23 Sep. 2022 @ UT

# 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: Small data
Function: Liner
Accuracy(Model fitting): Mid（Low?）
Interpretability : High
Good understanding travel behavior ?

## Machine Learning

Black Box

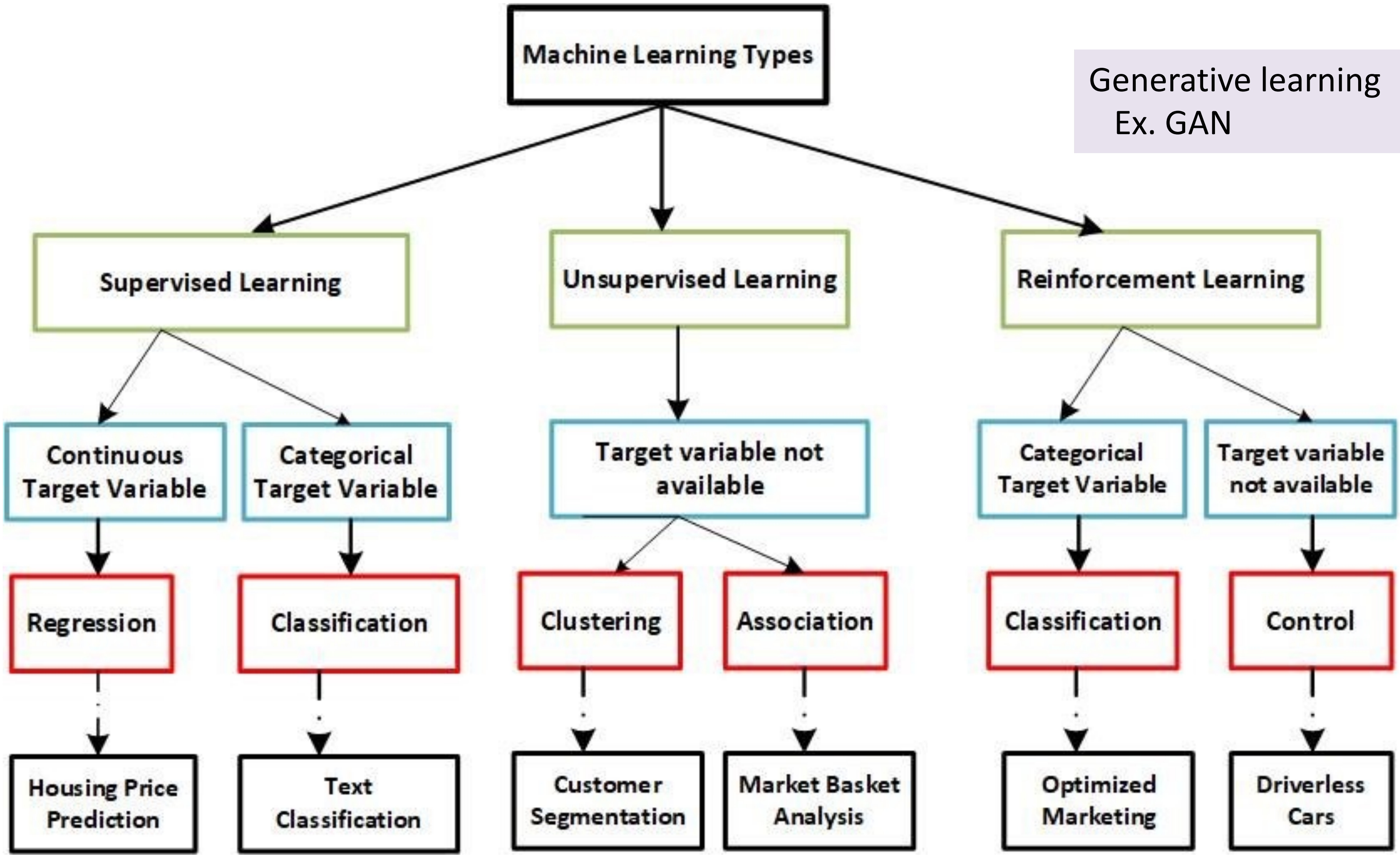
Source: Big data
Function: Non-Liner
Accuracy(Model fitting): High
Interpretability: Low
NOT understanding travel behavior ?

