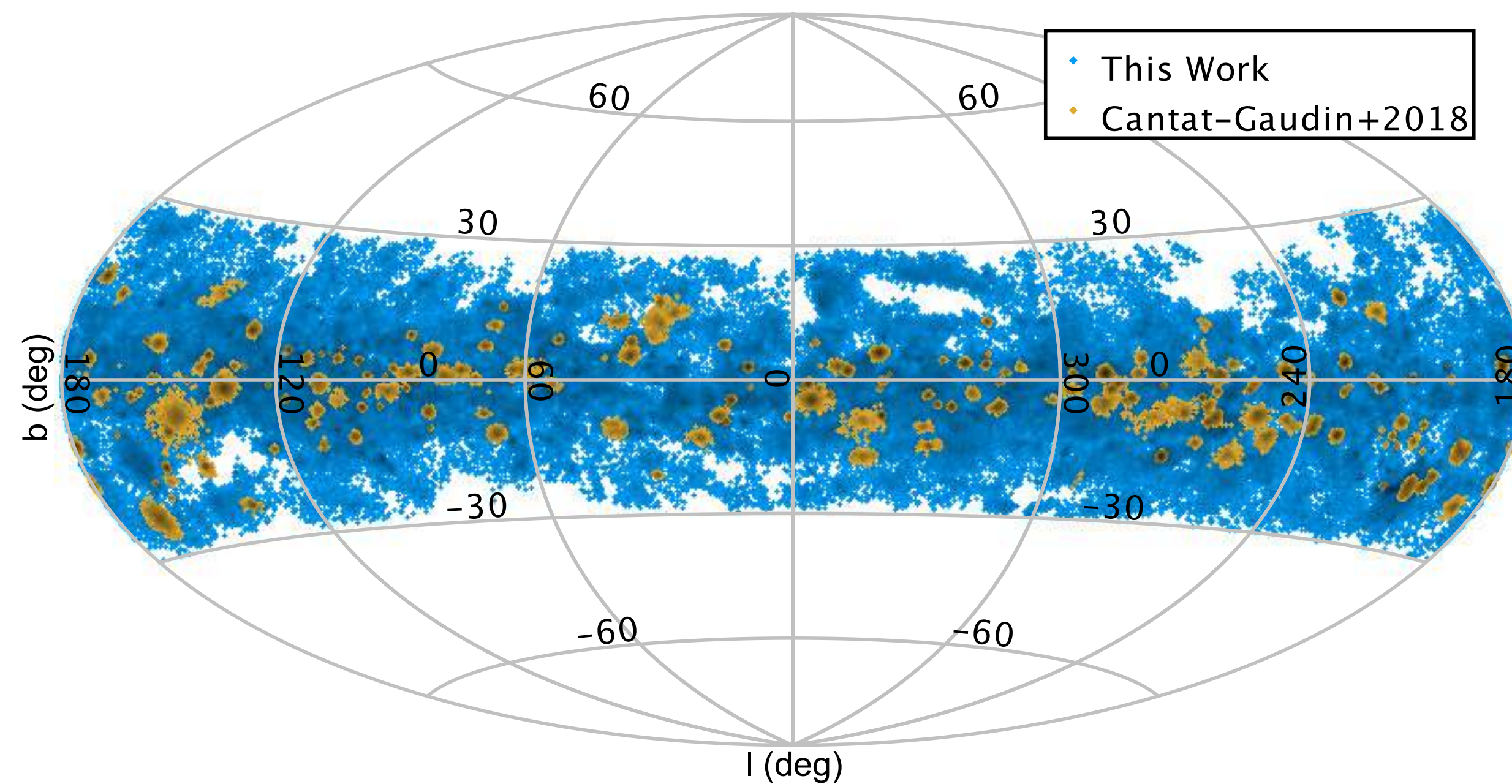
# Clustering

## Discovering open clusters with Gaia data

**Stars in an open cluster have similar position and velocity ( $\mathbf{x}, \mathbf{v}$ )**

>> **DBSCAN** can discover open clusters with **Gaia's astrometric data**.

>> There are ~2000 open clusters within 1 kpc from the Sun.

