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Machine Learning for Behavior Model

How to collaborate DCM and ML ?

Tokyo University of Science

Hideki YAGINUMA

yaginuma@rs.tus.ac.jp

DCM vs ML

To develop **more better** infrastructure and services, we are conducting analysis based on behavior models.

- ☐ **Prediction Accuracy**: issue of model parameter estimation
- ☐ **Model Interpretability**: issue of understanding model (behavior)

Discrete choice model

$$P(i)=\frac{\exp(\mu V_i)}{\sum_{j\in C}\exp(\mu V_j)}$$

Source: Sampling small data
Function: Liner
Accuracy(Model fitting): Mid（Low?）
Interpretability : High
Good understanding travel behavior ?

Machine Learning

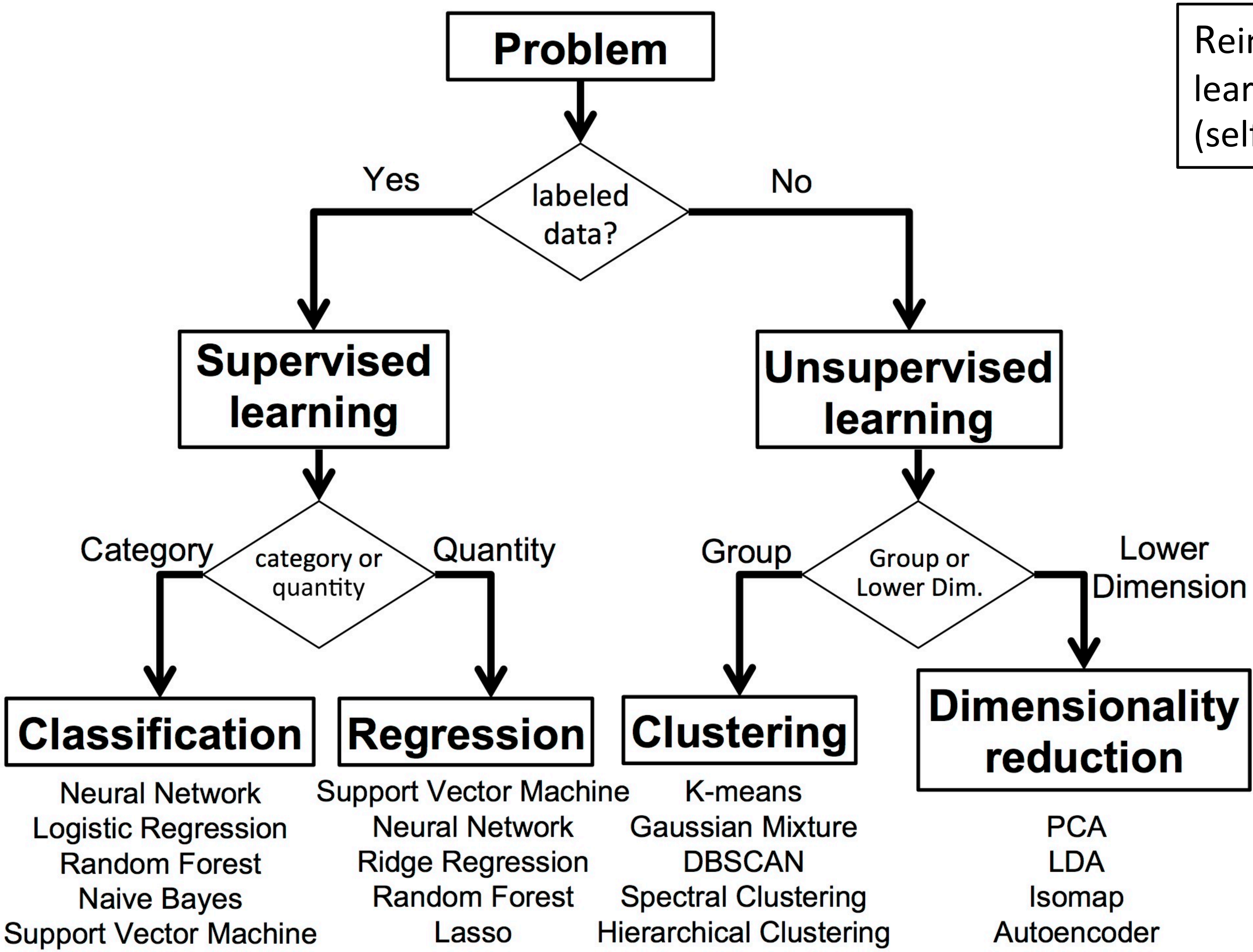
Black Box

Source: Big data
Function: Non-Liner
Accuracy(Model fitting): High
Interpertability: Low
NOT understanding travel behavior ?