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

# Overview of ML



Generative learning
Ex. GAN



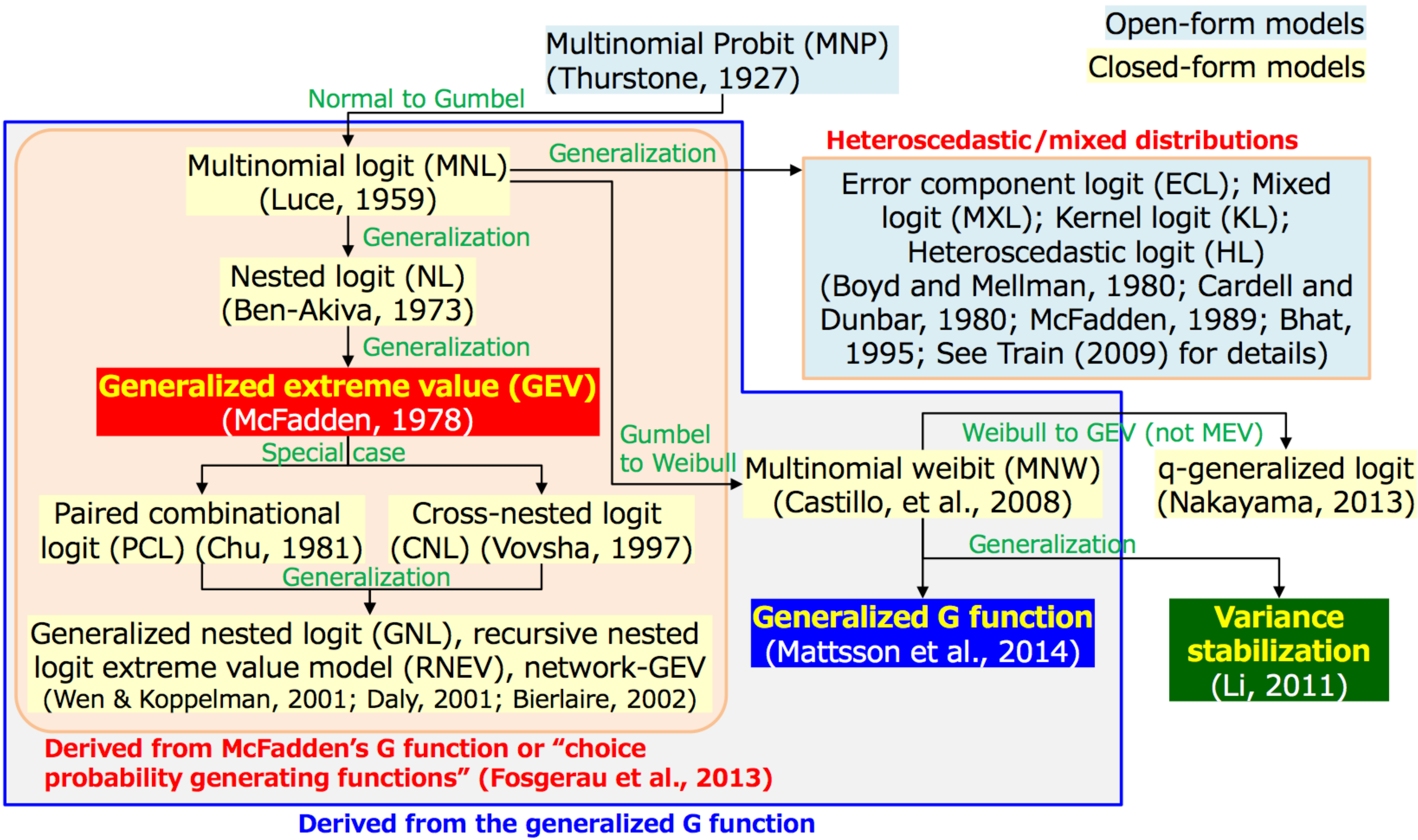

https://ieeexplore.ieee.org/document/8612259

# 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**

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

$\nu$ dist.: assume any G function

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

$\eta$ 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.).

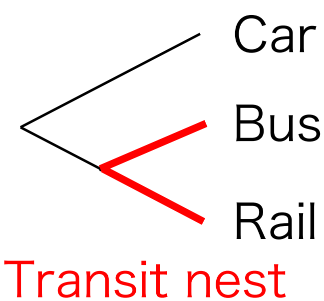
- Error Component: approximate to any GEV model
- Random Coefficient: Consider the heterogeneity

# MXL : Error Component Model

## Approximation of Nested Logit (NL)

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

**Ex: model choice**




Normal ⇒ nest

$$U_{car} = \beta \mathbf{X}_{car} + \quad + \nu_{car}$$
$$U_{bus} = \beta \mathbf{X}_{bus} + \sigma_{transit}\eta_{transit} + \nu_{bus}$$
$$U_{rail} = \beta \mathbf{X}_{rail} + \sigma_{transit}\eta_{transit} + \nu_{rail}$$

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)

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

# MXL : Random Coefficient Model

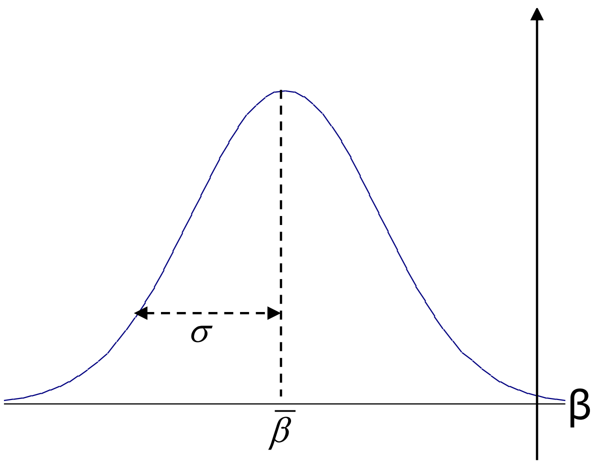
## Approximation of unobservable heterogeneity

Assume the heterogeneity of parameter

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

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

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




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

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

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

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

Hyper-parameter can describe using observable variables

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

$\beta$ 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 can not 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 method



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)
- ✓ Nested Pseudo Likelihood …
- ✓ MPEC

**Machine Learning (ML)**

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

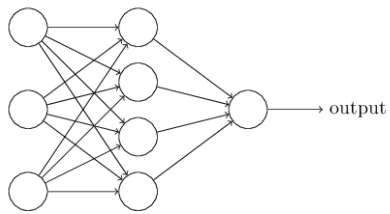
⇒ Several methodologies are useful for DCM parameter estimation !

# Collaboration of DCM and ML

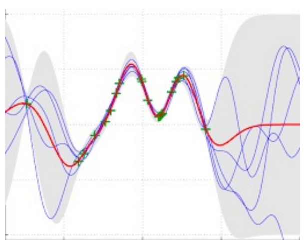


Estimation methods in the field of machine learning can be applied to DCM estimation.


**Neural network**
**(Back propagation)**

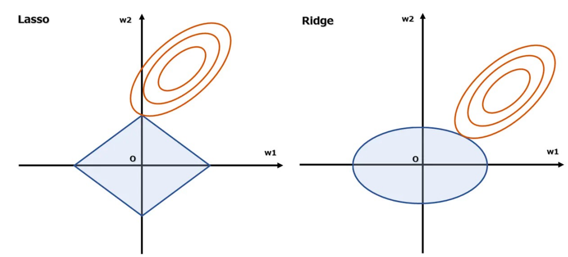



**Gaussian Process**



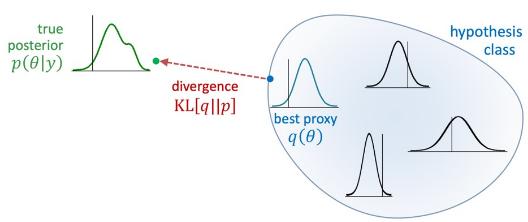
Estimation considering complex nonlinear structures

