

WELCOME.



WORLD STATISTICS
CONGRESS

2025

THE HAGUE

CPS 14
Ordinal Data and Tree-Based Methods

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Wednesday 8 October, 4:00PM - 5:00PM

Research Subject: Ordinal Regression

Title is “Mixture-Based Approximately Unimodal Likelihood Model for Ordinal Data”.

Subject is prediction (**ordinal regression; OR**) for **ordinal data** $(x_1, y_1), (x_2, y_2), \dots \sim (X, Y)$:

- Estimation of $\Pr(y|x)$
- Classification
- Explanatory variable $X \in \mathbb{R}^d$ can be in any format
- Target variable $Y \in [K] := \{1, \dots, K\}$ is categorical and has a “**natural ordinal relation**” $1 < \dots < K$

Many OR applications:

age estimation from facial image; analysis of rating in EC site, credit rating & questionnaire

Facial image

$X = x$



Age $Y = y$

20

<

40



Aaa, Aa, A, Baa, Ba, B, Caa, Ca, C

strongly agree, ag., neutral, disag., strongly disag.

Mathematical characterization of “natural ordinal relation” is key for success in OR.

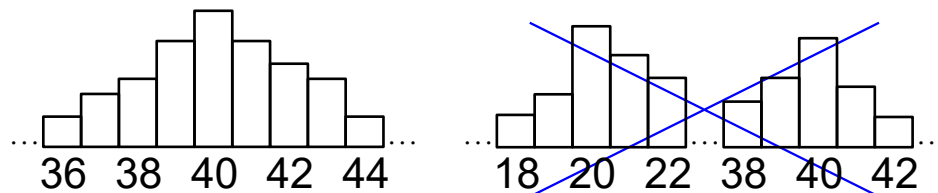
Previous works considered that **conditional probability distribution (CPD)** $(\Pr(y|\mathbf{x}))_{y \in [K]}$ should be **unimodal** in a large domain of X :

$\Pr(1|\mathbf{x}) \leq \dots \leq \Pr(M_x|\mathbf{x})$ and $\Pr(M_x|\mathbf{x}) \geq \dots \geq \Pr(K|\mathbf{x})$ with a conditional mode $M_x \in [K]$

Facial image
 $\mathbf{X} = \mathbf{x}$



CPD of age Y
 $(\Pr(y|\mathbf{x}))_{y \in [K]}$



- J. F. P. da Costa+, “Classification of ordinal data using neural networks,” *ECML*, 2005.
- M. Iannario+, “Cub models: statistical methods and empirical evidence,” in *Modern Analysis of Customer Surveys*, 2011.
- C. Beckham+, “Unimodal probability distributions for deep ordinal classification,” *ICML*, 2017.
- R. Yamasaki, “Unimodal likelihood models for ordinal data,” *TMLR*, 2022.

Setting:

- **21 real-world ordinal datasets** used in a survey (Gutierrez+,15)
- **100 trials, training data size: 800** (large), validation/test data size: 100/remaining
- Estimate CPD $(\Pr(y|x))_{y \in [K]}$ by **multinomial logit model** with a neural network
- Evaluate **unimodality rate (UR)** $\mathbb{E}[\mathbb{I}\{(\Pr(y|x))_{y \in [K]}$ is unimodal. $\}$] with test data

Result: **Many real-world ordinal data would have “high unimodality rate”.**

Tab.1: **mean \pm std of UR & evaluation for uniform random data** (for comparison in same K)