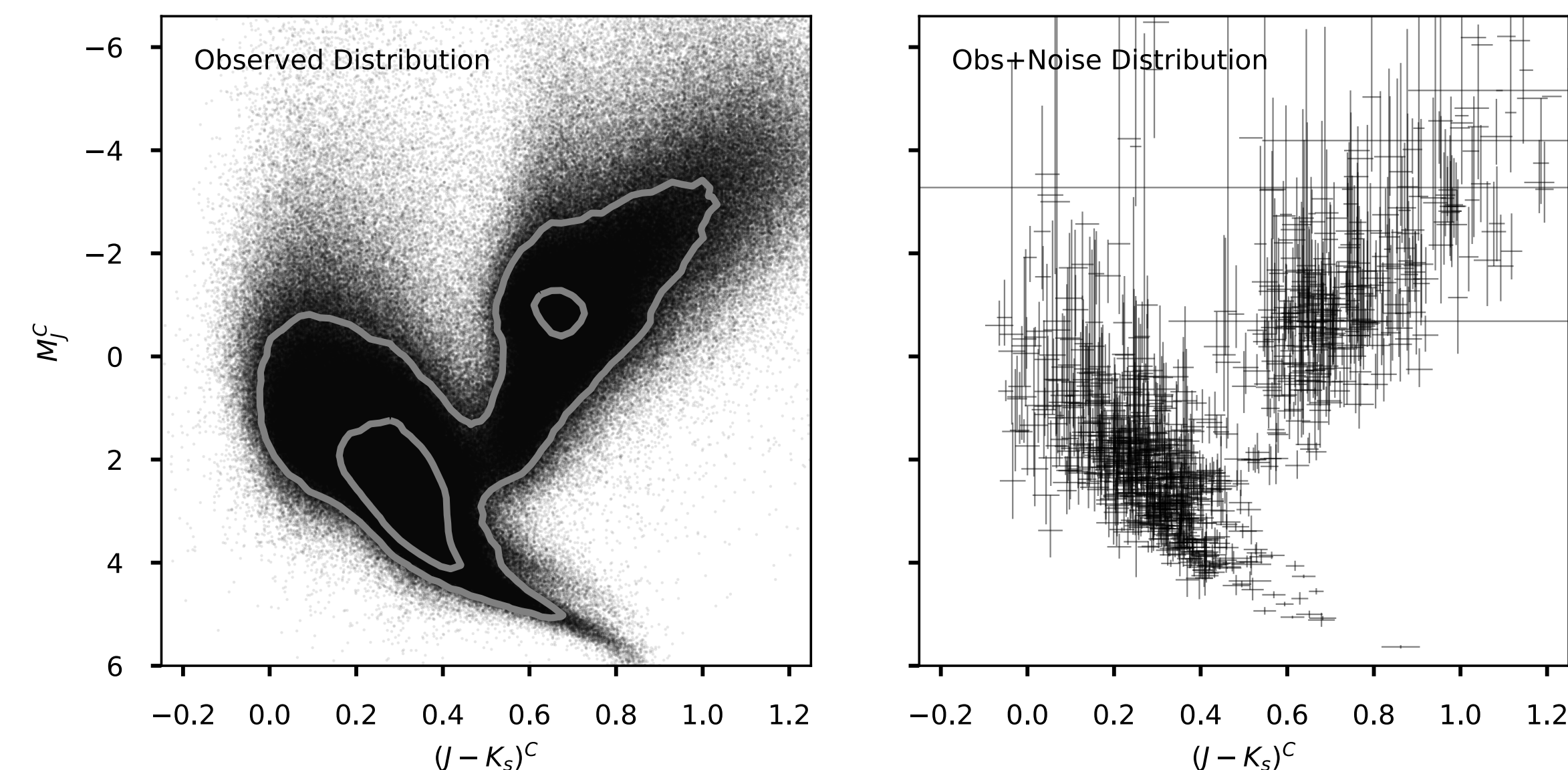


**Kounkel & Covey (2019)**

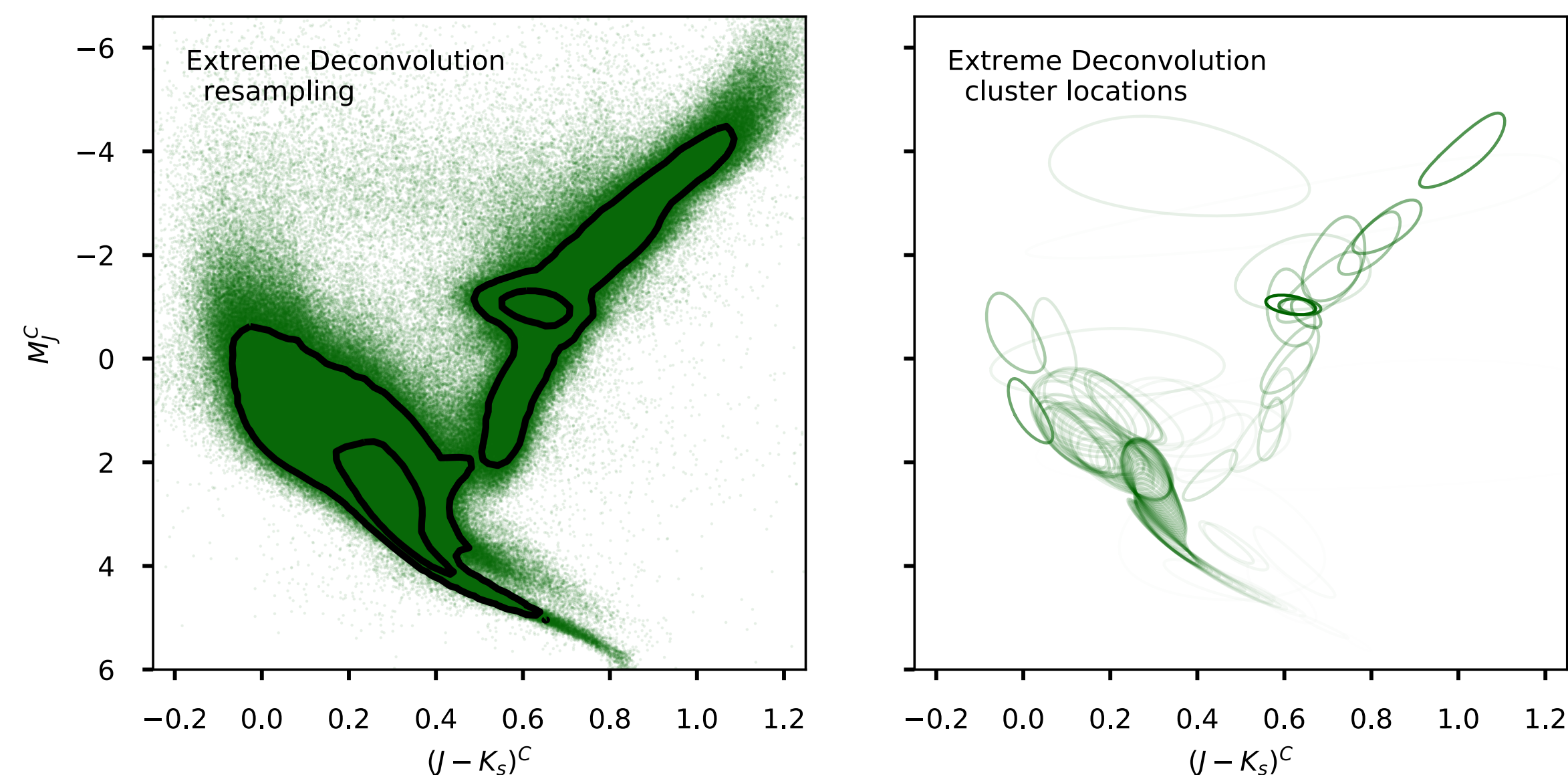


# Density estimation

## Color-magnitude diagram (CMD) of nearby stars in Gaia (DR1) data.



**Raw data**  
**... Blurred CMD due to distance error**



**Reconstructed CMD**  
**... Gaussian Mixture model**  
**after deconvolution of error**

**Anderson et al. (2017)**  
**[see also Leistedt et al. 2017]**

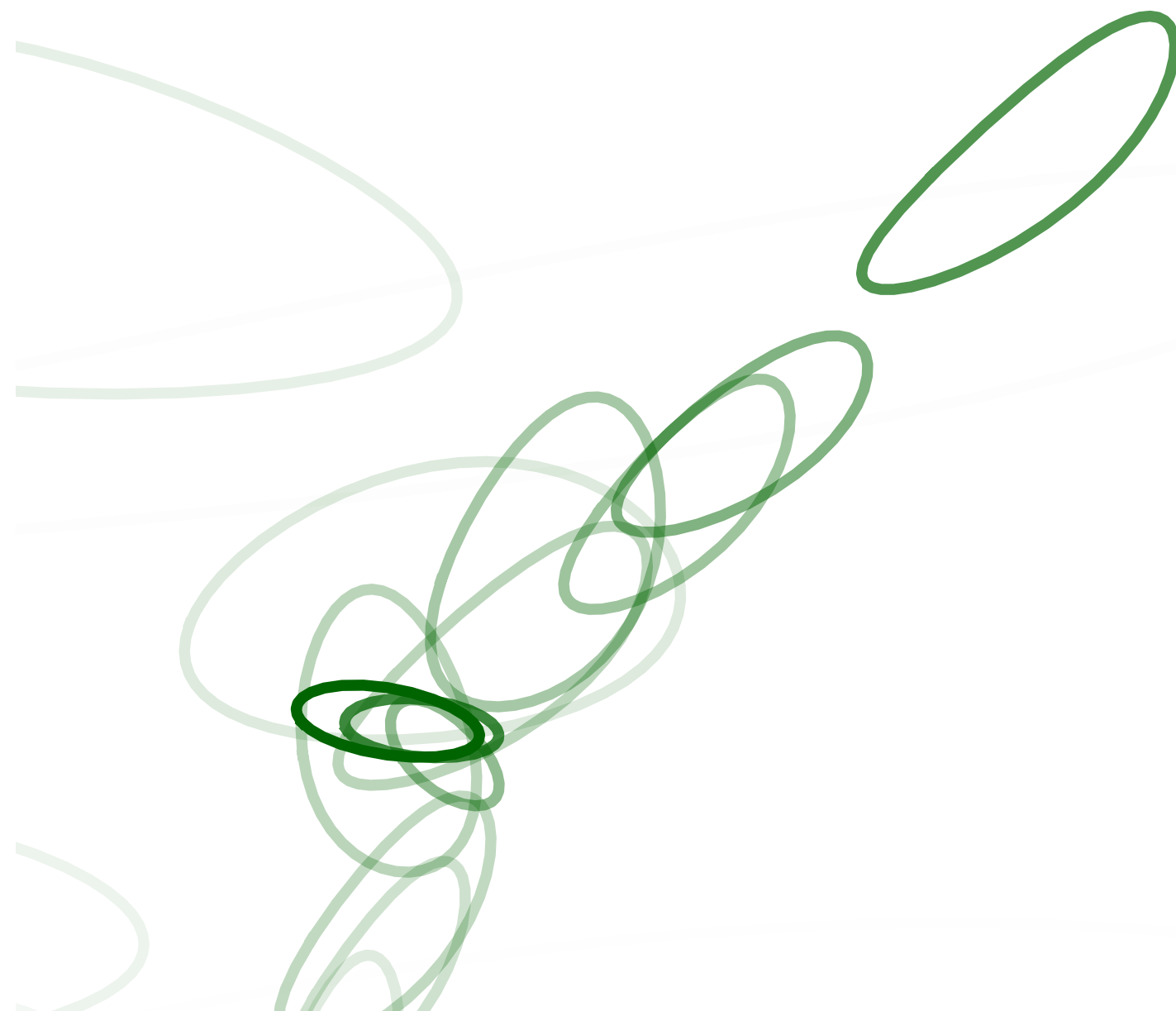


## Trends in machine learning

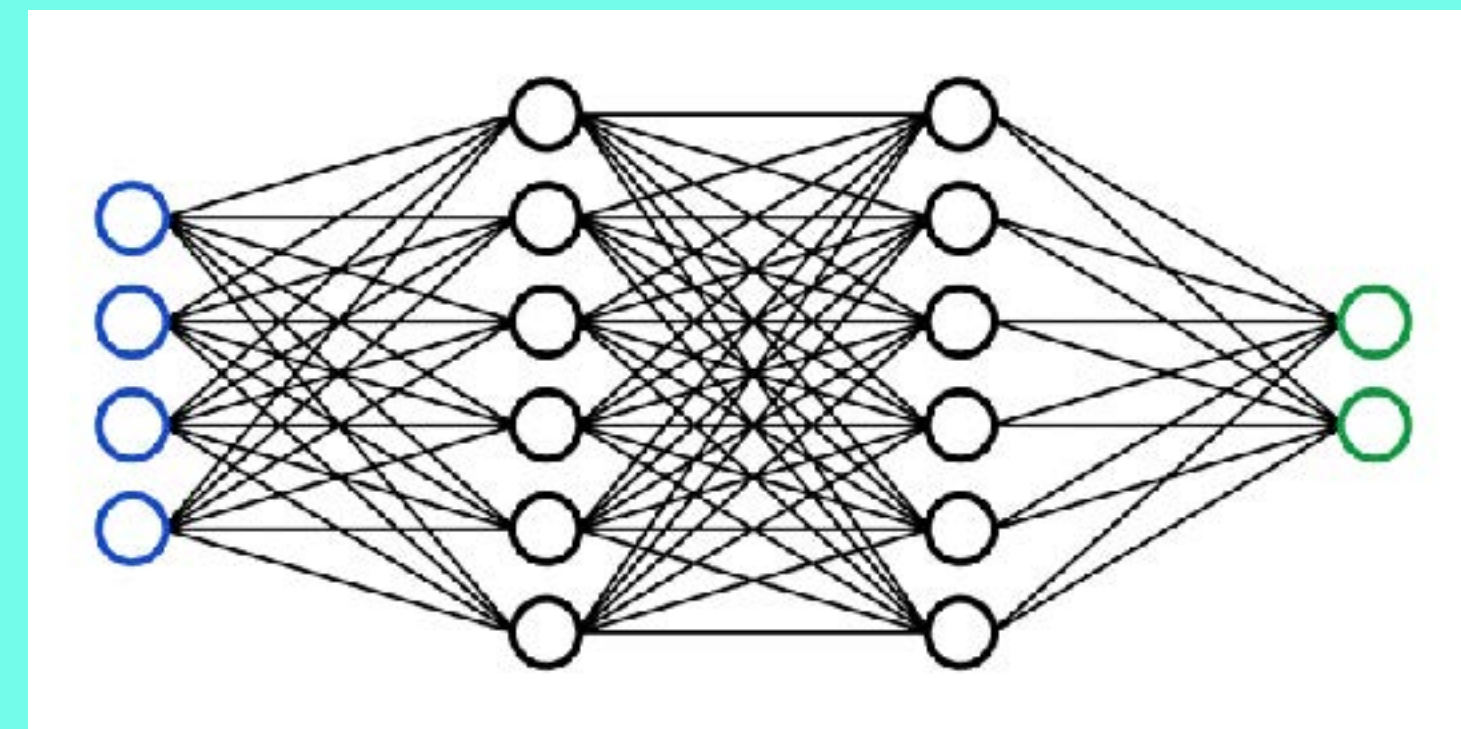
- (1) Era of big data
- (2) Dimensionality reduction
- (3) Sparsity
- (4) Bayesian analysis
- (5) Machine learning
- **(6) Neural network**
- (7) Data challenge

# Machine learning

## Classical methods



## Neural network



**Artificial Neural Network**

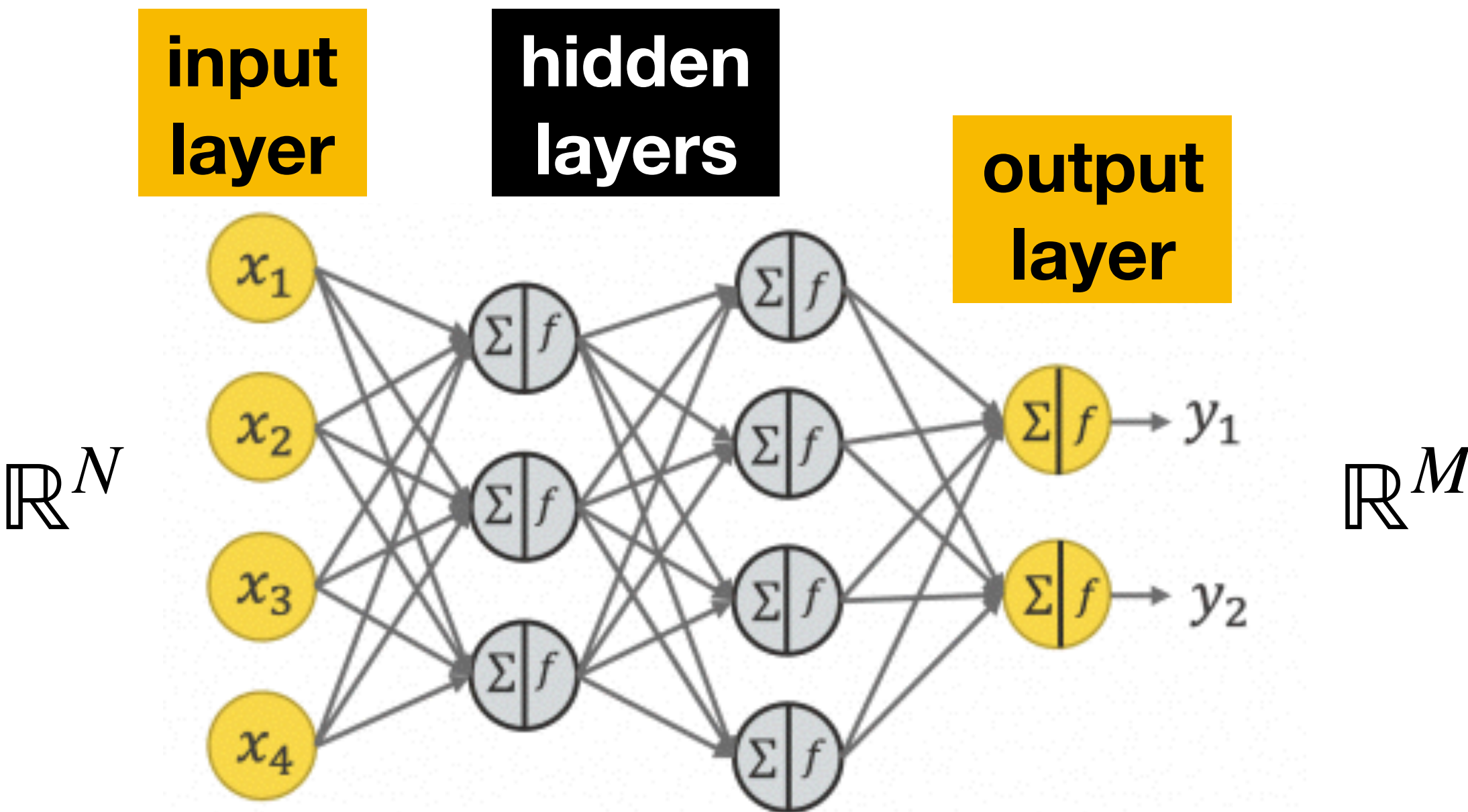
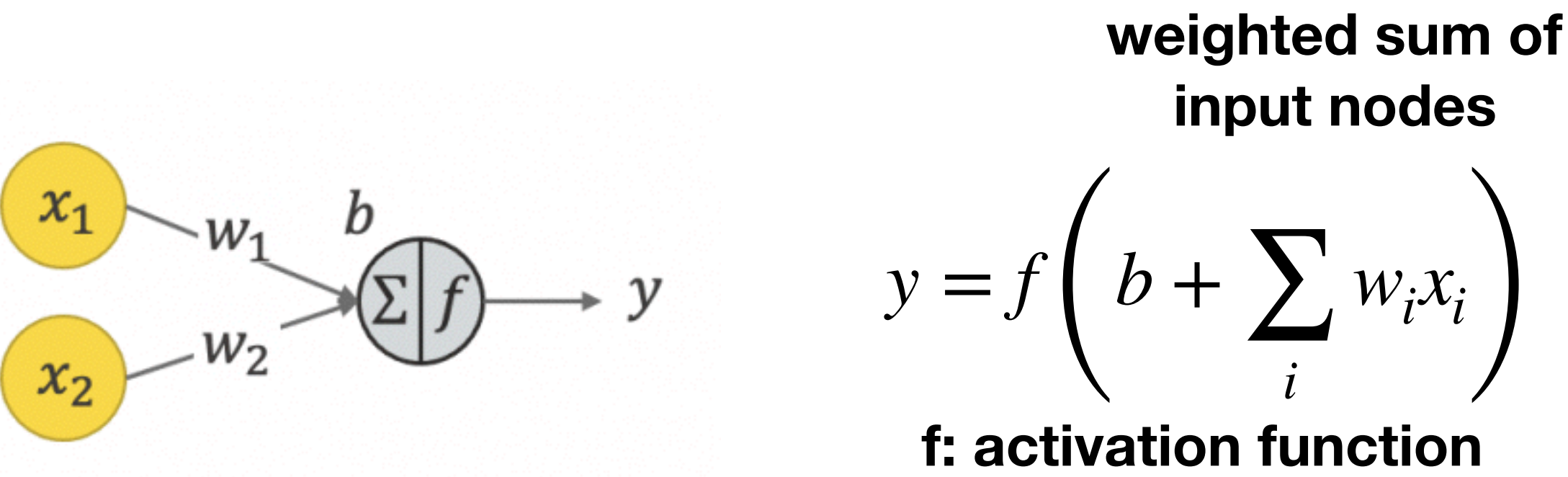
**Convolutional Neural Network**

**Auto-encoder**

**Generative Adversarial Network (GAN\*)**

\* Masato Shirasaki is an expert of GAN

# Neural network



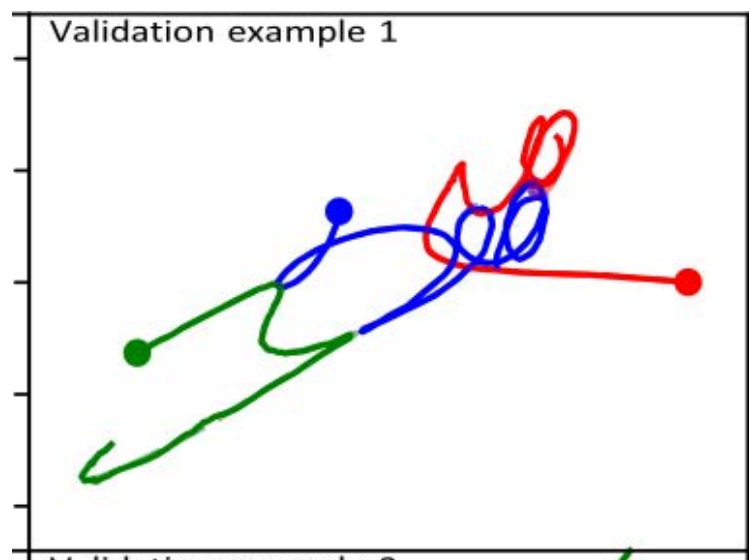
**hidden layers** =  $g : \mathbb{R}^N \rightarrow \mathbb{R}^M$

Many parameters (weights) allow large flexibility.  
We find the optimal weights by training.

If  $N > M$ , this can be seen as a **dimensionality reduction**.