Considering the possibility of collaboration between DCM and ML from the perspective of Aaccuracy and Interpretability

Overview of ML

Reinforcement learning (self-learning)



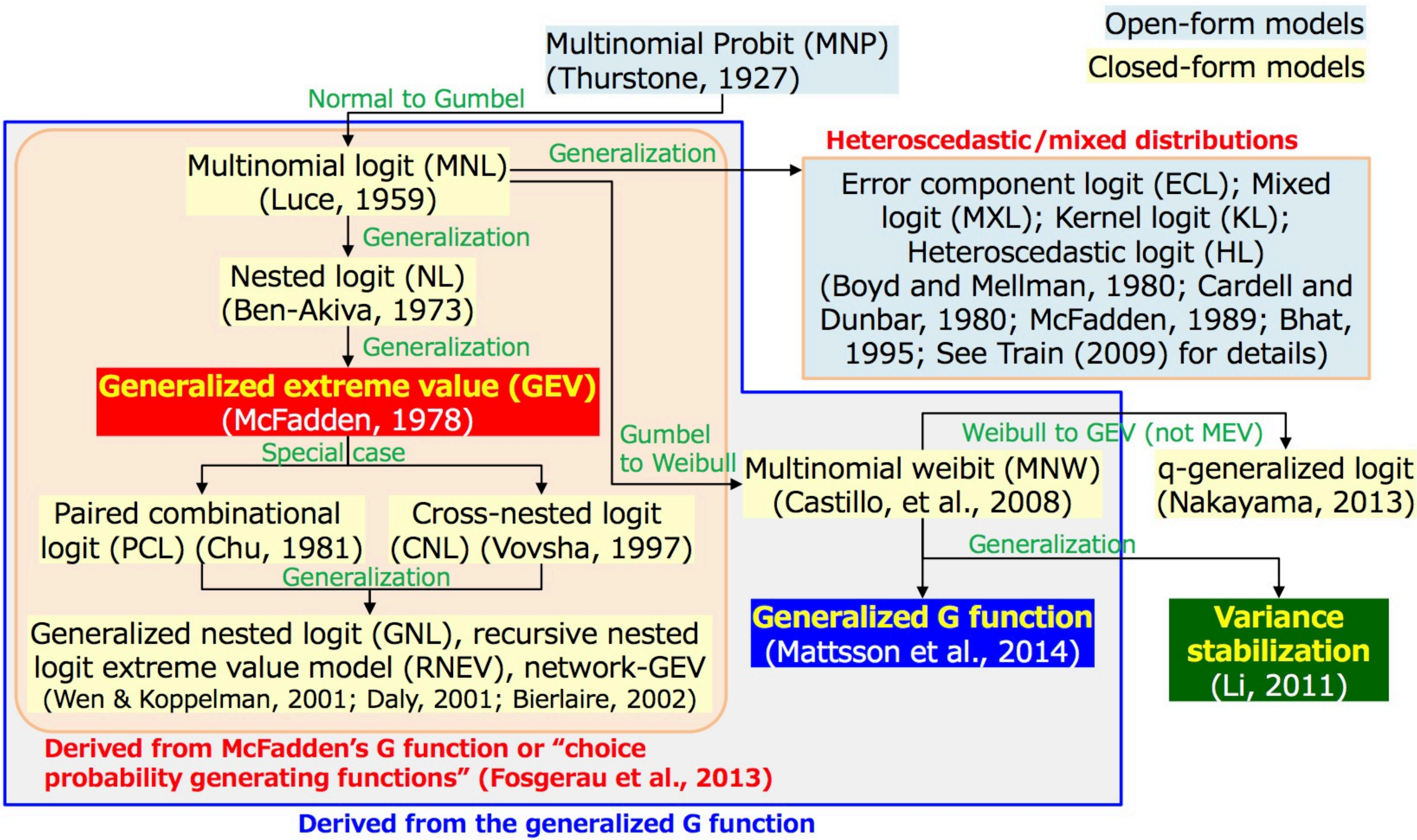
https://pythonnumericalmethods.berkeley.edu/notebooks/chapter25.01-Concept-of-Machine-Learning.html

How to collaborate DCM and ML ?

Part 1: Prediction Accuracy

- You can (not) estimate behavior model-

Overview of DCM



By Chikaraishi(Hiroshima Univ)

Flexible DCM

Mixed Loigt (Train 2000)

High flexible model structure by two error term.

Utility function

$$U_i = V_i + \boxed{\eta_i} + \boxed{\nu_i}$$

ν dist.: assume any G function

- IID Gamble (Logit Kernel) ⇒ MNL
- any G function (GEV Kernel) ⇒ NL, PCL, CNL, GNL…

η dist.: basically assume "*Normal dist.*"

In the case of normal distribution takes a non-realistic value, it can assume a variety of probability distribution (triangular distribution, cutting normal distribution, lognormal distribution, Rayleigh distribution, etc.).