**Sparse modeling**



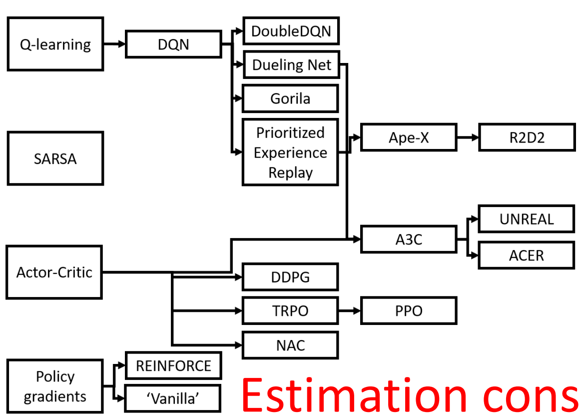

Estimation considering parameter dimension reduction

**Variational Bayesian**




Estimation considering complex probability distribution

**Reinforcement learning**




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

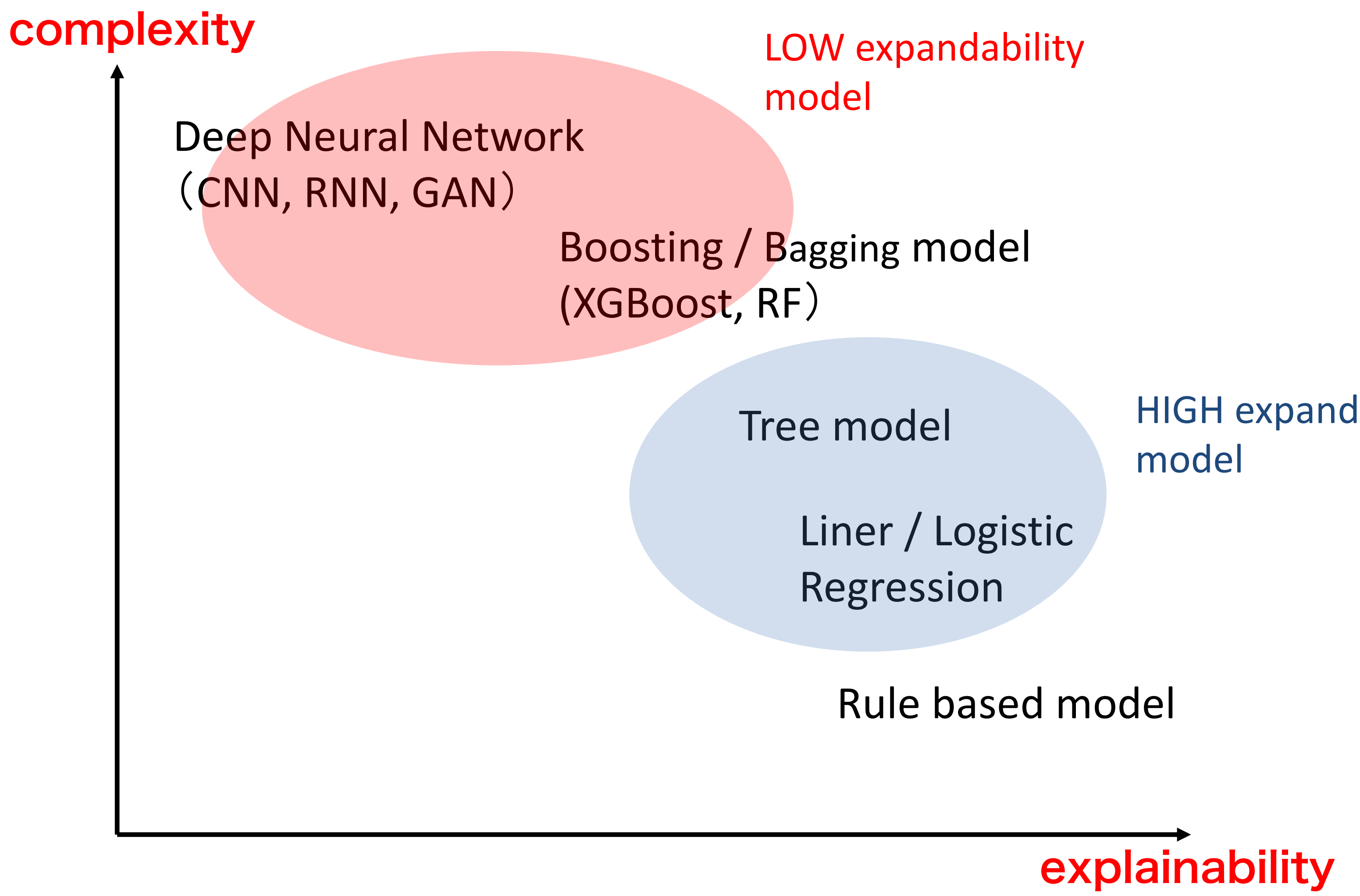
AI systems can present information that **users can understand**.

- 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



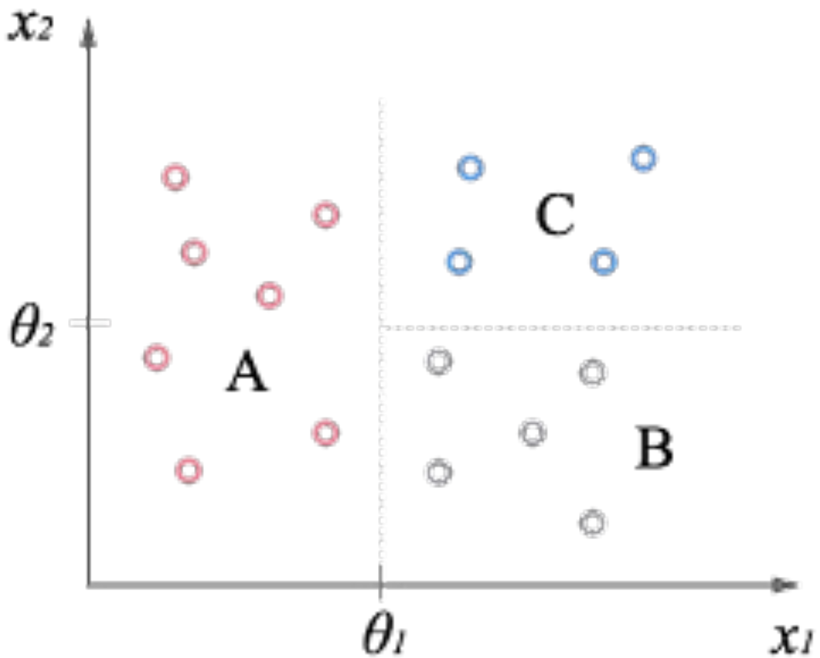
In machine learning, there is a **tradeoff** between the **complexity** (= accuracy) of the problem and its **explainability**.