# Model generation



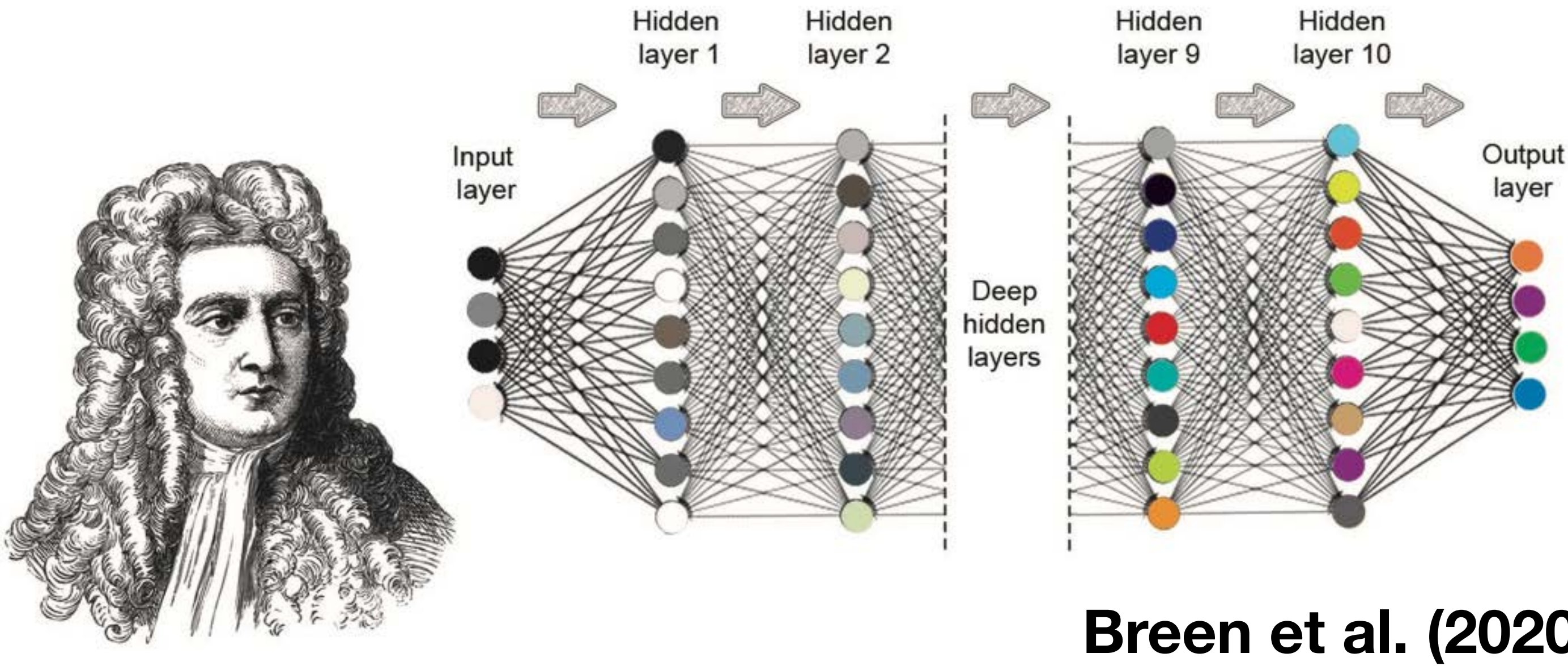
## 3-body problem in math.

$$\begin{bmatrix} x_1(T) \\ x_2(T) \\ x_3(T) \\ v_1(T) \\ v_2(T) \\ v_3(T) \end{bmatrix} = f \left( \begin{bmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \\ v_1(0) \\ v_2(0) \\ v_3(0) \\ T \end{bmatrix} \right)$$

Operator of  
“solving equation of motion”

# Newton vs the machine: solving the chaotic three-body problem using deep neural networks

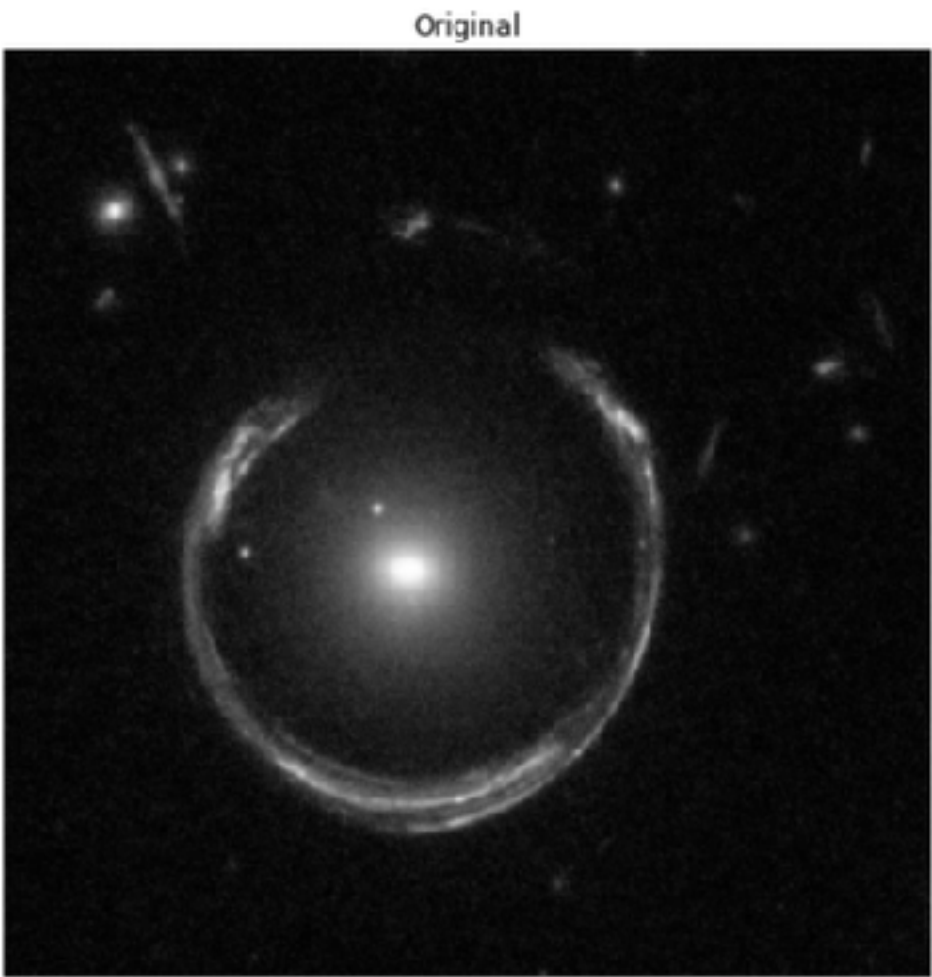
Philip G. Breen<sup>1</sup>★†, Christopher N. Foley<sup>2</sup> ★‡, Tjarda Boekholt<sup>3</sup>  
and Simon Portegies Zwart<sup>4</sup>



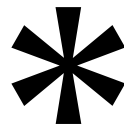
- (step 1) Solve 3-body problem with **various** initial conditions.
- (step 2) Train the NN.
- (step 3) NN solves 3-body problem with any initial condition **quickly**.

# CNN — Convolutional Neural Network

raw image



Convolution



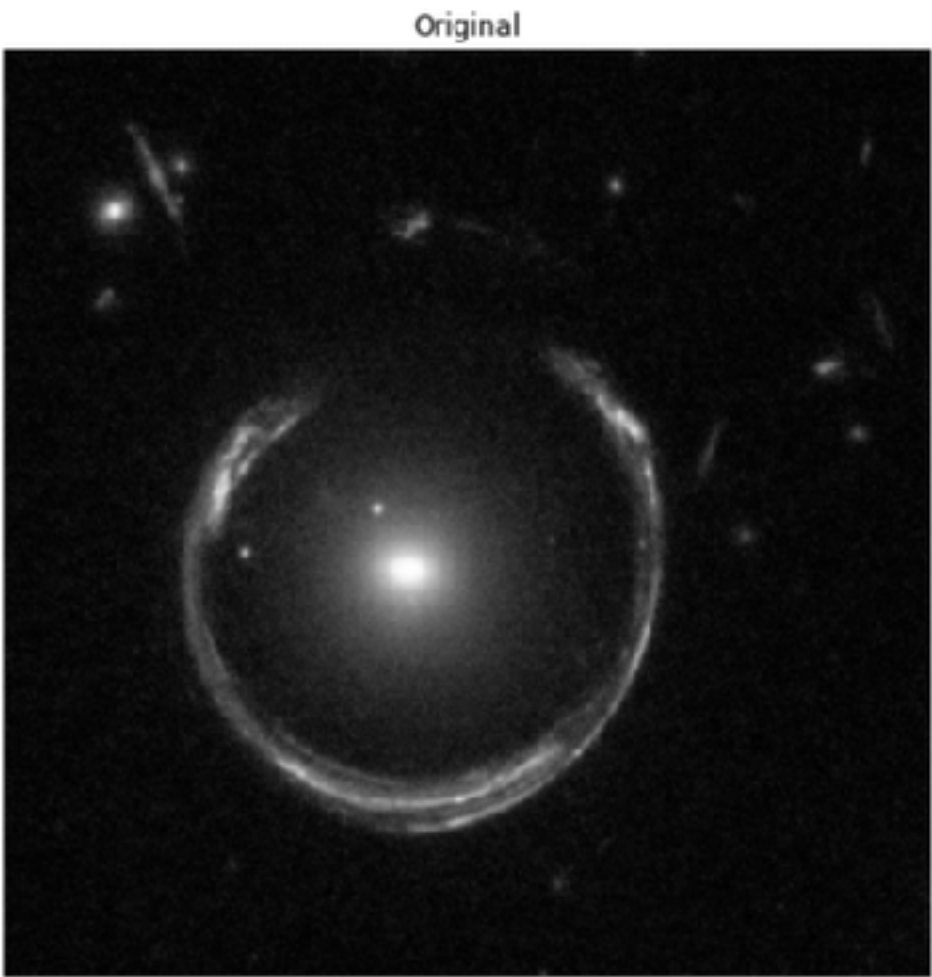
edge-detecting filter

-1	-1	-1	-1	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	-1	-1	-1	-1

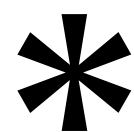


# CNN — Convolutional Neural Network

raw image

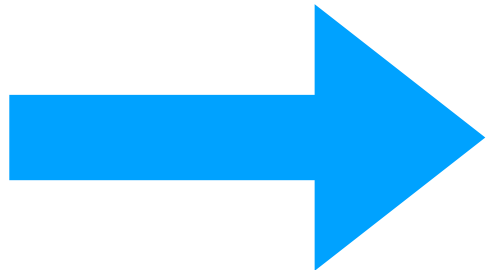


Convolution



edge-detecting filter

-1	-1	-1	-1	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	-1	-1	-1	-1



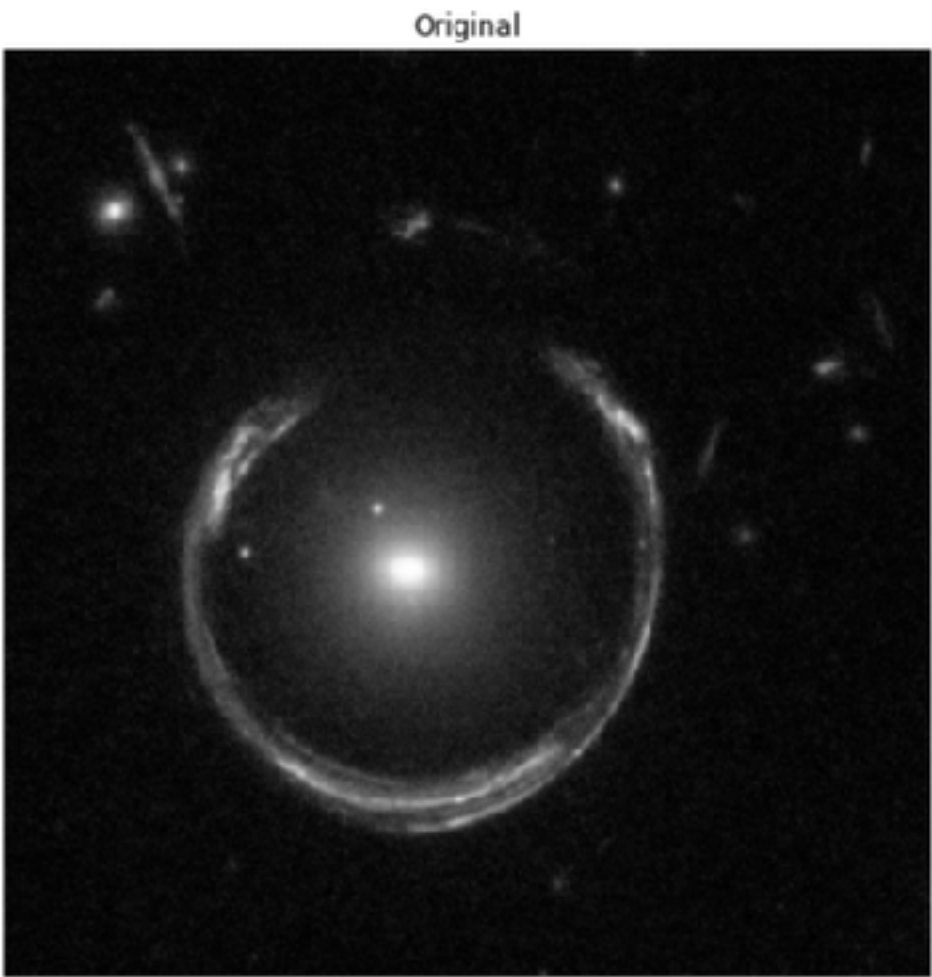
Smooth components disappear.