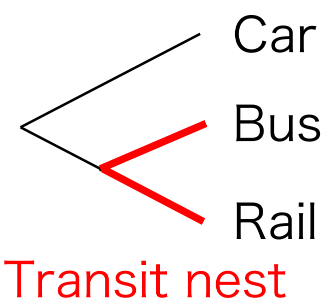
- Error Component: approximate to any GEV model
- Random Coefficient: Consider the heterogeneity

MXL : Error Component Model

Approximation of Nested Logit (NL)

Describe the nest (covariance) using structured $\boldsymbol{\eta}$.

Ex: model choice



Normal ⇒ nest

$$
\begin{aligned}
U_{car} &= \beta \mathbf{X}_{car} + \qquad\qquad\qquad\qquad + \nu_{car} \\
U_{bus} &= \beta \mathbf{X}_{bus} + \sigma_{transit}\eta_{transit} + \nu_{bus} \\
U_{rail} &= \beta \mathbf{X}_{rail} + \sigma_{transit}\eta_{transit} + \nu_{rail}
\end{aligned}
$$

IID Gamble ⇒ Logit

Choice prob. (open-form)

$$
P_{rail} = \int_{\eta_{transit}} \frac{e^{V_{rail}+\sigma_{transit}\eta_{transit}}}{e^{V_{car}} + e^{V_{bus}+\sigma_{transit}\eta_{transit}} + e^{V_{rail}+\sigma_{transit}\eta_{transit}}} f\left(\eta_{transit}\right) d\eta_{transit}
$$

$$
\eta_{transit} \approx N(0,1)
$$

Choice prob. (Simulated)

$$
P_{rail} = \frac{1}{N} \sum_{N} \frac{e^{V_{rail}+\sigma_{transit}\eta_{tranist}^{N}}}{e^{V_{car}} + e^{V_{bus}+\sigma_{transit}\eta_{tranist}^{N}} + e^{V_{rail}+\sigma_{transit}\eta_{tranist}^{N}}}
$$

MXL : Random Coefficient Model

Approximation of unobservable heterogeneity

Assume the heterogeneity of parameter

⇒In the case of parameter following Normal dist., we estimate the dist.'s hyper-parameter (mean and variance).

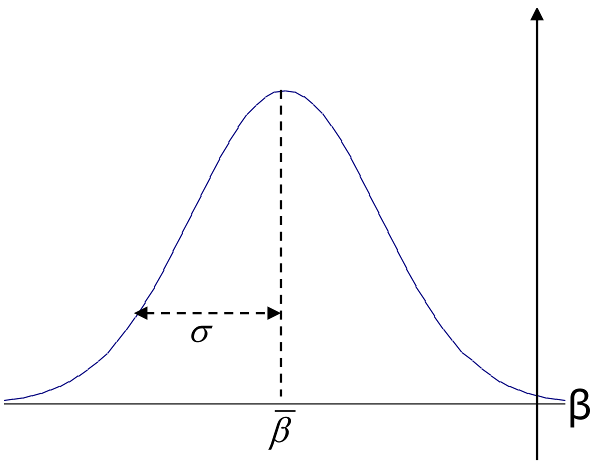
$$U_{car,n} = \boxed{\beta_n} T_{car,n} + \nu_{car,n}$$

$$\beta_n \approx N\left(\bar{\beta}, \sigma^2\right)$$

$$U_{car,n} = \bar{\beta} T_{car,n} + \sigma \eta_n T_{car,n}$$

$$U_{bus,n} = \bar{\beta} T_{bus,n} + \sigma \eta_n T_{bus,n}$$

$$U_{rail,n} = \bar{\beta} T_{rail,n} + \sigma \eta_n T_{rail,n}$$



$\eta_n \approx N(0,1)$ $\bar{\beta}, \sigma : unknown\ parameter$

Hyper-parameter can describe using observable variables

$$\bar{\beta}_n = \gamma_0 + \gamma_1 income_n$$

β depend on observable income variable

Difficulty of Estimation

Why estimation methods is important ?

- ✓ Advance GEV model (CNL, GNL, n-GEV…) has many parameter.
  ⇒ Convergence becomes unstable (Hessian passed away…)
- ✓ non-GEV model requires multiple integral calculations .
  ⇒ ML estimation cannot be used
- ✓ Stricture of utility function (non-liner, complex distribution)
- ✓ Dynamic choice behavior (Dynamic Programing:DP)
- ✓ Interaction between decision-maker (Endogeneity)
- ✓ high dimensional data ⇒ N of Sample < N of Variable

The analyst needs to select an appropriate estimation method corresponding to the model !