dataset	d	K	UR	dataset	d	K	UR	dataset	d	K	UR	dataset	d	K	UR
BA5'	32	5	.9999 \pm .0006	LEV	4	5	.9594 \pm .0570	CO10	12	10	.8308 \pm .1917	uniform on Δ_3	-	4	.3326 \pm .0135
SWD	10	4	.9996 \pm .0031	CAR	21	4	.9380 \pm .1693	CE10'	16	10	.7239 \pm .2580	" Δ_4	-	5	.1314 \pm .0108
WQR	11	6	.9959 \pm .0186	CH5	8	5	.9334 \pm .0924	ERA	4	9	.7122 \pm .1581	" Δ_5	-	6	.0443 \pm .0065
CO5'	21	5	.9958 \pm .0250	CE5	8	5	.8866 \pm .1102	BA10'	32	10	.6805 \pm .3600	" Δ_8	-	9	.0009 \pm .0010
CO5	12	5	.9889 \pm .0459	BA10	8	10	.8831 \pm .2141	CH10	8	10	.5086 \pm .3127	" Δ_9	-	10	.0001 \pm .0003
CE5'	16	5	.9814 \pm .0366	AB5	10	5	.8785 \pm .1024	CE10	8	10	.4535 \pm .2263				
BA5	8	5	.9760 \pm .0894	CO10'	21	10	.8605 \pm .1948	AB10	10	10	.3232 \pm .1989				

Low: .0001~.3326

High: .3232~.9999

- P. A. Gutierrez et al., “Ordinal regression methods: survey and experimental study,” *TKDE*, 2015.

(Yamasaki,22) developed a UL model for modeling “high unimodality rate” data:

Multinomial logit model:

$$P_{\text{sm},y}(\mathbf{g}(\mathbf{x}))$$

with

$$\mathbf{g} : \mathbb{R}^d \rightarrow \mathbb{R}^K$$

$$P_{\text{sm},y}(\mathbf{u}) \equiv \frac{e^{u_y}}{\sum_{k=1}^K e^{u_k}}$$

UL model:

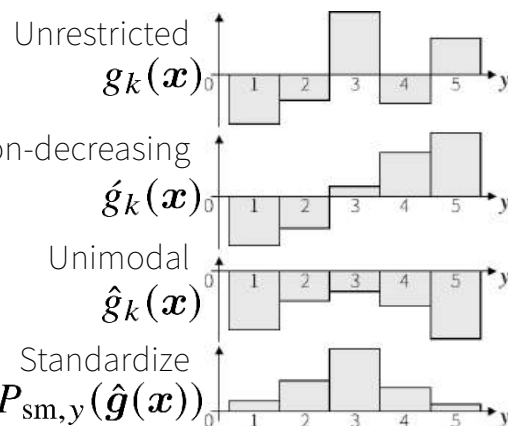
$$P_{\text{sm},y}(\hat{\mathbf{g}}(\mathbf{x}))$$

with

$$\mathbf{g} : \mathbb{R}^d \rightarrow \mathbb{R}^K$$

$$\hat{g}_k(\mathbf{x}) \equiv \begin{cases} g_1(\mathbf{x}) & \text{for } k = 1 \\ \hat{g}_{k-1}(\mathbf{x}) + \{g_k(\mathbf{x})\}^2 & \text{for } k \geq 2 \end{cases}$$

$$\hat{g}_k(\mathbf{x}) \equiv -\{\hat{g}_k(\mathbf{x})\}^2 \quad \text{for } k = 1, \dots, K$$



Theorem (simplified)

UL model is ensured to be unimodal & can represent any unimodal CPD:

$$\{(P_{\text{sm},y}(\hat{\mathbf{g}}(\cdot)))_{y \in [K]} \mid \mathbf{g} : \mathbb{R}^d \rightarrow \mathbb{R}^K\} = \{\mathbf{p} : \mathbb{R}^d \rightarrow \hat{\Delta}_{K-1}\} \text{ with } \hat{\Delta}_{K-1} \equiv \{\text{unimodal } \mathbf{p} \in \Delta_{K-1}\}$$

Motivation:

In many ordinal data, CPD $(\Pr(y|x))_{y \in [K]}$ would be **non-unimodal at some points** $X = x$:

Tab.1: **mean \pm std of UR & evaluation** for uniform random data (for comparison in same K)

dataset	d	K	UR	dataset	d	K	UR	dataset	d	K	UR	dataset	d	K	UR
BA5'	32	5	.9999 \pm .0006	LEV	4	5	.9594 \pm .0570	CO10	12	10	.8308 \pm .1917	uniform on Δ_3	-	4	.3326 \pm .0135
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CE5'	16	5	.9814 \pm .0366	AB5	10	5	.8785 \pm .1024	CE10	8	10	.4535 \pm .2263				
BA5	8	5	.9760 \pm .0894	CO10'	21	10	.8605 \pm .1948	AB10	10	10	.3232 \pm .1989				

High but not 1

UL model has a bias at points with a non-unimodal CPD.