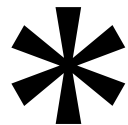


# CNN — Convolutional Neural Network

raw image

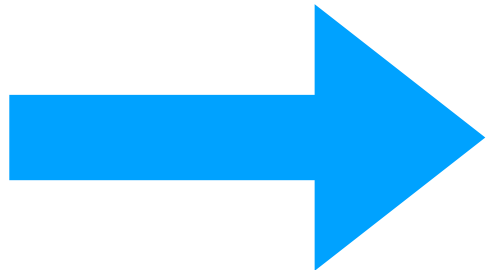


Convolution



edge-detecting filter

-1	-1	-1	-1	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	-1	-1	-1	-1



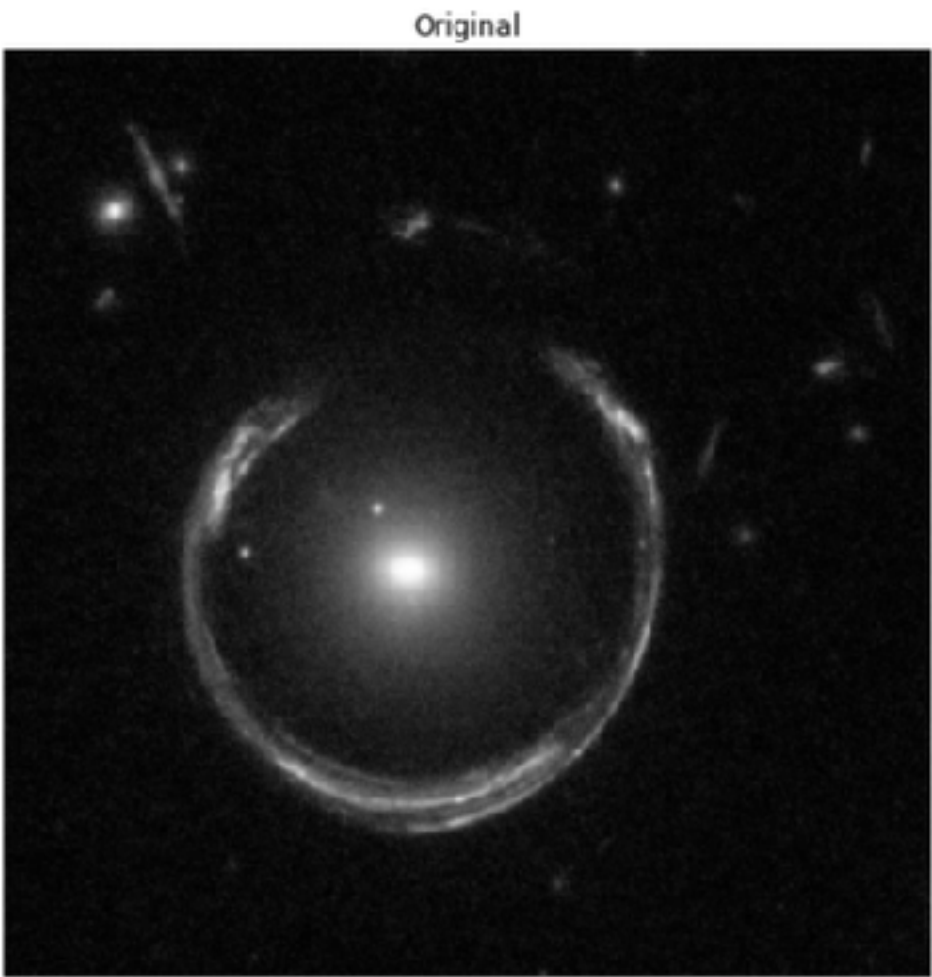
Smooth components disappear.



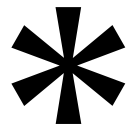
Convolutions extract the local pattern (e.g., “edge”) in the data.

# CNN — Convolutional Neural Network

raw image

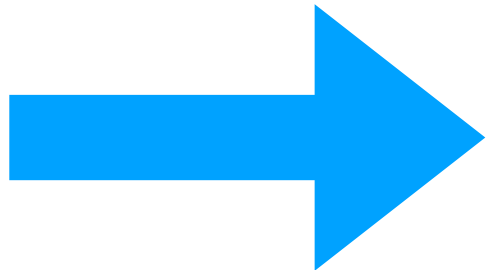


Convolution



edge-detecting filter

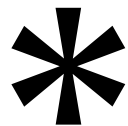
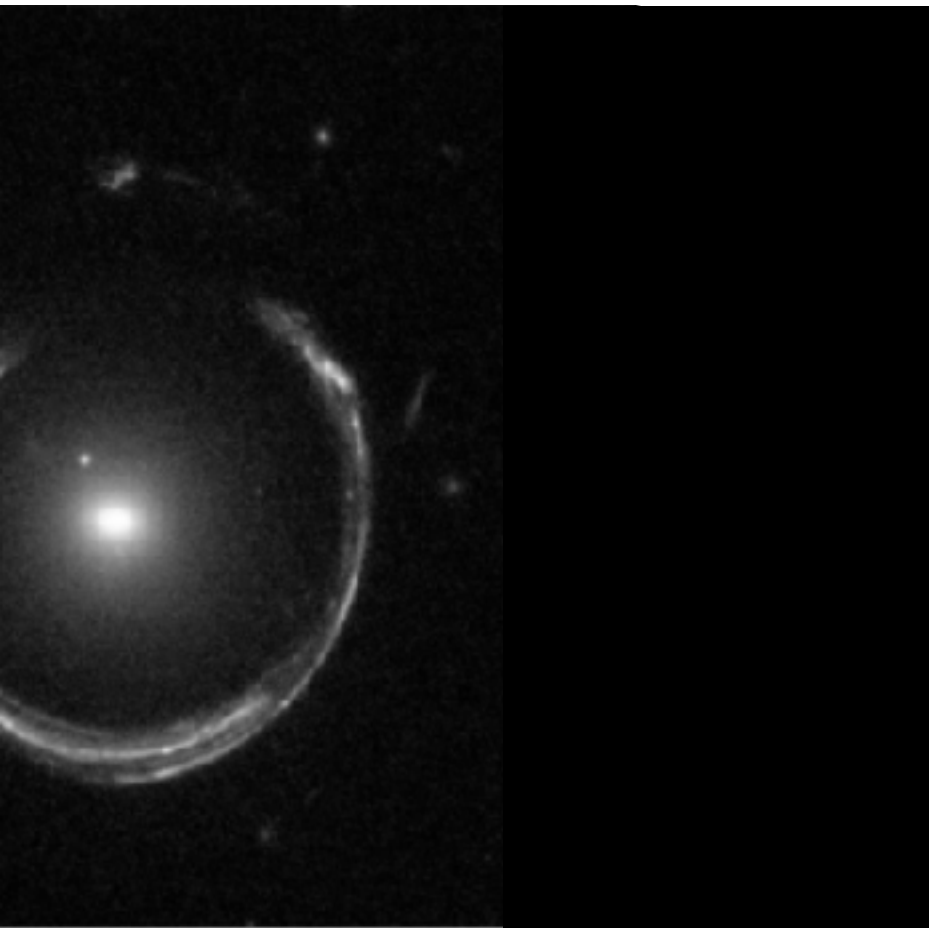
-1	-1	-1	-1	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	-1	-1	-1	-1



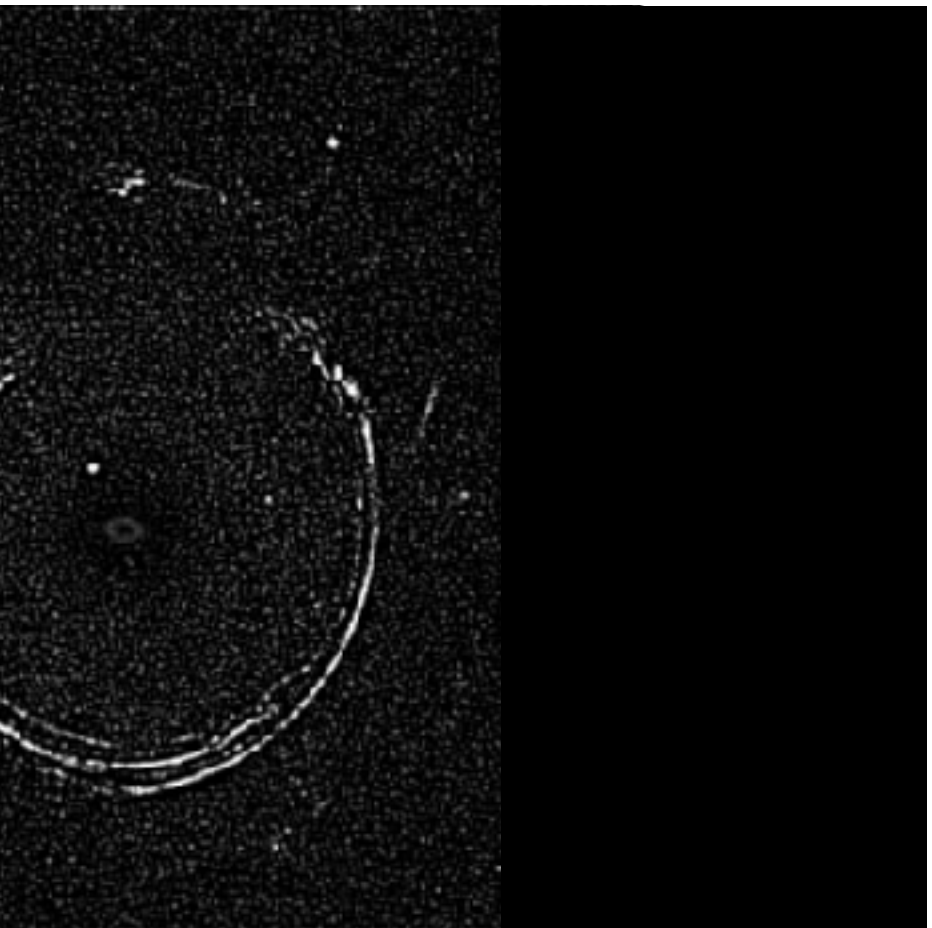
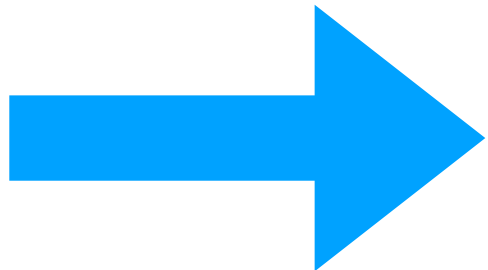
Smooth components disappear.



Convolutions extract the **local pattern** (e.g., “edge”) in the data.  
The extracted information is **translation invariant**.



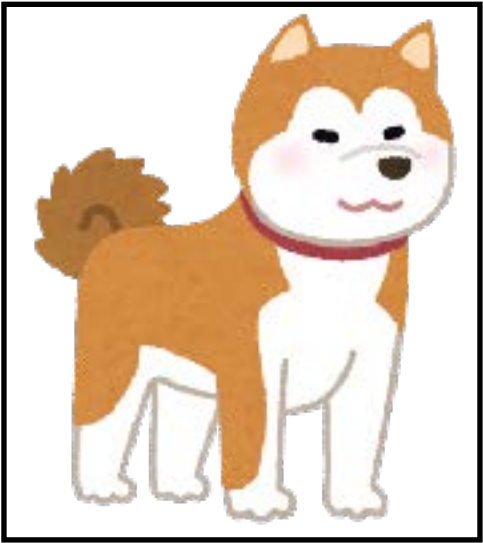
-1	-1	-1	-1	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	1.78	1.78	1.78	-1
-1	-1	-1	-1	-1





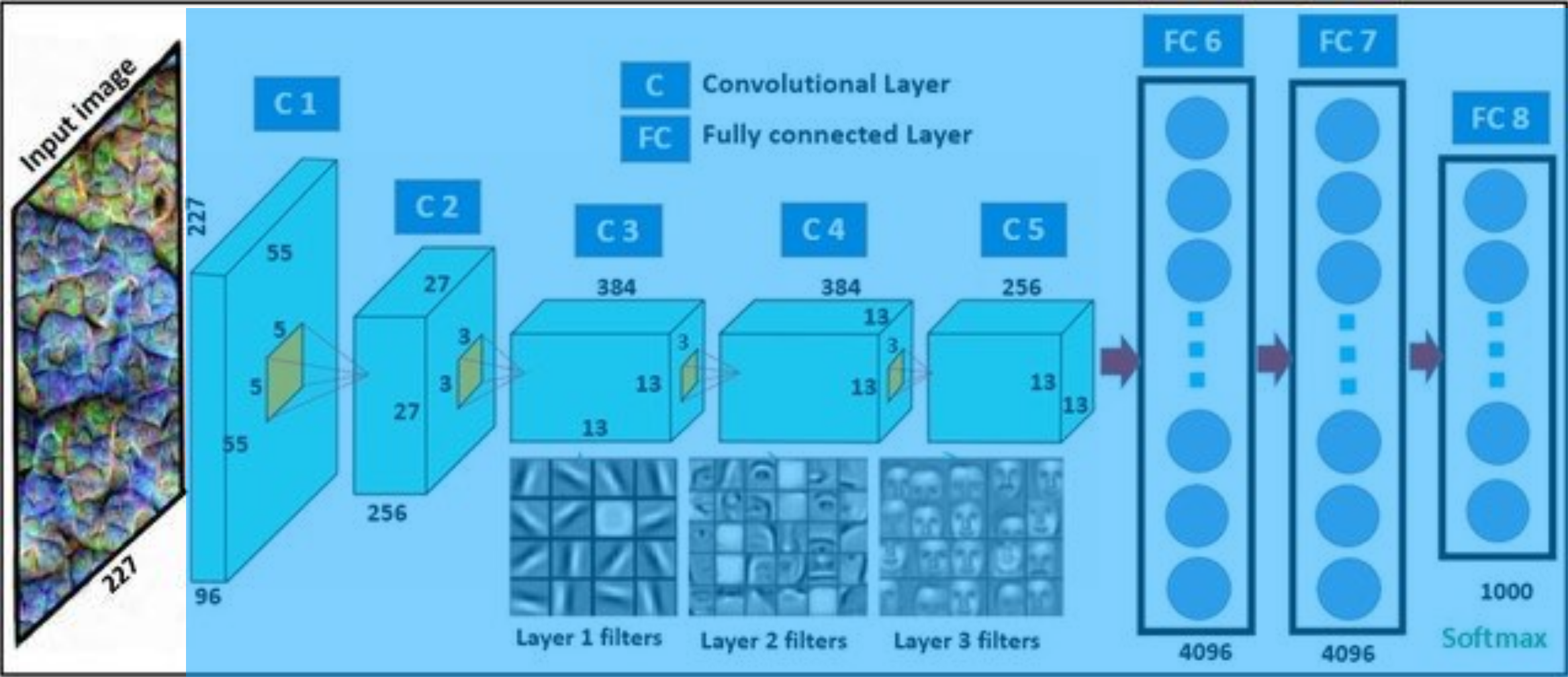
# CNN — Convolutional Neural Network

AlexNet 2012  
Krizhevsky et. al. (2012)  
Hassan & Gousev (2019)