Overview of Estimation

To solve Integral

Maximum Likelihood estimation

To Consider Dynamics Interaction

Bayesian estimation

To general

Numerical method

- ✓ Newton-Cotes rules
- ✓ Simpson's rule

Low-dimensional

Analytical approximation

- ✓ Series approximation
- ✓ Clark approximation
- ✓ MACML

Random approximation

- ✓ Maximum Simulated Likelihood
  （Monte Carlo integral, GHK…）
- ✓ MCMC
  （Gibbs, MH, HM…）

High-dimensional

Structural estimation

- ✓ Heckman's 2-step
- ✓ Pseudo Likelihood
- ✓ nested Fixed Point (NFXP)
- ✓ Nestef Pseudo Likelihood …
- ✓ MPEC

Machine Learning (ML)

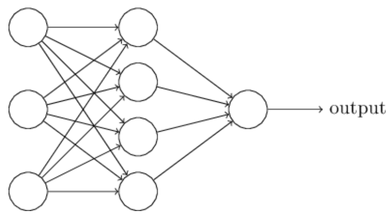
Neural network, (reverse) Reinforcement learning, Sparse modeling, Gaussian Process…

⇒ Several methodologies are useful for DCM parameter estimation !

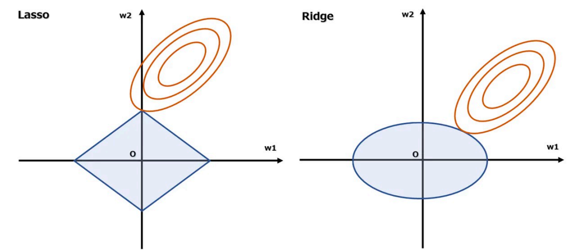
Collaboration of DCM and ML

Estimation methods in the field of machine learning can be applied to DCM estimation.

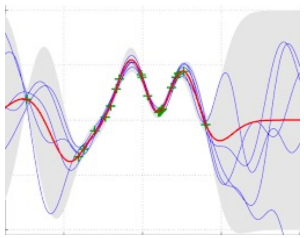
Neural network (Back propagation)



Sparse modeling



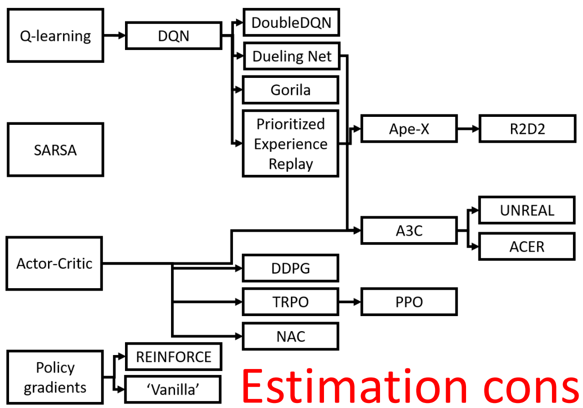
Gaussian Process



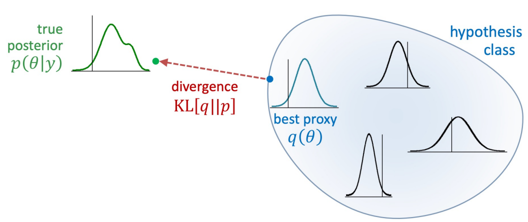
Estimation considering complex nonlinear structures

Estimation considering parameter dimension reduction

Reinforcement learning



Variational Bayesian



Estimation considering complex probability distribution

Estimation considering complex and dynamic choice

How to collaborate DCM and ML ?

Part 2: Model Interpretability

- You can (not) understand behavior model-

XAI: eXplainable AI

Recent issue in AI

- In recent years, Accuracy and explainability of AI (ML) has been required in practice situation.
- XAI: provides **reasons and evidence** that humans can understand for the results by AI.
- Three requirements were presented in G20 AI principles

  Human centered values
  - Fairness（公平性）
  - Accountability（説明責任）
  - Transparency（透明性）

https://www.mofa.go.jp/policy/economy/g20_summit/osaka19/en/documents/final_g20_osaka_leaders_declaration.html

ANNEX

G20 AI Principles [1]

The G20 supports the Principles for responsible stewardship of Trustworthy AI in Section 1 and takes note of the Recommendations in Section 2.

Section 1: Principles for responsible stewardship of trustworthy AI

1.1. Inclusive growth, sustainable development and well-being
Stakeholders should proactively engage in responsible stewardship of trustworthy AI in pursuit of beneficial outcomes for people and the planet, such as augmenting human capabilities and enhancing creativity, advancing inclusion of underrepresented populations, reducing economic, social, gender and other inequalities, and protecting natural environments, thus invigorating inclusive growth, sustainable development and well-being.