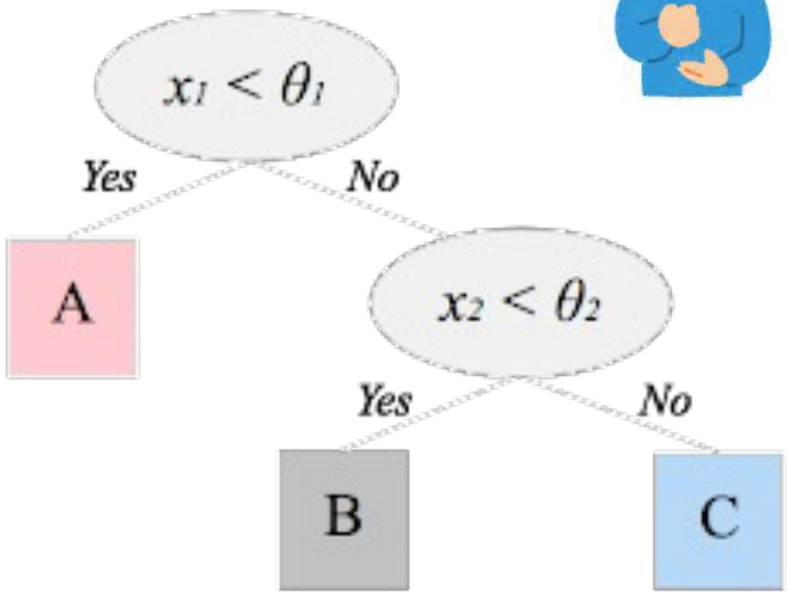


# Explainability of ML methods



## Tree model

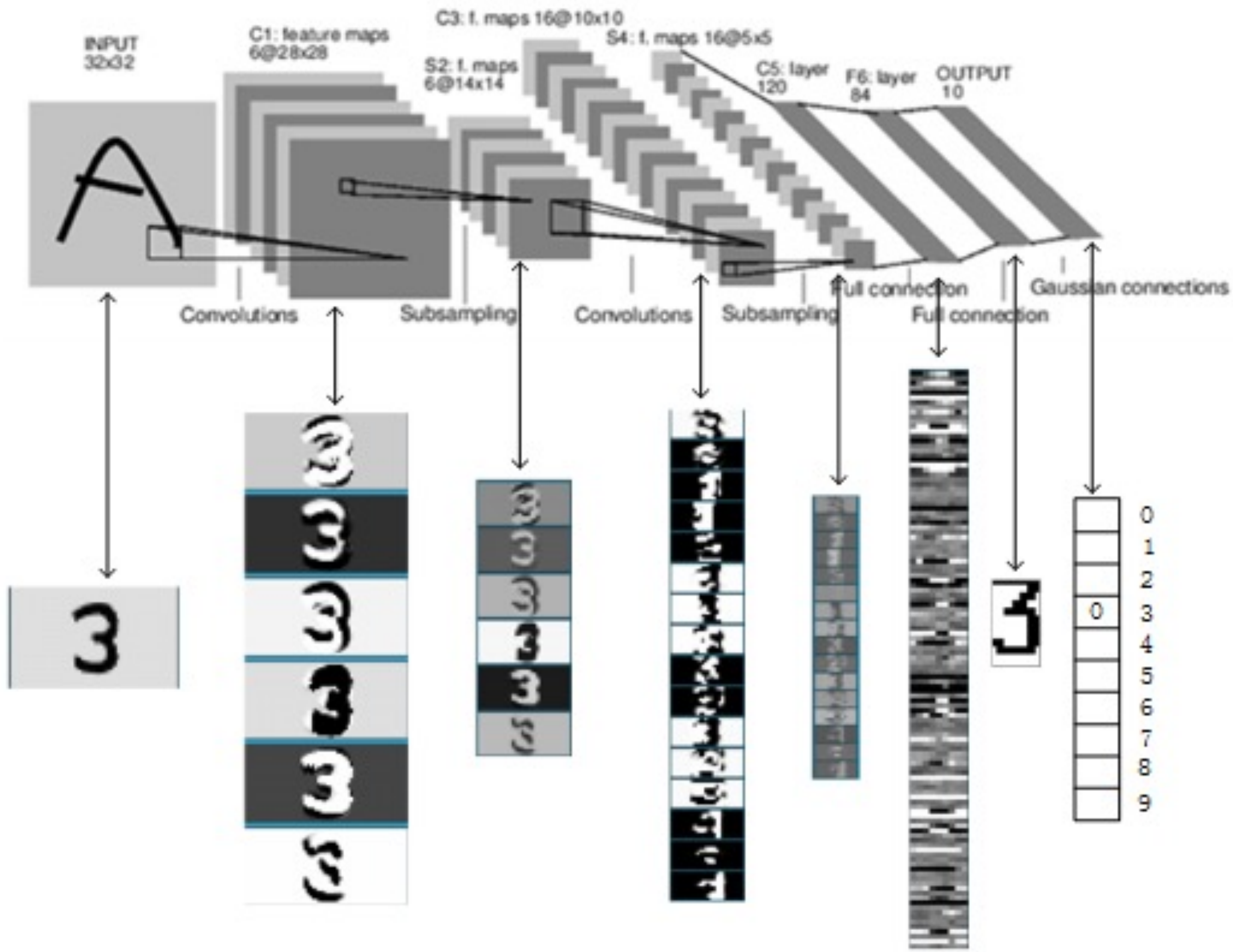



# Explainability of ML methods



## 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)

PD
(Partial Dependence)

CPD
(Conditional 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

- Calculating the **feature importance** in models.
- Shuffle (**permutation**) the features sample data and evaluate the importance based on the **prediction error** of the model.