(c) いらすとや

input  
image



output  
array

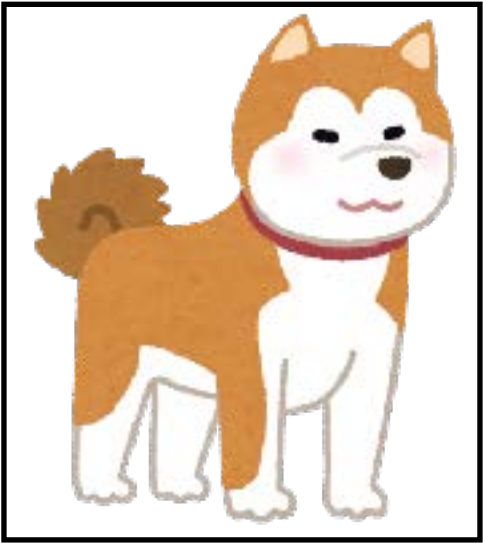
$$\begin{bmatrix} 0.01 \\ 0.00 \\ \vdots \\ 0.94 \\ 0.02 \end{bmatrix} \quad \text{P(dog)} = 0.94$$



# CNN — Convolutional Neural Network

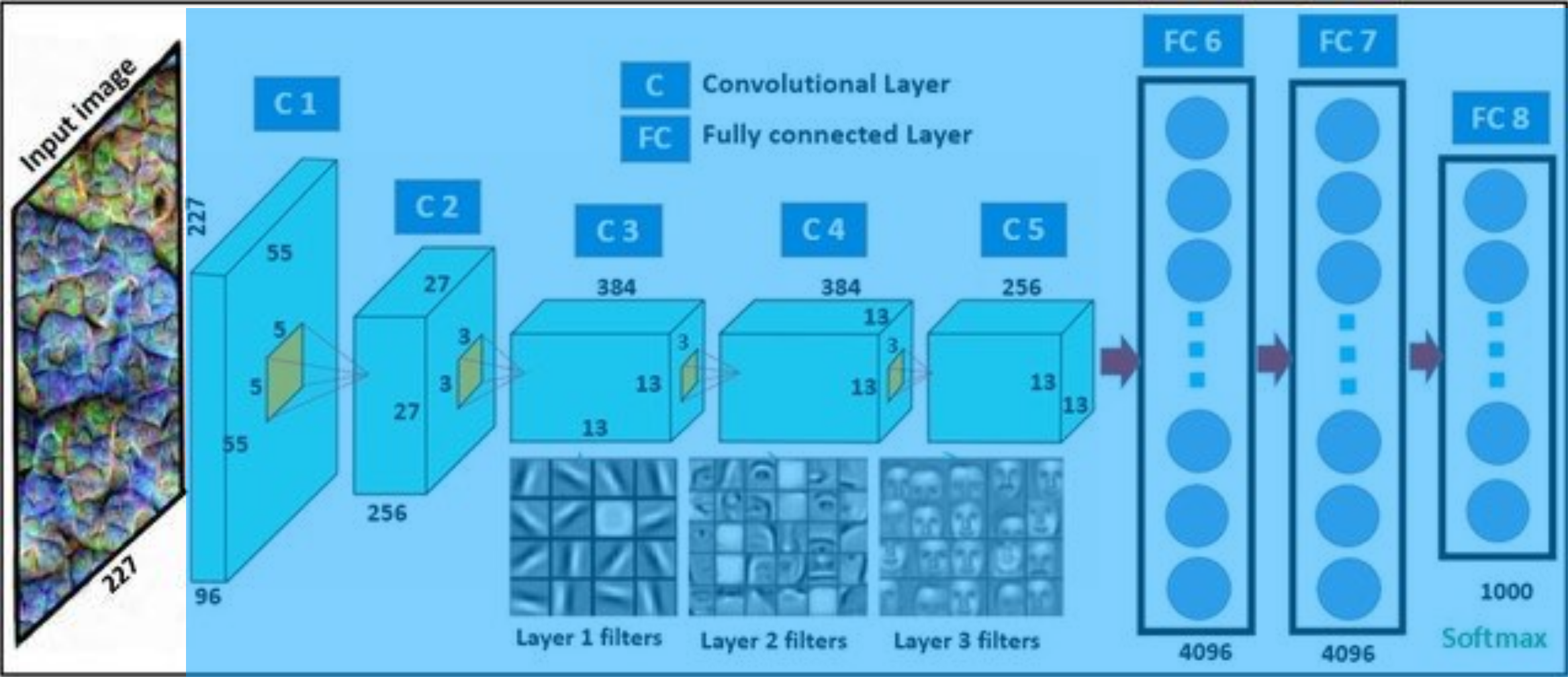
AlexNet 2012

Krizhevsky et. al. (2012)  
Hassan & Gousev (2019)



(c) いらすとや

input  
image



output  
array

$$\begin{bmatrix} 0.01 \\ 0.00 \\ \vdots \\ 0.94 \\ 0.02 \end{bmatrix} \quad \begin{matrix} P(\text{dog}) \\ = 0.94 \end{matrix}$$

Convolution = Extract “local patterns” that are translation invariant.  
Various filters are used = Various patterns are extracted.

-1	-1	-1
-1	8	-1
-1	-1	-1

-1	0	1
-1	0	1
-1	0	1

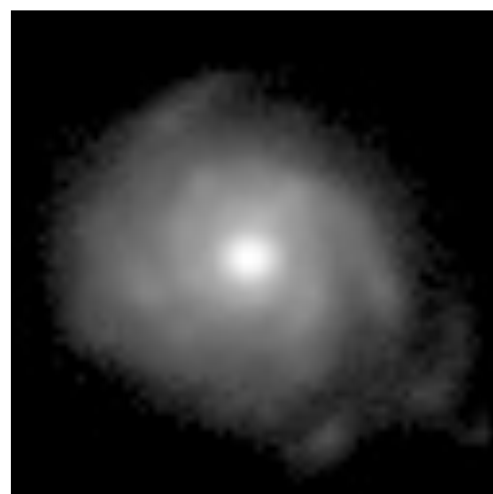
-1	-1	-1
0	0	0
1	1	1

(original work) input = 2D image ... (N x N x 3) array for RGB color image

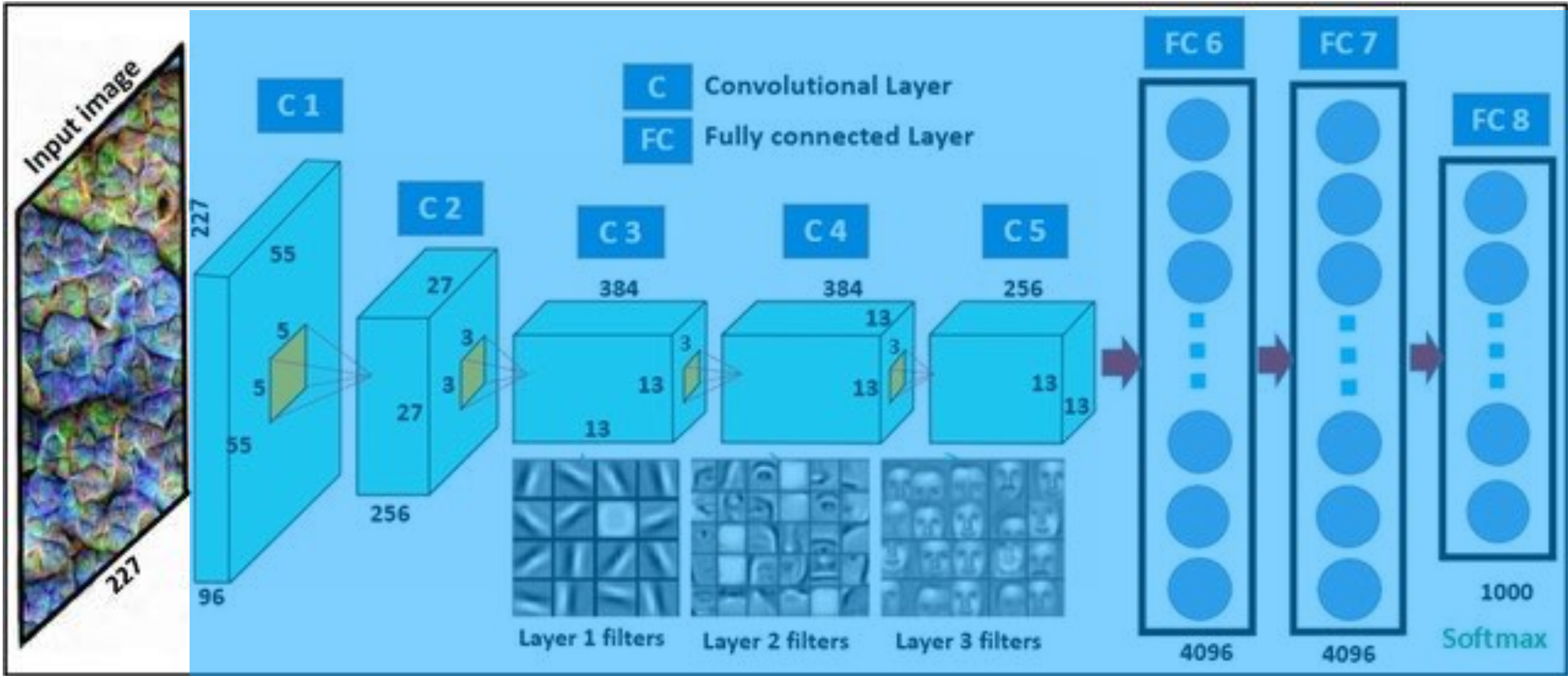
# CNN — Convolutional Neural Network

AlexNet 2012

Krizhevsky et. al. (2012)  
Hassan & Gousev (2019)



input  
image



output  
array

$$\begin{bmatrix} 0.01 \\ 0.00 \\ \vdots \\ 0.94 \\ 0.02 \end{bmatrix} \quad \text{P(spiral)} = 0.94$$

Convolution = Extract “local patterns” that are translation invariant.  
Various filters are used = Various patterns are extracted.

-1	-1	-1
-1	8	-1
-1	-1	-1

-1	0	1
-1	0	1
-1	0	1

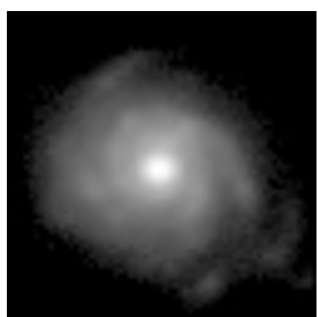
-1	-1	-1
0	0	0
1	1	1

- (original work) input = 2D image ... (N x N x 3) array for RGB color image
- (astro works) input = 2D image ... (N x N x 1) array for gray-scale image
- (astro works) input = 1D vector ... 1D spectra

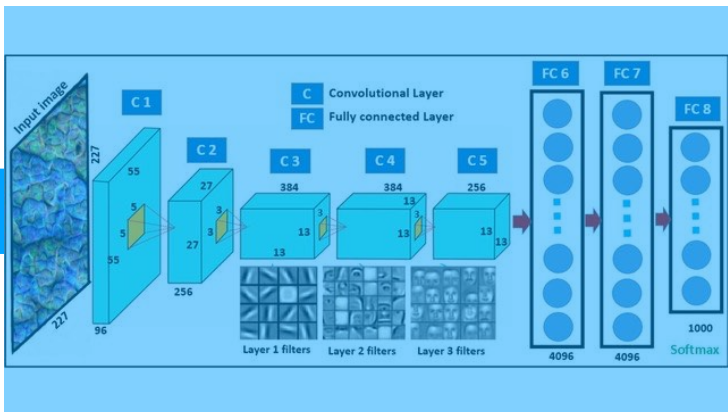


# CNN — Convolutional Neural Network

2D image (galaxy)



CNN

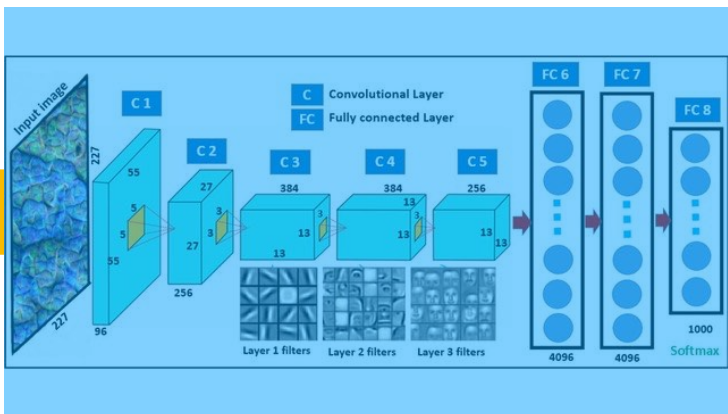
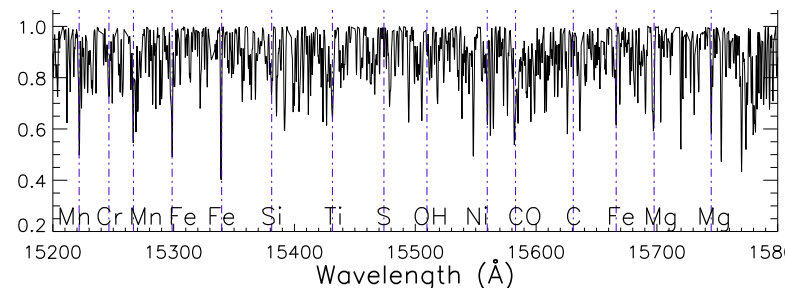


Tadaki et al. (2020)

classification

galaxy  
morphology

1D stellar spectrum (stellar physics)