1.2. Human-centered values and fairness
a) AI actors should respect the rule of law, human rights and democratic values, throughout the AI system lifecycle. These include freedom, dignity and autonomy, privacy and data protection, non-discrimination and equality, diversity, fairness, social justice, and internationally recognized labor rights.
b) To this end, AI actors should implement mechanisms and safeguards, such as capacity for human determination, that are appropriate to the context and consistent with the state of art.

1.3. Transparency and explainability
AI Actors should commit to transparency and responsible disclosure regarding AI systems. To this end, they should provide meaningful information, appropriate to the context, and consistent with the state of art:
i. to foster a general understanding of AI systems;
ii. to make stakeholders aware of their interactions with AI systems, including in the workplace;
iii. to enable those affected by an AI system to understand the outcome; and,
iv. to enable those adversely affected by an AI system to challenge its outcome based on plain and easy-to-understand information on the factors, and the logic that served as the basis for the

AI principles

Fairness

Eliminate **biases** that cause unfairness so that AI can provide fair services regardless of **differences in user attributes**.

- Bias in training data (input): historical bias, sampling bias
- Users with certain attributes cannot receive the service. And they cannot receive the same level of service as other users.

Accountability

Clarify where the **cause of the error lies** and who (or what) is responsible for it.

→ In complex models, it may be difficult to identify where the cause of the problem lies. (ex. DNN)

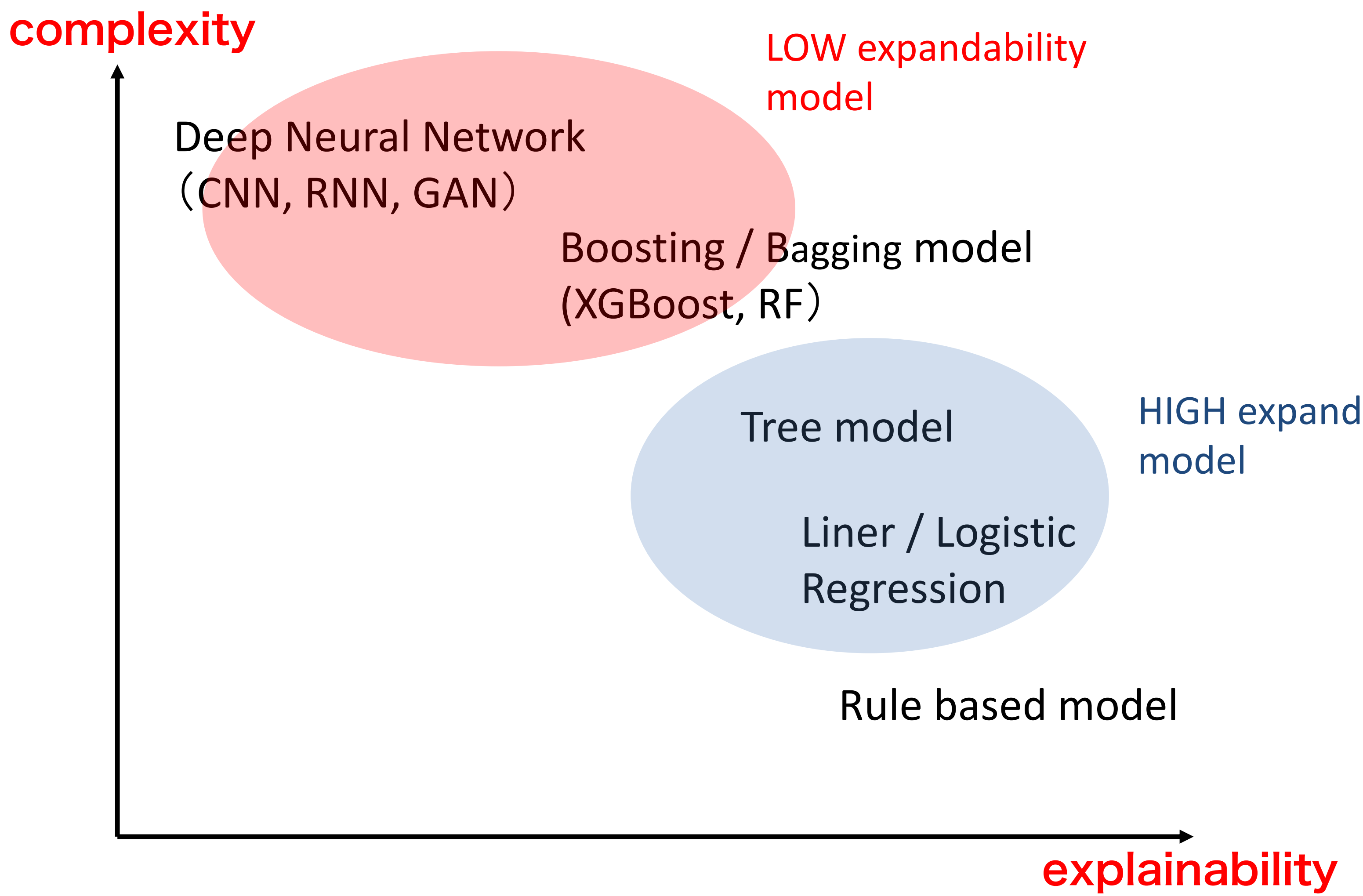
Transparency

AI systems can present information that **users can understand**.