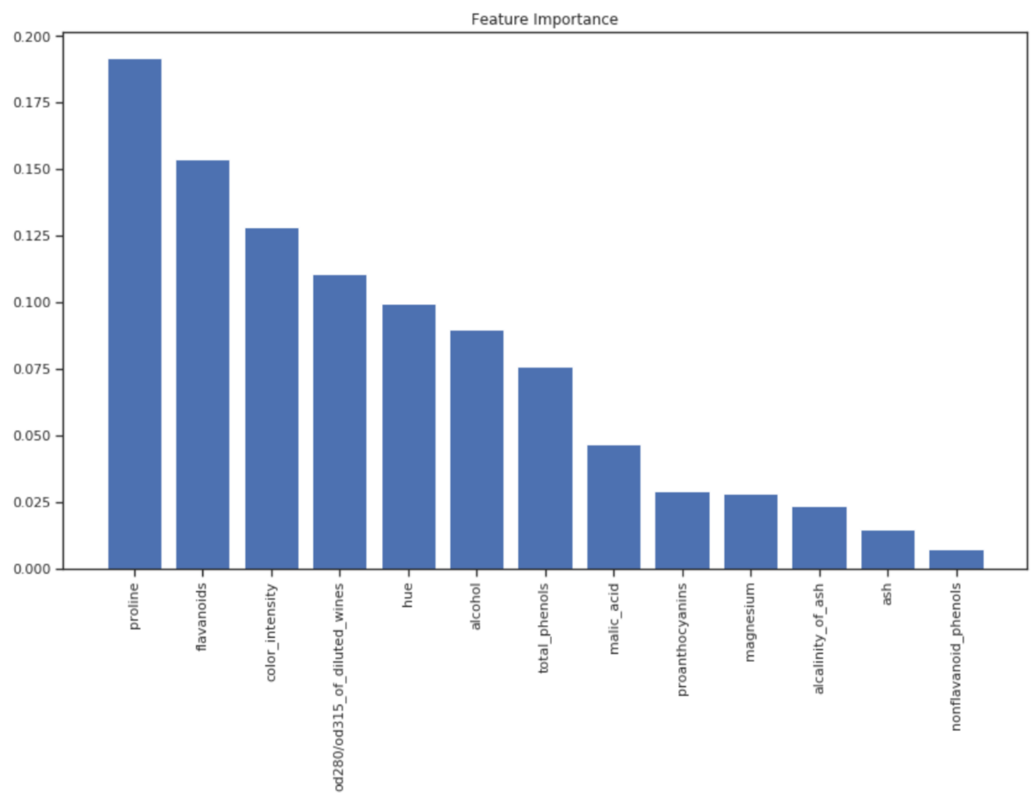
**Trained model**

$$y = f(x)$$

Error Function

**Test data**

| | value_1 | value_2 | value_3 | value_4 | value_5 | value_6 | value_7 | value_8 | value_9 | value_10 |
|---|---|---|---|---|---|---|---|---|---|---|
| **dataname** | | | | | | | | | | |
| 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

◆ 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 feature's shuffle 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 |

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

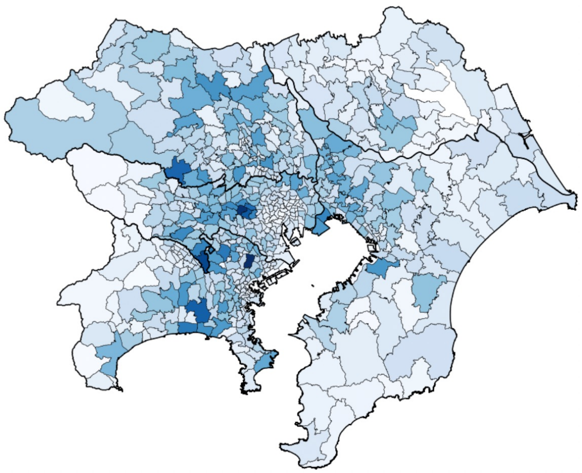
$$FI_i = \frac{e_{prem}(f)}{e_{base}(f)}$$