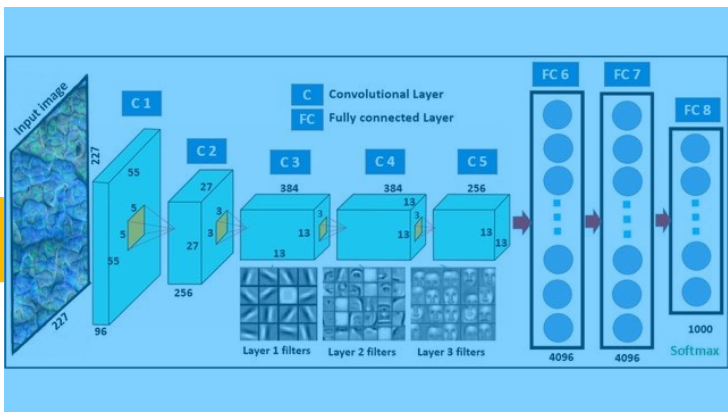
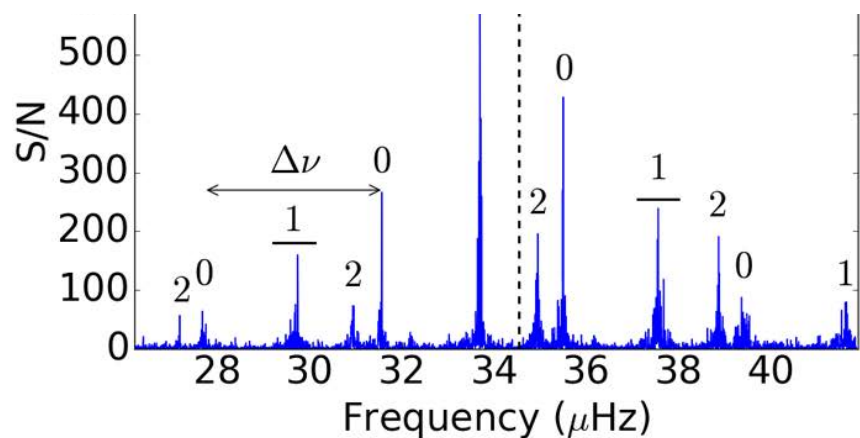


Leung & Bovy (2019)

inference

chemical  
abundances

1D power spectrum (asteroseismology)

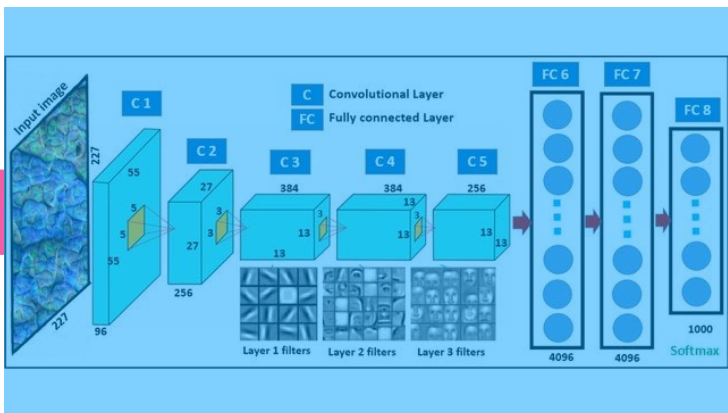
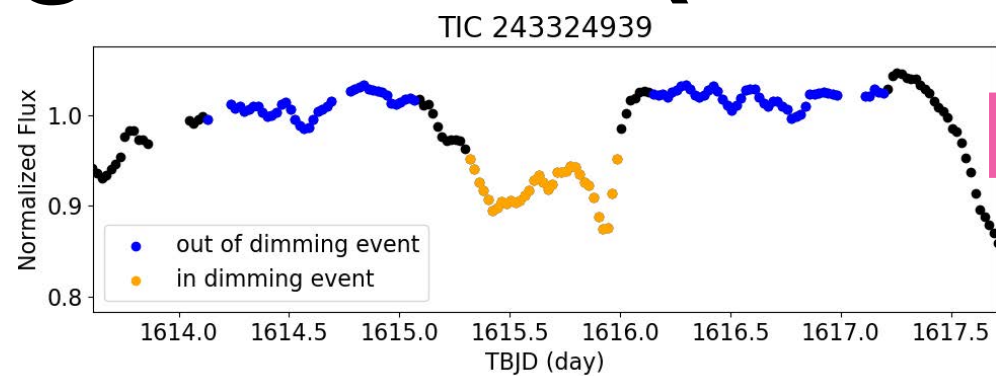


Hon et al. (2017)

inference

stellar  
parameters

1D light curve (dimming stars)



Tajiri et al. (2020)

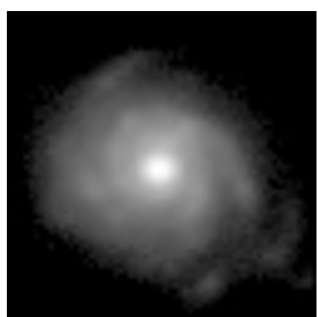
identification

Find a specific  
type of stars

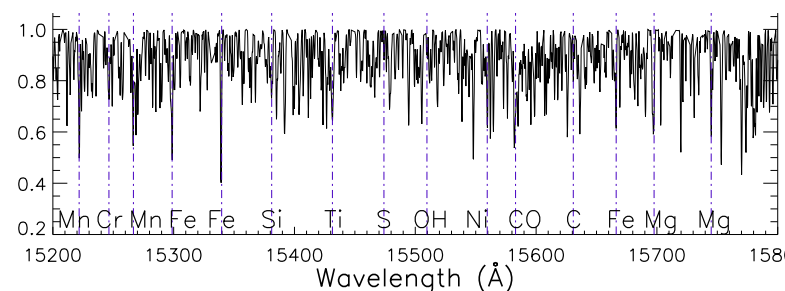


# CNN — Convolutional Neural Network

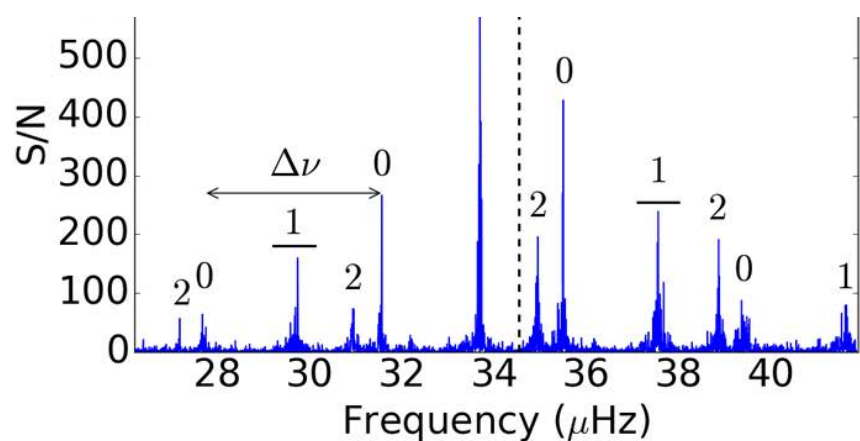
2D image (galaxy)



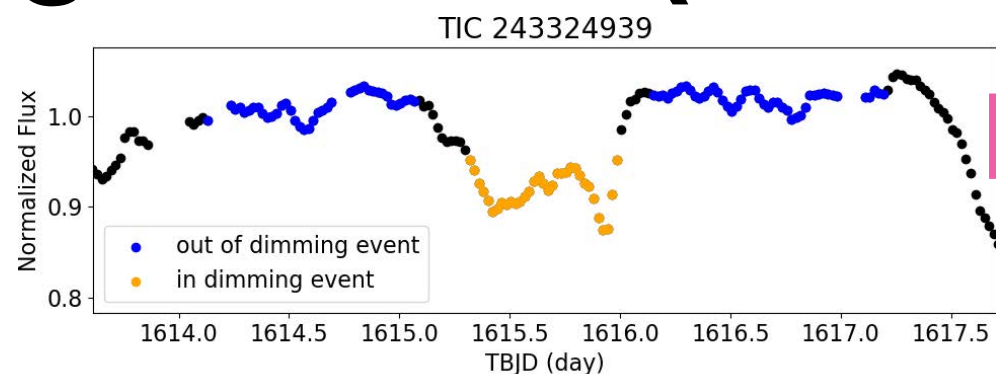
1D stellar spectrum (stellar physics)



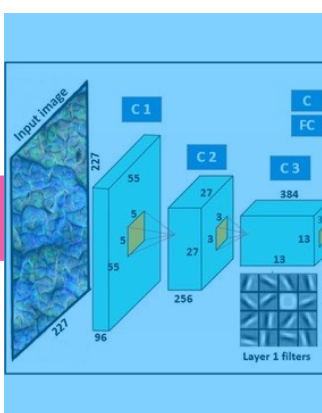
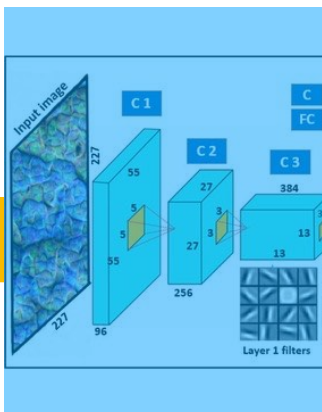
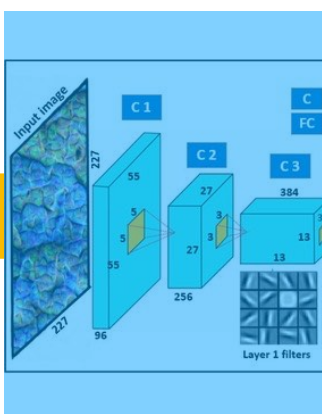
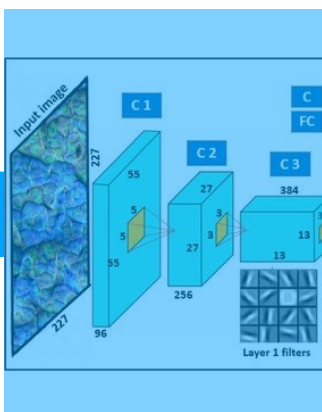
1D power spectrum (asteroseismology)



1D light curve (dimming stars)



CNN



Why CNN works for various data?  
— “**Translational invariance**”

2D image: Freedom to choose the origin

1D stellar spectrum: Doppler shift

1D power spectrum:  $\Delta\nu$

1D light curve: Freedom to choose the origin

CNN is suited for natural science.

— Reason for  
“**Inflation of ML universe**”

# Some concerns about neural network

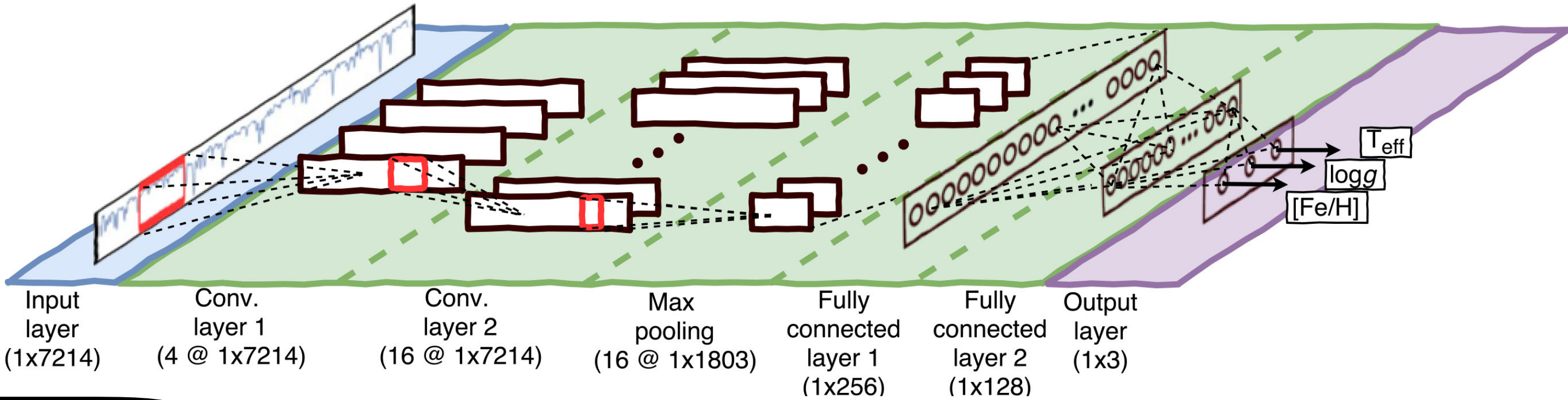
NN is sometimes described as a “black box.”

- **Bias in the test data**
- **Interpretability of NN — “Explainable AI” (XAI)**
- **Uncertainty quantification — Bayesian NN**
- **High degrees of freedom — No unique solution.**

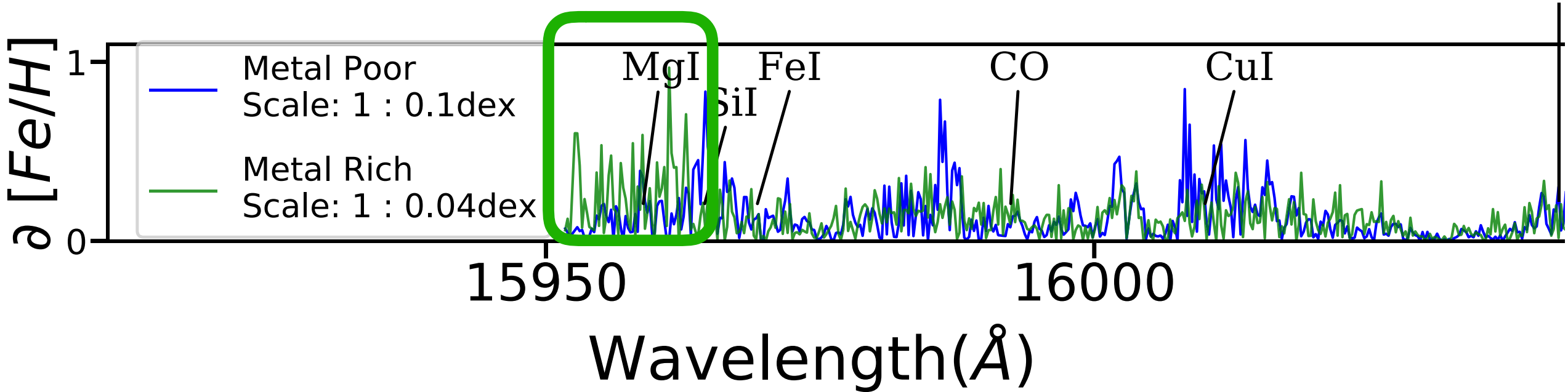


# Bias in the test data

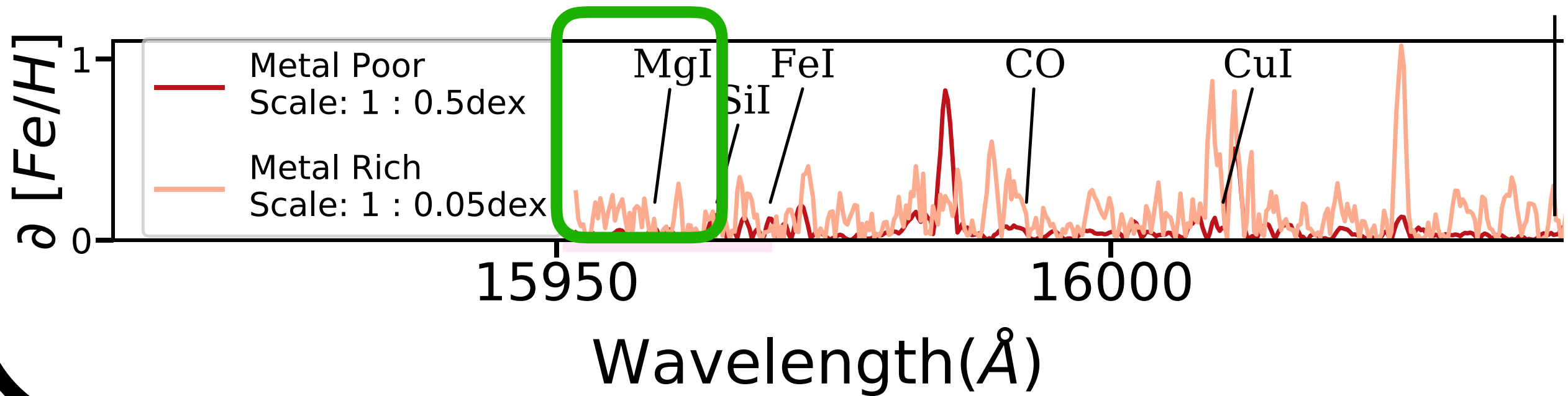
**Example** Fabbro et al. (2018)