- Information that should be presented model (processing criteria), data was used to train it, validation, etc...
- This is important when dealing with issues related to medical, safety and policy making.

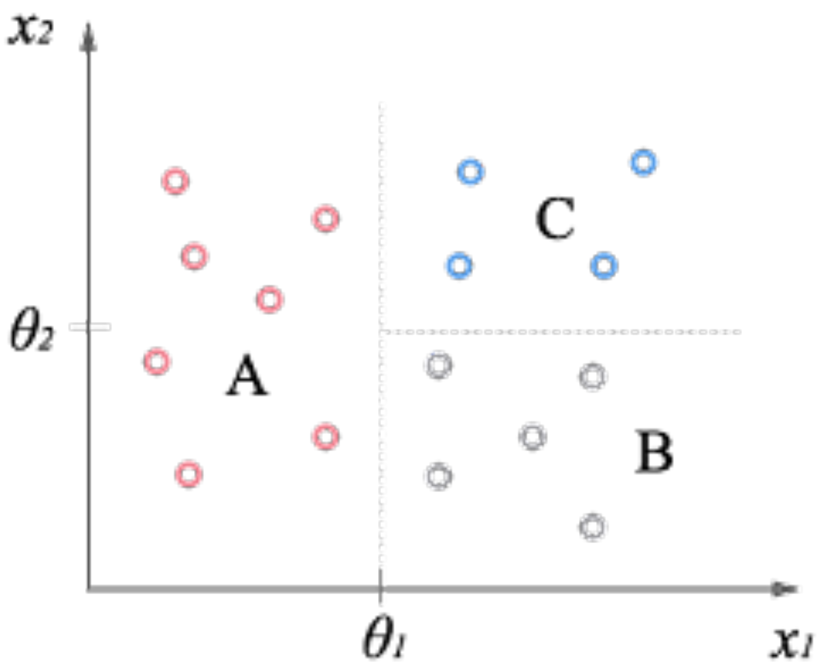
Explainability of ML methods

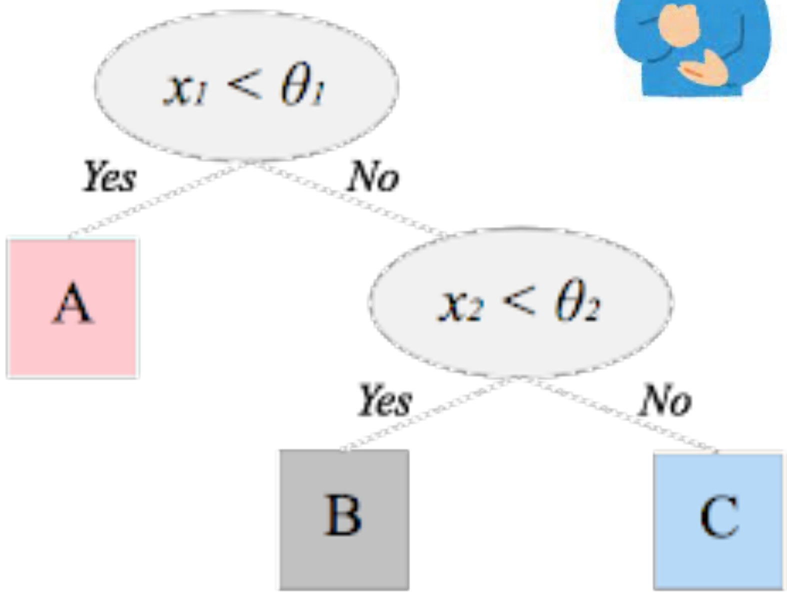
In machine learning, there is a **tradeoff** between the **complexity** (= accuracy) of the problem and its **explainability**.