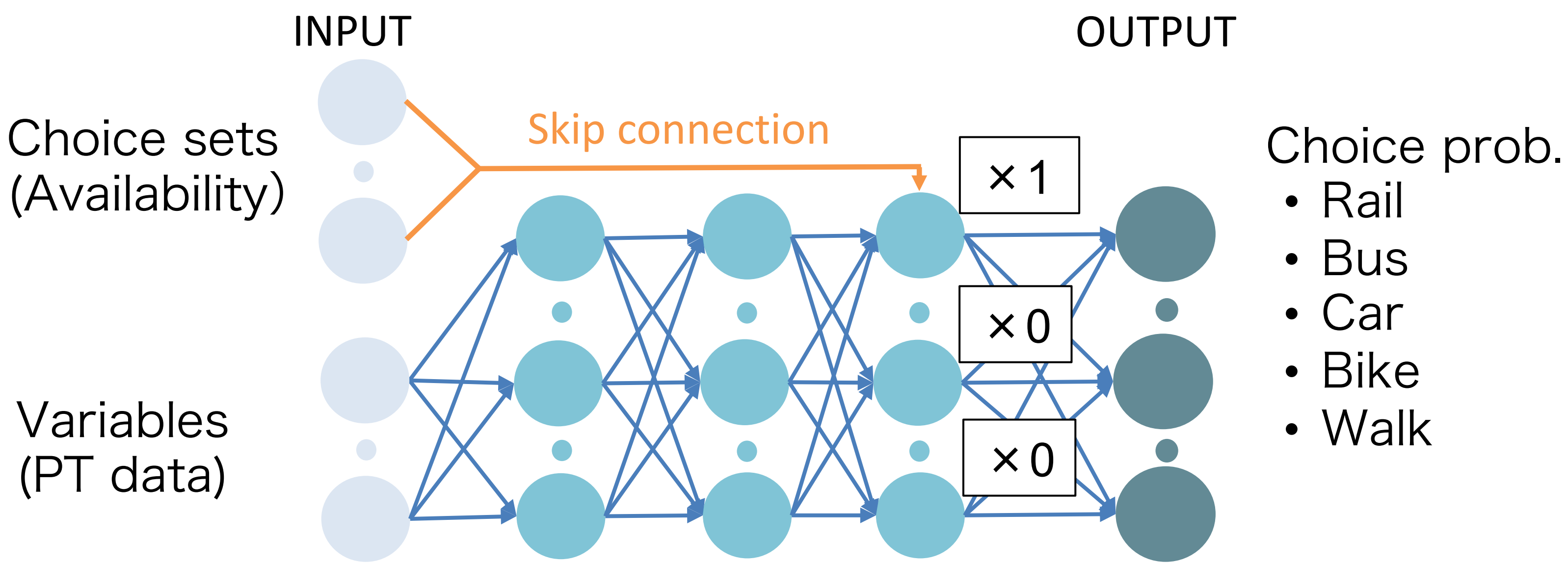
Repeat to 2-4
for all features

# Application : mode choice

## Mode choice model based on NN

- Simple NN considering choice sets by skip connection.
- Apply to the Tokyo Metropolitan area.
- Data: Tokyo PT 2018






Hidden layer: 4
Units: 100, 100, 50, 10

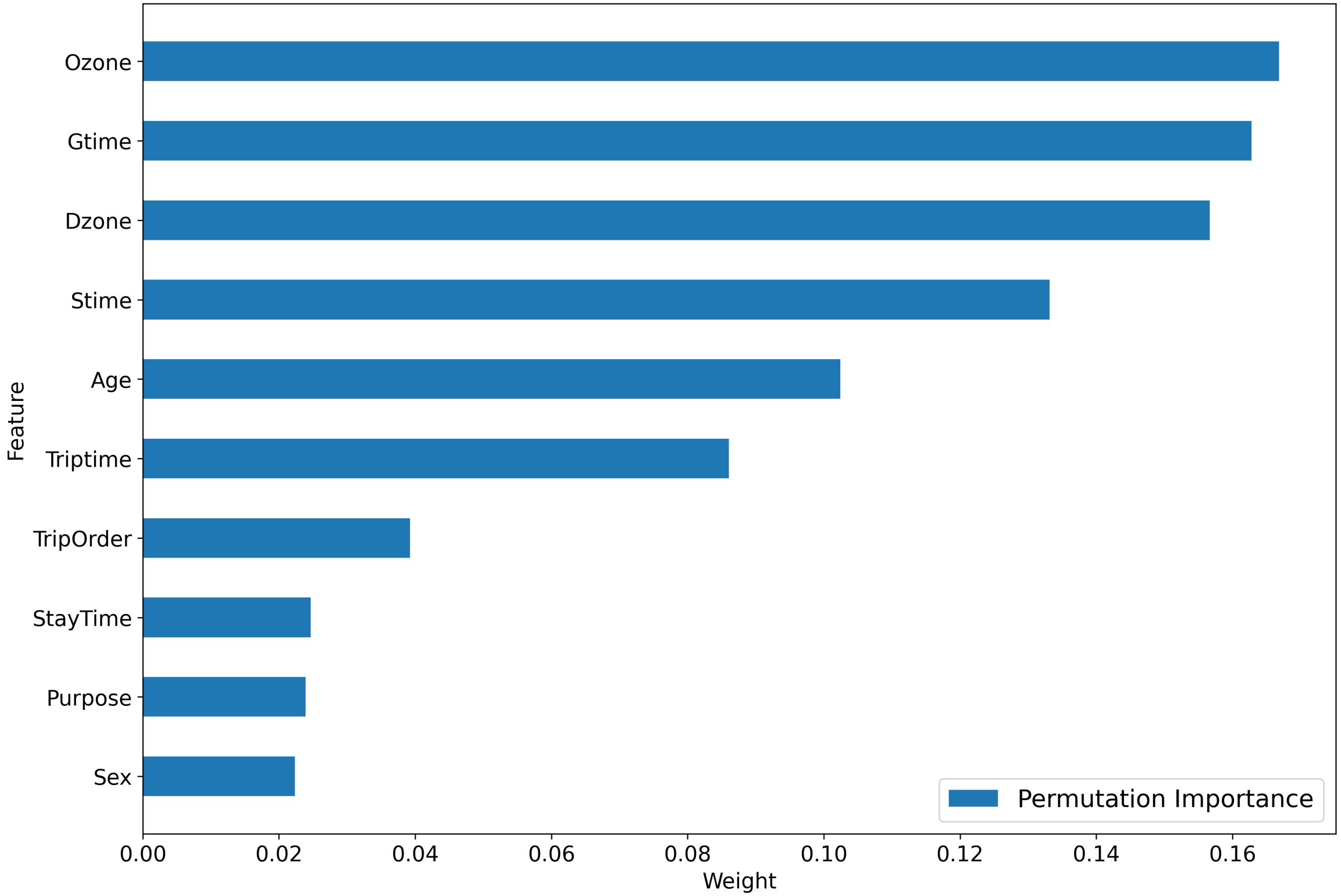
Ishijima, Yaginuma etc.: Interpretability of machine-learning based travel behavior models using XAI [accepted IATBR]