(1) Train a NN to learn the relationship between  $[\text{X}/\text{H}]$  and spectra using **APOGEE spectra**



(2) Train the same NN to learn the relationship between  $[\text{X}/\text{H}]$  and spectra using **synthetic spectra**



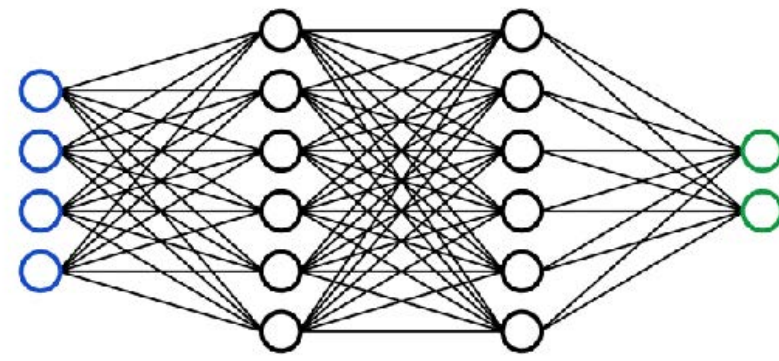
## Result:

NNs prioritize different lines to infer  $[\text{X}/\text{H}]$ , because **synthetic spectra**  $\neq$  **APOGEE**

**A bias in test data will affect performance.**

When designing stellar spectra pipeline, this bias should be kept in mind.

# Interpretability of NN



## A **funny** example

Train NN to learn the relationship between chemistry ( $[\text{Fe}/\text{H}]$ ) and observation data using

- (1) **observation fits file (spectra, date, observer's name etc..)**
- (2)  $[\text{X}/\text{H}]$  from another catalog

... Supervised learning.

**Result:**

**NN learned how to measure  $[\text{Fe}/\text{H}]$  from fits file.**

This result ***might*** be wrong!

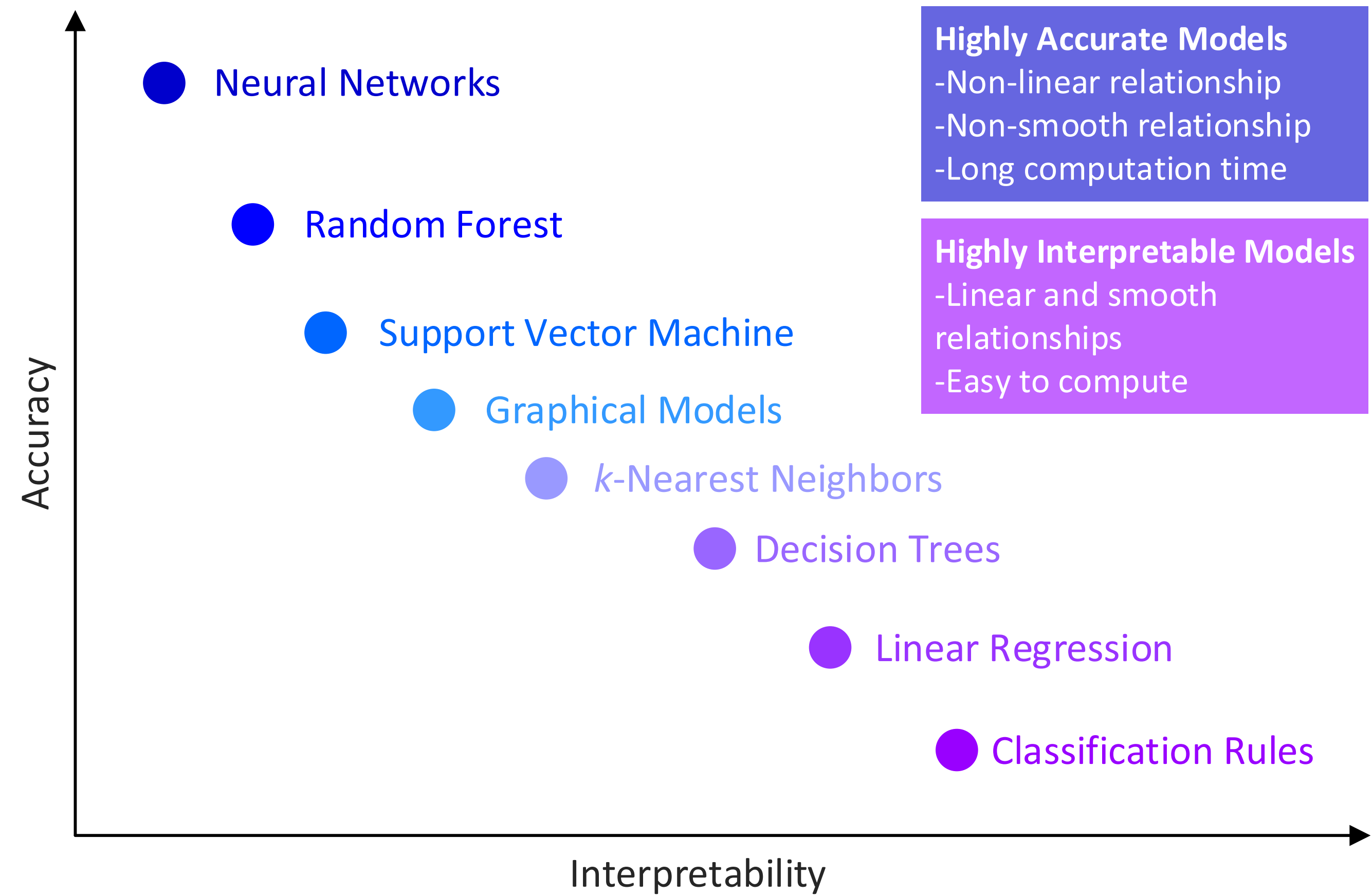
**NN might learn the correlation between **observer's name** and chemistry.)**  
(“Dr. AAA only observes low- $[\text{Fe}/\text{H}]$  stars,” etc.)

**Do not use NN as a black-box.**



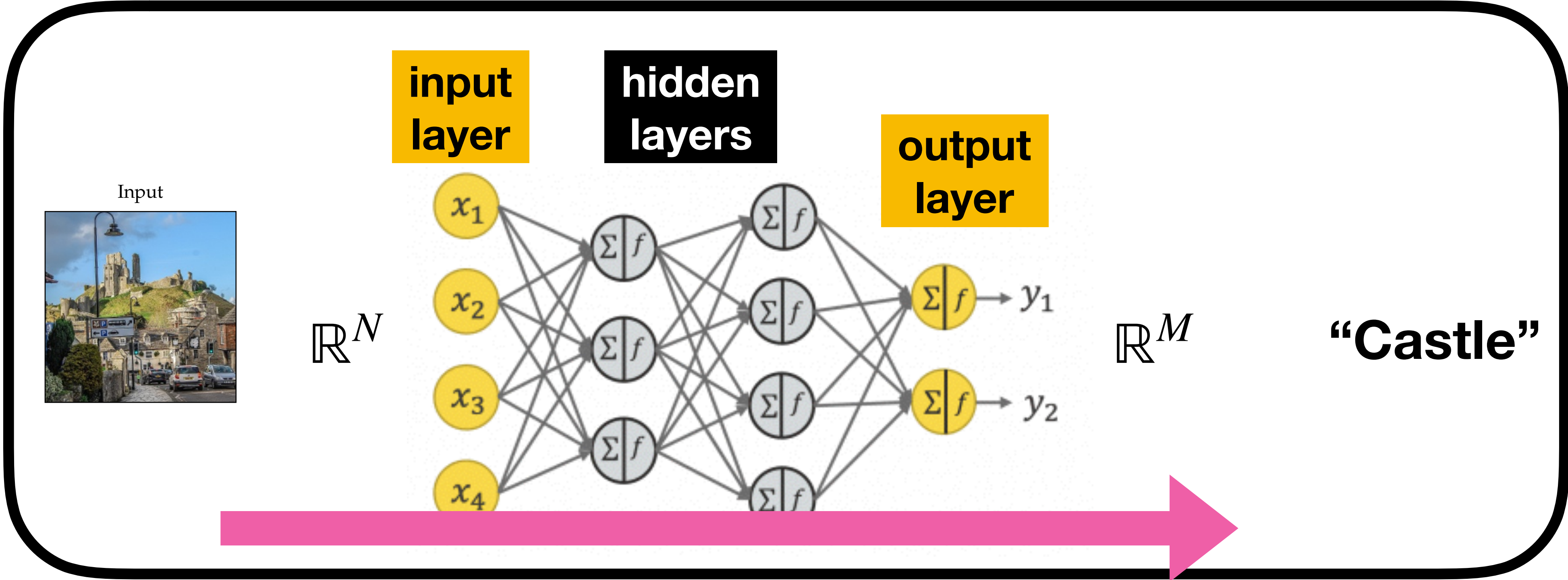
# Trade-off: interpretability vs accuracy

accuracy

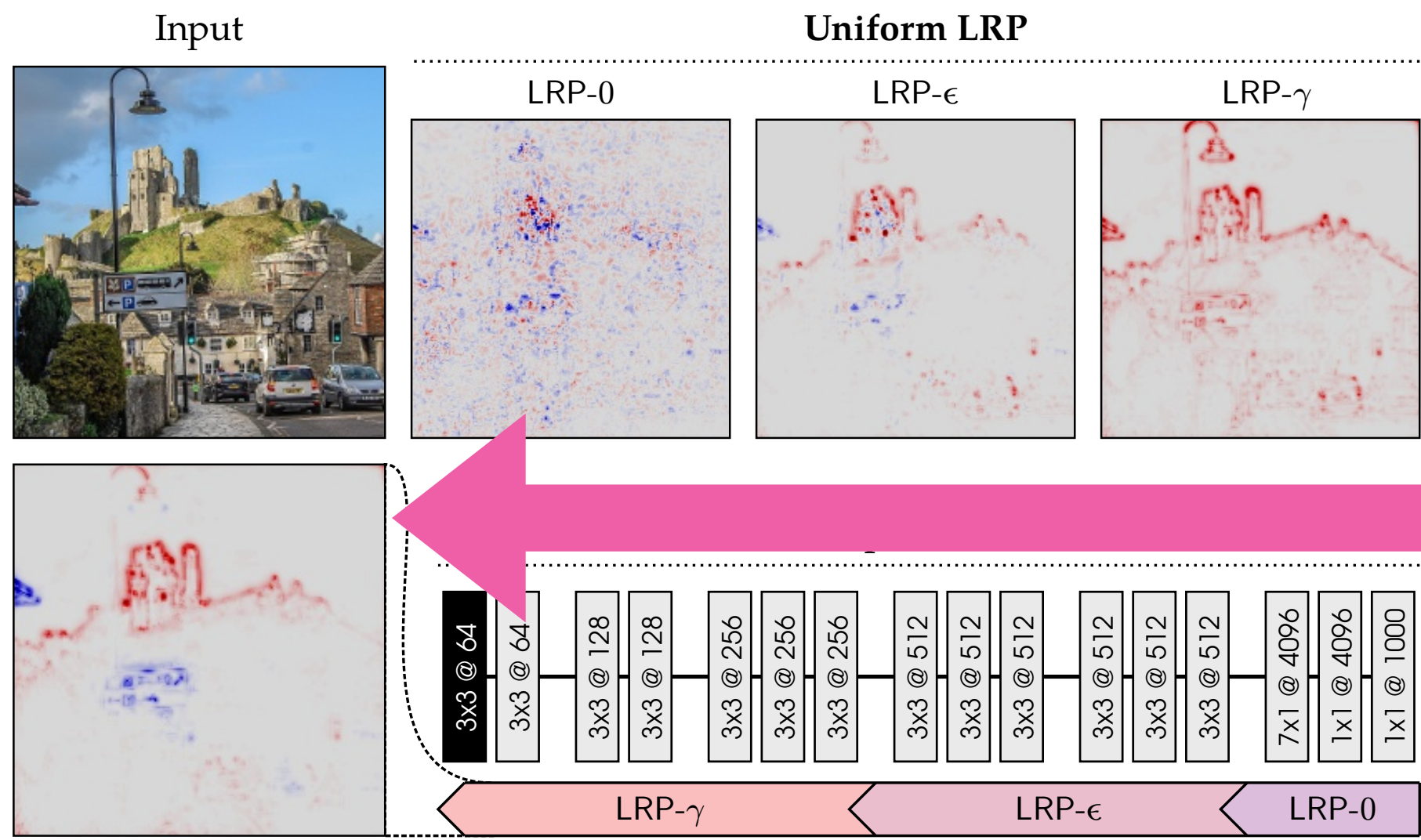


interpretability

# Toward explainable AI: Layer-wise Relevance Propagation



**“Red** part of the image was useful for classification”



**“Castle”**



- (1) Era of big data
- (2) Dimensionality reduction
- (3) Sparsity
- (4) Bayesian analysis
- (5) Machine learning
- (6) Deep learning