Explainability of ML methods

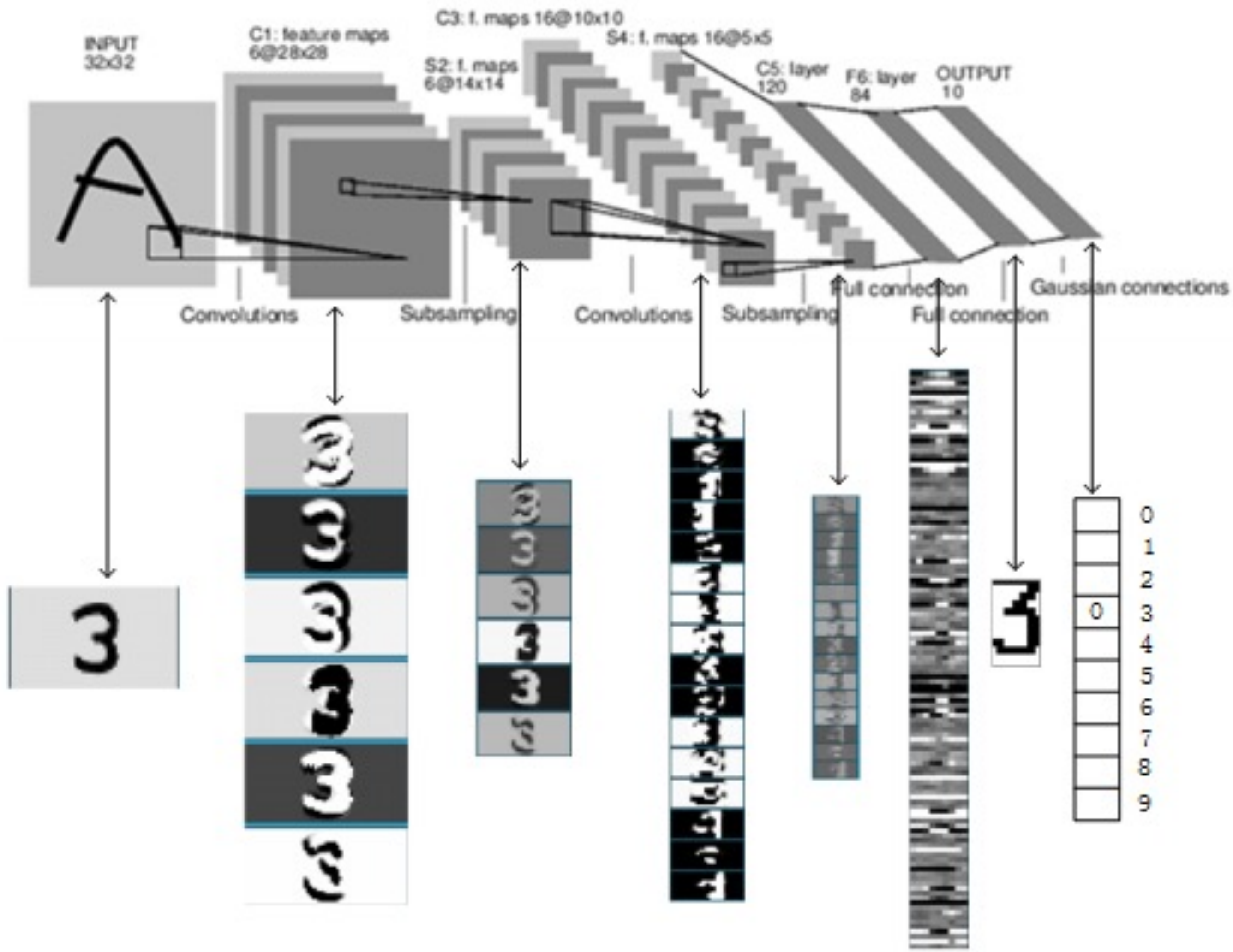
Tree model





Explainability of ML methods

CNN model



XAI method

◆ Global or Local explanation: Domains that the model can explain

- Global: Understand the overall behavior of AI models.
- Local: Understand the reasoning behind each prediction.

Model in-dependent XAI

Global Explanation

↕

PFI
(Permutation Feature Importance)
- Leave One Covariate Out FI
- Grouped PFI

PD
(Partial Dependence)

ICE
(Individual Conditional Expectation)

Local Explanation

SHAP
(SHapley Additive exPlanations)

LIME

Model dependent XAI

CAM/ Grad-CAM

Integrated Gradients

Tree Surrogate

Attention

Global XAI : PFI

PFI: Permutation Feature Importance

- ◆ A method for calculating the **feature importance** in models.
- ◆ Shuffle (**permutation**) the features sample data and evaluate the importance based on the **prediction error** of the model.