# Application : XAI



## Results of PI (Permutation Importance)

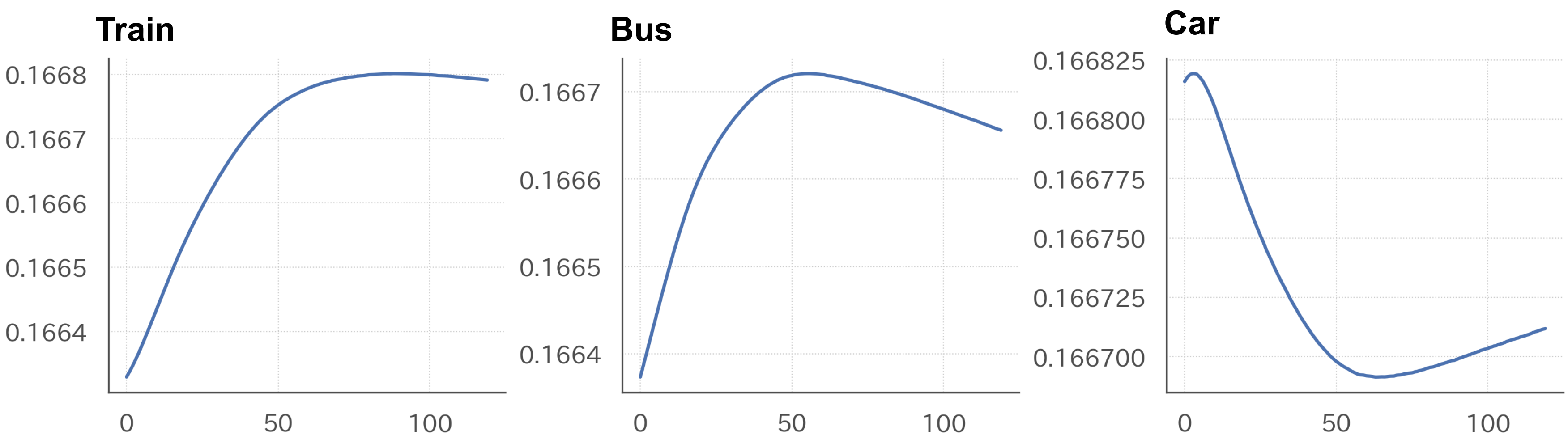
- ◆ Calculating the **feature importance** in models.
- ◆ Determining important features for improving model accuracy



# Application : XAI

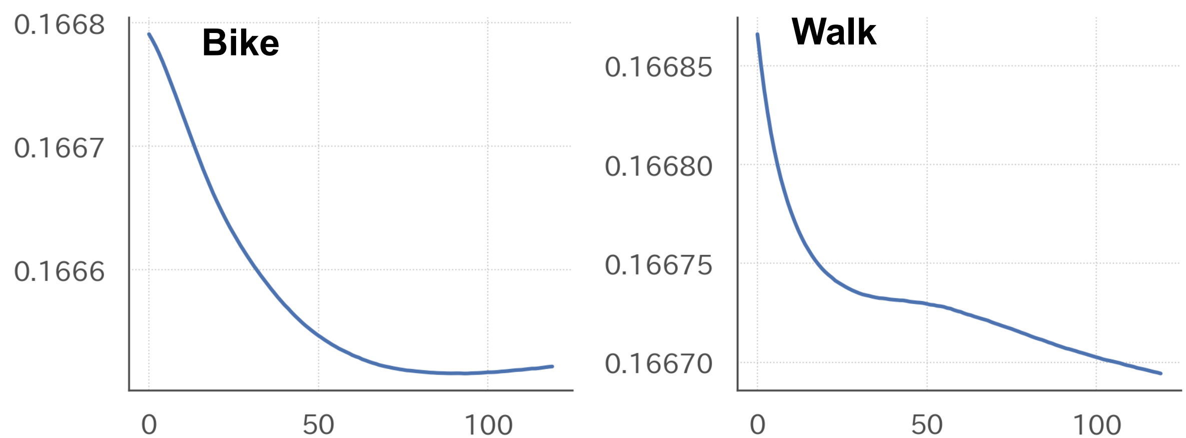
## Results of PD(Partial Dependence)

- ◆ Calculating the **relationship** between output and each feature.
- ◆ Change point can be detected by **expected sensitivity**




X-axis: travel time

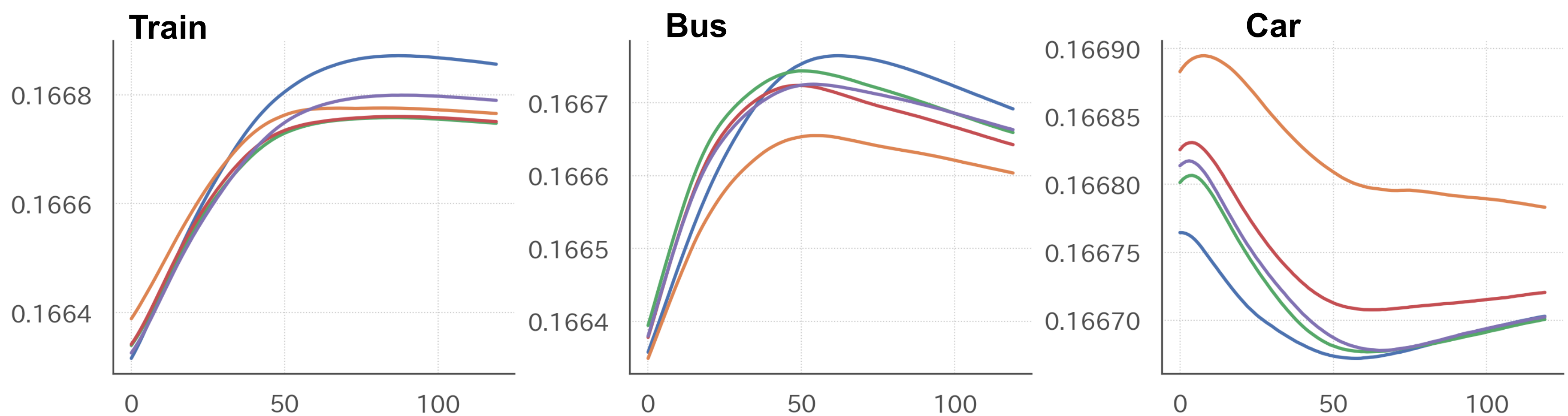
Y-axis: choice prob.