**Robustness / reliability  
of new methods**

- [ • (7) **Data challenge**

# Data Challenge (Test to validate methods)

- Photometric **LSST** Astronomical Time-Series Classification Challenge (<https://www.kaggle.com/c/PLAsTiCC-2018>)
- **Exoplanet: ARIEL** Mission Data Challenges (<https://www.ariel-datachallenge.space/ML/documentation/description>)
- **Radio astronomy: SKA** Data Challenge Competition #1 (<https://astronomers.skatelescope.org/ska-science-data-challenge-1/>)
- **Microlensing** Data Challenge (<https://microlensing-source.org/data-challenge/>)
- **Galaxy Zoo: galaxy morphology** classification challenge (<https://www.kaggle.com/c/galaxy-zoo-the-galaxy-challenge>)
- **Mapping dark matter** competition (<https://www.kaggle.com/c/mdm/overview>)
- **Strong lensing** data challenge (<https://bolognalensfactory.wordpress.com/home-2/blfkids-lens-finding-challenge/>)
- **Gaia challenge** (<http://astrowiki.ph.surrey.ac.uk/dokuwiki/doku.php>)



# Photometric LSST Astronomical Time-Series Classification Challenge

**Kaggle-based competition of classifying mock LSST data**  
with generous prize money :)

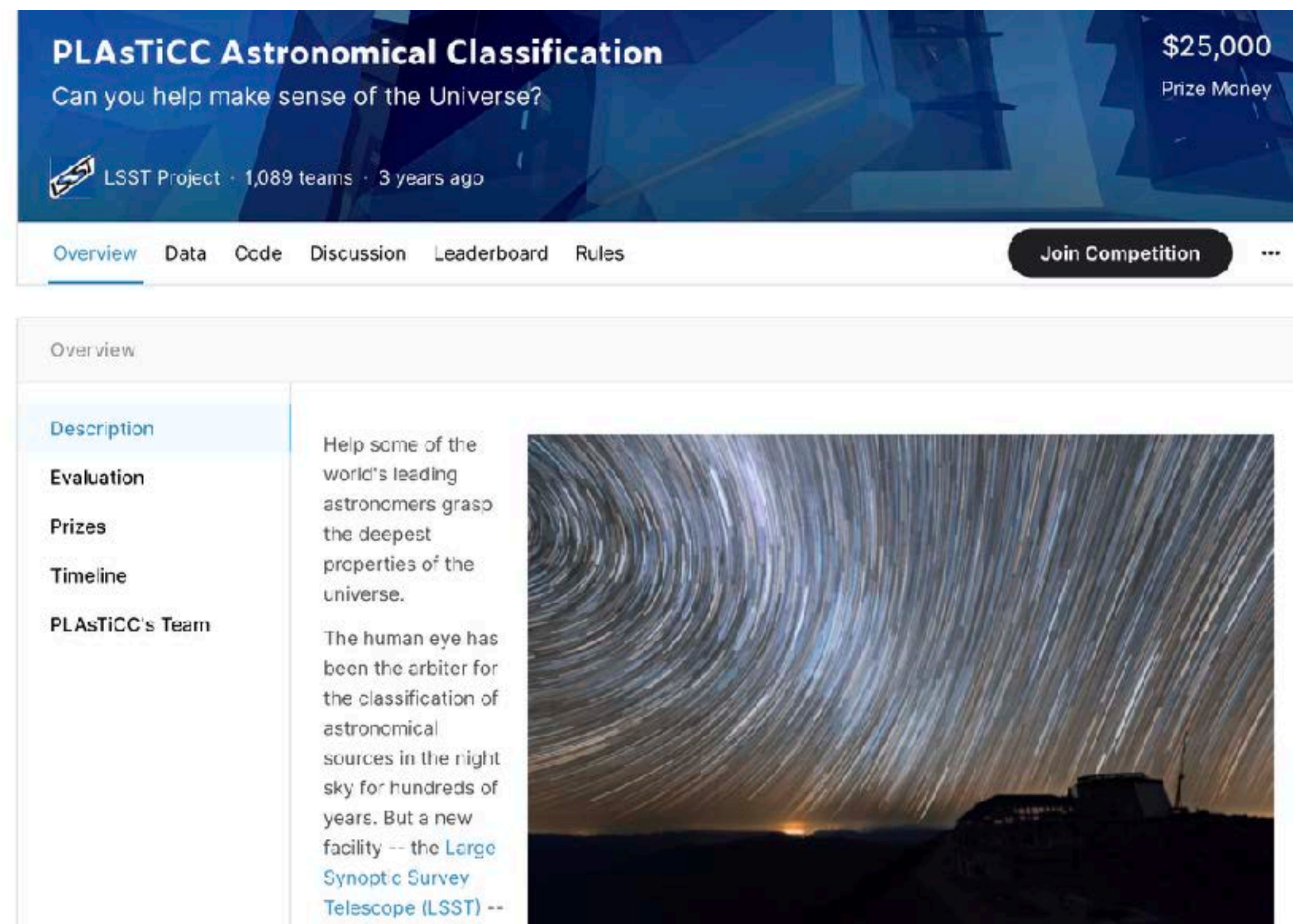
1st prize: Kyle Boone (Astro PhD student)  
2nd prize: Mike & Silogram (**Non-astro group**)  
3rd prize: Major Tom, mamas & nyanp (**Non-astro group**)

**Inflation of ML universe.**

**Is our community open to data scientists,  
given the need for ML talents?**

**Data challenges for**

- mock **ULTIMATE-Subaru** data?
- mock **JASMINE** data?
- mock [your favorite project] data?
- ... These will **galvanize young/enthusiastic members of astro/non-astro community!!**



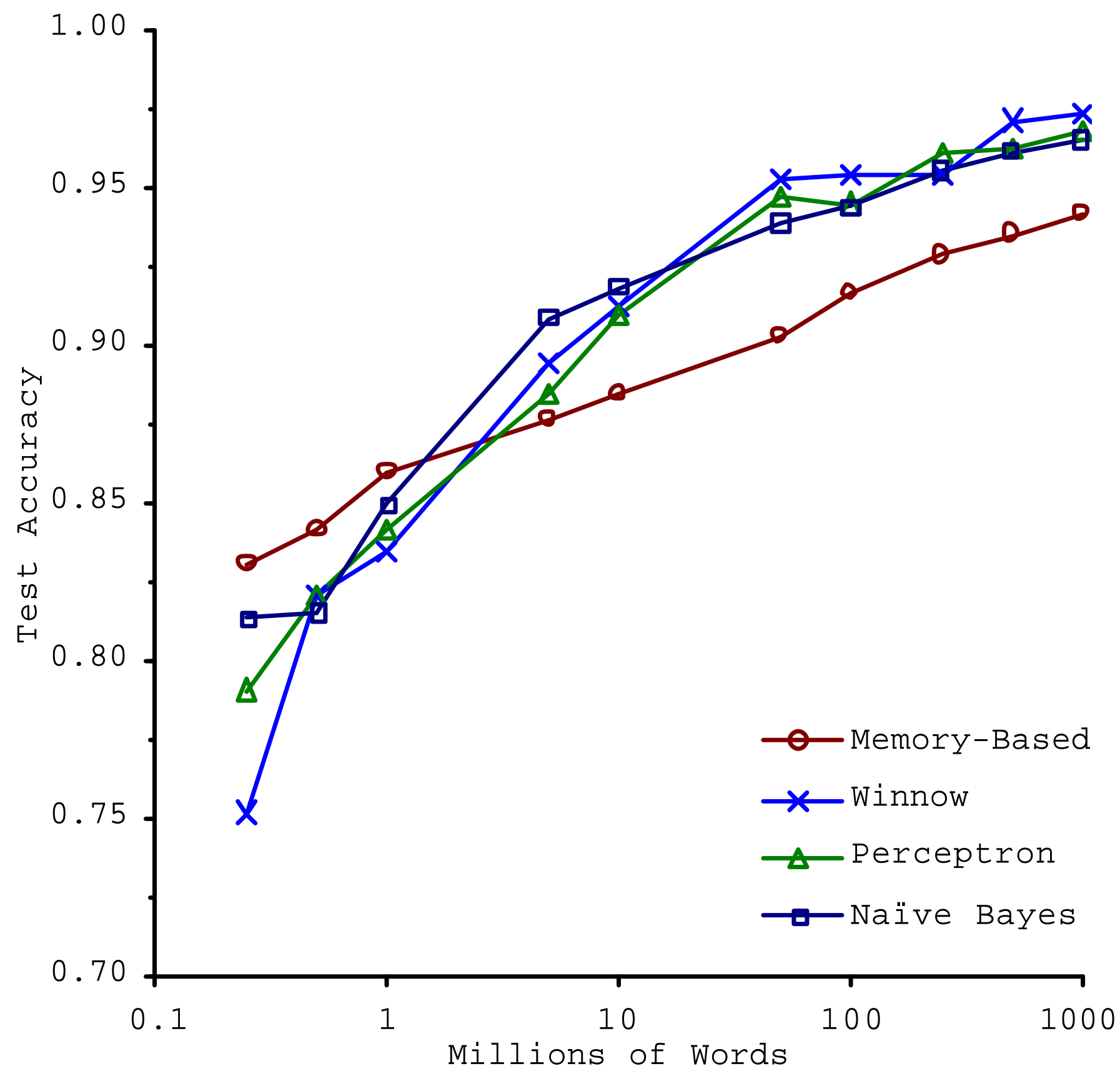


# Concluding remarks: Era of Big Data

## Natural language tasks

[自然言語処理=機械英文チェックのテスト]

Score  
(Accuracy)



Data size

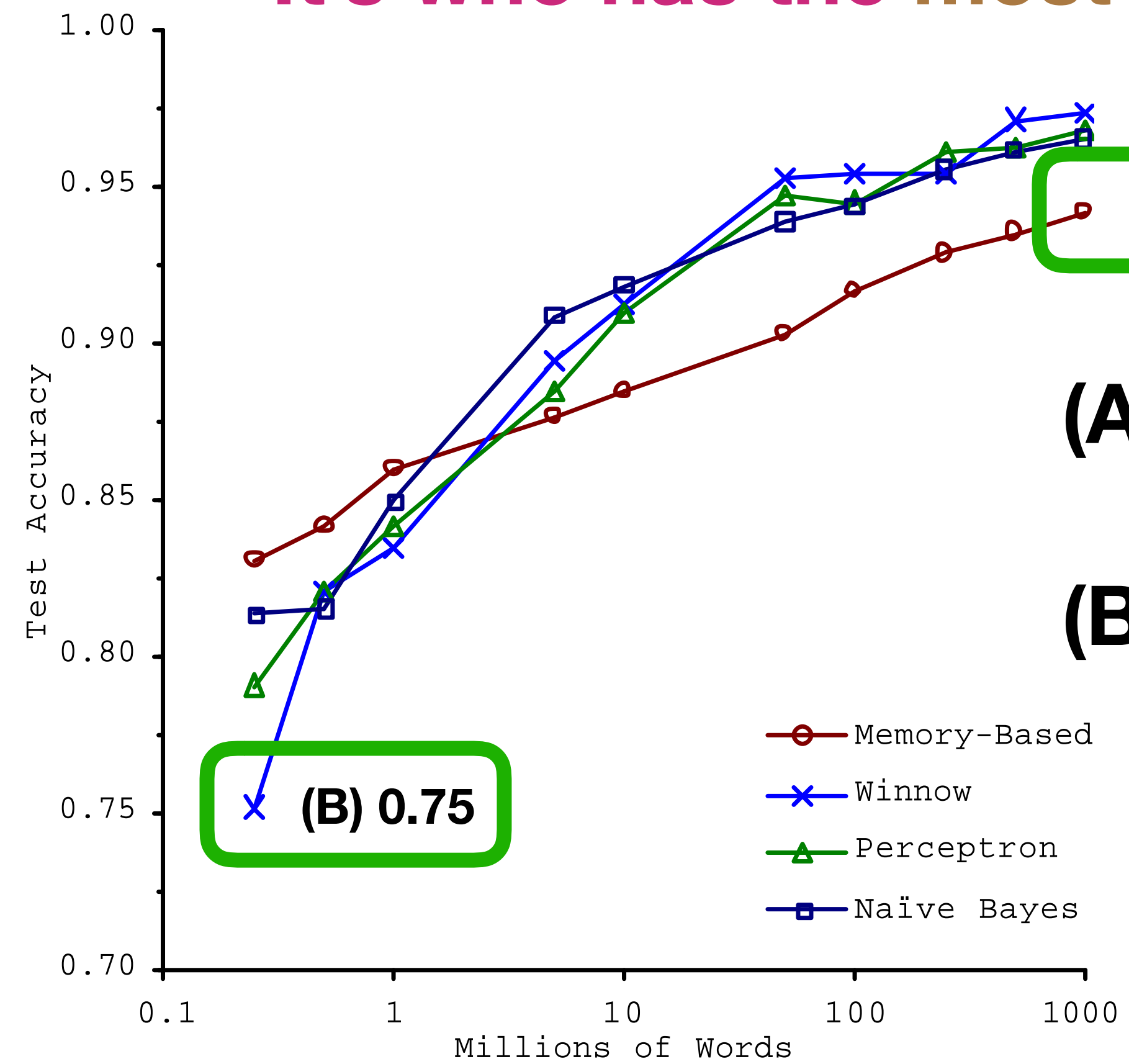


Banko & Brill (2001) “Scaling to Very Very Large Corpora for Natural Language Disambiguation”

# Concluding remarks: Era of Big Data

It's **NOT** who has the best algorithms that wins.  
It's who has the **most data**.

Score  
(Accuracy)



(A) **Poor algorithm + Big data**

vs

(B) **Good algorithm + Small data**

Data size



# Concluding remarks: Era of Big Data

We have the biggest data.  
We need a scope for fostering data scientists,  
because the future of NAOJ is on the shoulders of  
grad students, postdocs, and young researchers.