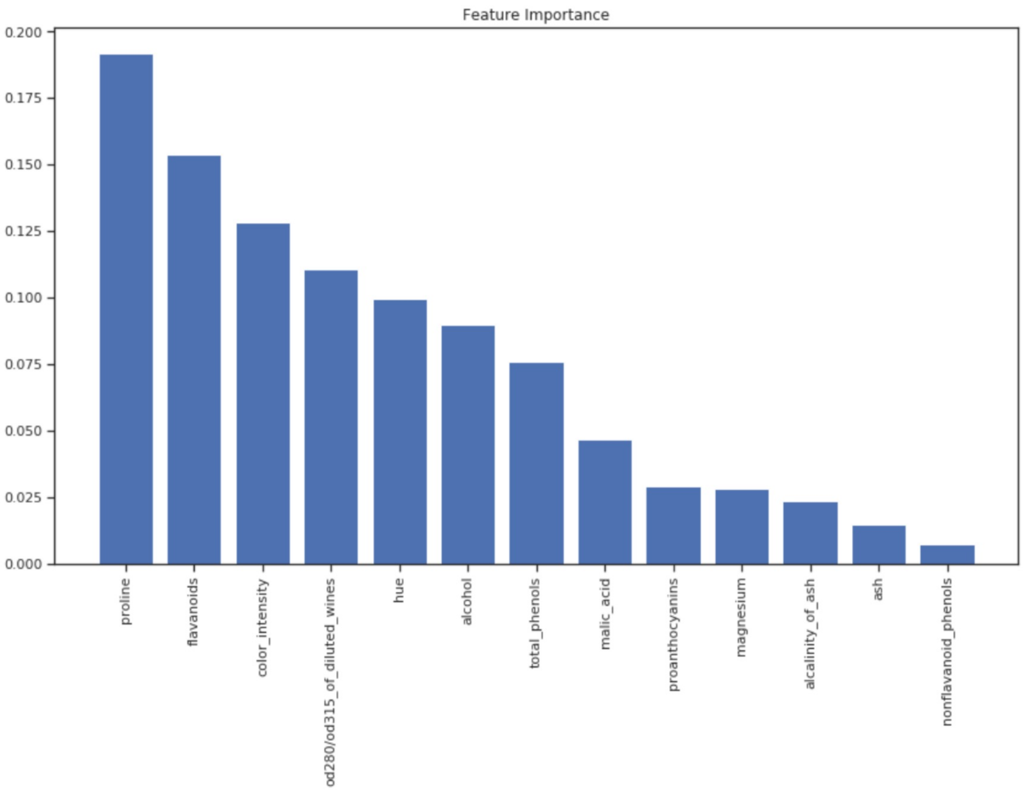
Trained model

$$y = f(x)$$

Error Function

Test data

dataname	value_1	value_2	value_3	value_4	value_5	value_6	value_7	value_8	value_9	value_10
data_1	12	91	30	22	39	63	75	53	17	91
data_2	29	61	87	9	24	55	57	3	11	45
data_3	59	33	28	61	86	81	52	90	29	48
data_4	11	79	16	41	30	79	57	57	25	89
data_5	75	9	84	31	50	58	21	71	74	38
...	...	...	...	...	...	...	...	...	...	...
data_121	16	94	29	60	14	95	74	14	46	2
data_122	30	70	82	58	36	44	47	90	7	85
data_123	27	29	24	9	29	4	47	94	88	43
data_124	21	66	45	33	69	99	43	91	34	78
data_125	95	39	19	89	70	38	72	29	72	52



Global XAI : PFI

PFI: Algorithm

◆ A method for calculating the **feature importance** in models.

1. Calculate Baseline Prediction Error

Baseline prediction error

$$e_{base}(f) = \mathbb{E}[L(f(x), y)]$$

Error evaluation index
(ex. RMSE)

Trained model $y = f(x)$

Obs. Value   Prediction Value

2. Create shuffle data of feature

dataname	value_1	value_2	value_3	value_4	value_5	value_6	value_7	value_8	value_9	value_10
data_1	12	91	30	22	39	63	75	53	17	91
data_2	29	61	87	9	24	55	57	3	11	45
data_3	59	33	28	61	86	81	52	90	29	48
data_4	11	79	16	41	30	79	57	57	25	89
data_5	75	9	84	31	50	58	21	71	74	38
...	...	...	...	...	...	...	...	...	...	...
data_121	16	94	29	60	14	95	74	14	46	2
data_122	30	70	82	58	36	44	47	90	7	85
data_123	27	29	24	9	29	4	47	94	88	43
data_124	21	66	45	33	69	99	43	91	34	78
data_125	95	39	19	89	70	38	72	29	72	52

Random Shuffle

X_i

3. Calculate shuffle data's Prediction Error

$$e_{prem}(f) = \mathbb{E}[L(f(X_i), y)]$$

4. Calculate FI index

$$FI_i = \frac{e_{prem}(f)}{e_{base}(f)}$$

Repeat to 2-4
for all features

Collaboration of DCM and ML

◆ XAI methods are powerful tools for more deep understanding for DCM.

→ Especially, model in-dependent methods (PFI, PD, SHAP) is good for us !

Thank you for your attention !