# Application : XAI

## Results of CPD(Partial Dependence)

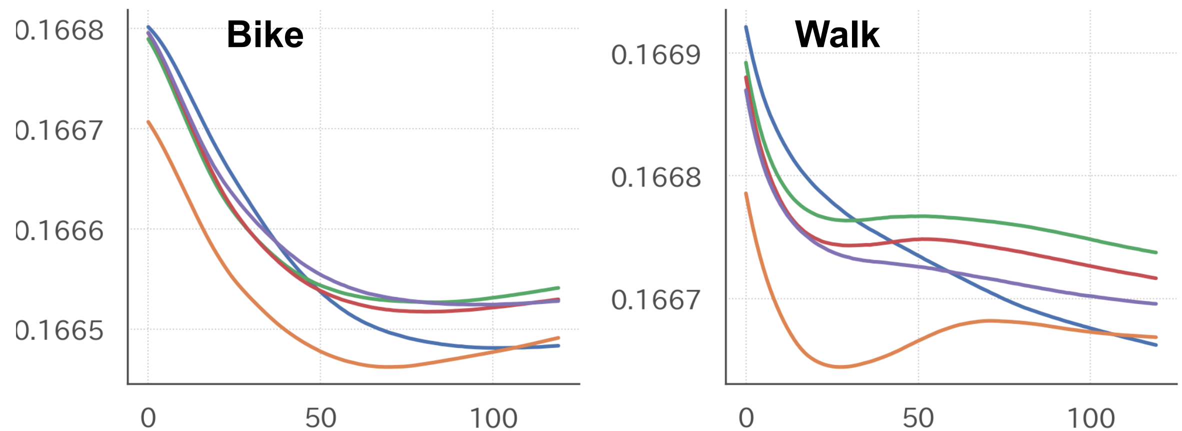
- Calculating the **relationship** between output and each feature.
- Change point can be detected by **gruop sensitivity**




X-axis: travel time

Y-axis: choice prob.

Travel Purpose

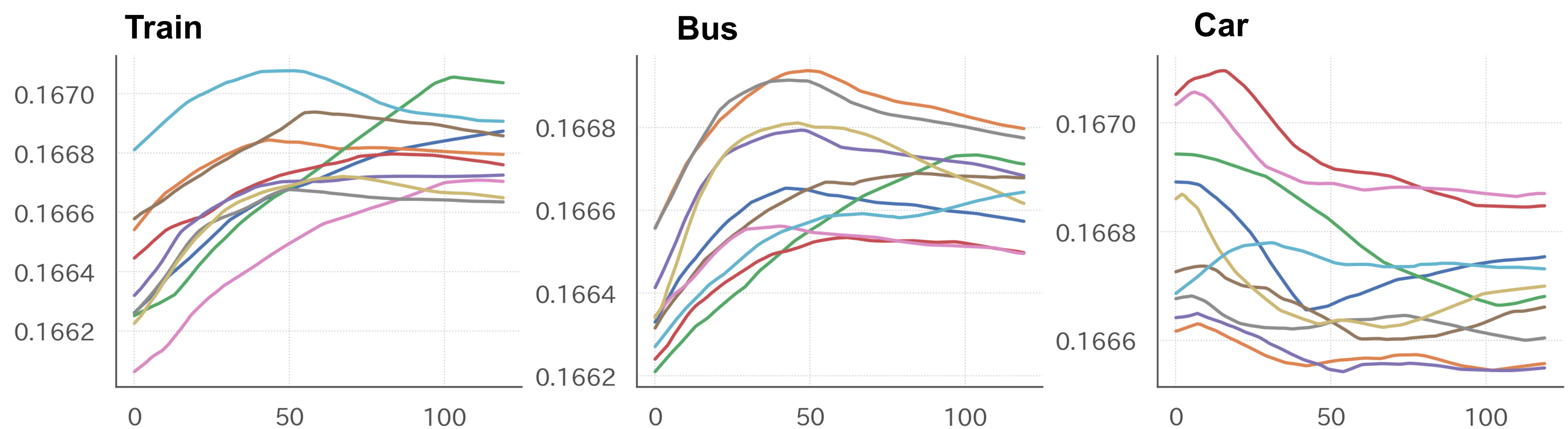


# Application : XAI



## Results of ICE(Individual Conditional Expectation)

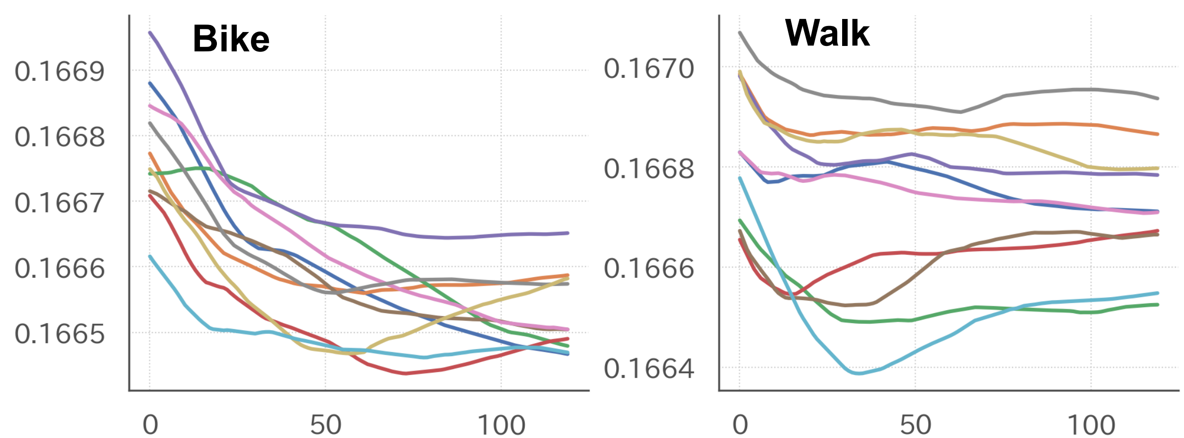
- ◆ Calculating the **relationship** between output and each feature.
- ◆ Change point can be detected by **individual sensitivity**




X-axis: travel time

Y-axis: choice prob.

Indevidual



# Results of DCM vs ML



| | DCM | ML |
|---|---|---|
| Explainability | • Value of parameter and sign (+/-)<br>• **Elasticity**<br>• **Sensitivity** | • **Feature's importance**<br>• **Feature's sensitivity**<br>• **Degree of contribute**<br>• **Group Heterogeneity**<br>• **Individual parameter** |
| Accuracy | • Mid/Low (depend on N of alternatives)<br>• Low calc. speed | • **High**<br>• **High** calc. speed |
| Methodological | • **RUM** | • **Data driven** |

# 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 such as specification of utility function !

◆Use different models depending on the situation.

→ DCM: Policy making, Explanation to citizen’s etc.
ML: Monitoring, short-term forecasting, service design etc.


Thank you for your attention !