Goal:

To decrease bias and improve prediction performance, develop a novel likelihood model with better representation of ordinal data (higher representation ability).

Working Hypothesis

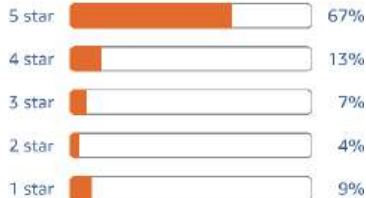
We consider that CPD $(\Pr(y|x))_{y \in [K]}$ of ordinal data should be **close to be unimodal** at points $X = x$ where $(\Pr(y|x))_{y \in [K]}$ is not strictly unimodal.

Rating distribution in EC site
(amazon.com)

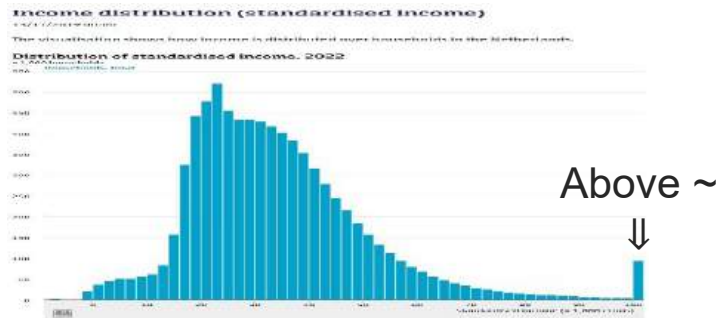
Customer reviews

★★★★☆ 4.2 out of 5

1,486 global ratings



Frequency distribution of Household income
(cbs.nl/en-gb/visualisations/income-distribution)



Mathematically, using Hausdorff distance $D_H(p, S) \equiv \min_{q \in S} \|p - q\|$ and unimodal set $\hat{\Delta}_{K-1} \equiv \{\text{unimodal } p \in \Delta_{K-1}\}$, we further assume that **unimodality deviation** $D_H((\Pr(y|x))_{y \in [K]}, \hat{\Delta}_{K-1})$ of CPD $(\Pr(y|x))_{y \in [K]}$ is low at most $X = x$.

Setting:

- **21 real-world ordinal datasets** used in a survey (Gutierrez+,15)
- **100 trials, training data size: 800** (large), validation/test data size: 100/remaining
- Estimate CPD $(\Pr(y|x))_{y \in [K]}$ by **multinomial logit model** with a neural network
- Evaluate **mean unimodality deviation (MUD)** $\mathbb{E} \left[D_H \left((\Pr(y|x))_{y \in [K]}, \hat{\Delta}_{K-1} \right) \right]$ with test data

Result: **Many real-world ordinal data would have “low unimodality deviation”.**

Tab.2: **mean±std of MUD & evaluation for uniform random data** (for comparison in same K)

dataset	d	K	MUD	dataset	d	K	MUD	dataset	d	K	MUD
BA5'	32	5	.0000±.0000	LEV	4	5	.0003±.0007	CO10	12	10	.0009±.0019
SWD	10	4	.0000±.0002	CAR	21	4	.0003±.0010	CE10'	16	10	.0017±.0023
WQR	11	6	.0000±.0001	CH5	8	5	.0009±.0017	ERA	4	9	.0048±.0049
CO5'	21	5	.0000±.0000	CE5	8	5	.0020±.0024	BA10'	32	10	.0012±.0018
CO5	12	5	.0001±.0003	BA10	8	10	.0000±.0001	CH10	8	10	.0061±.0072
CE5'	16	5	.0004±.0007	AB5	10	5	.0017±.0022	CE10	8	10	.0058±.0052
BA5	8	5	.0000±.0001	CO10'	21	10	.0003±.0009	AB10	10	10	.0105±.0086

dataset	d	K	MUD	
uniform on Δ_3	-	4	.0752±.0026	
"	Δ_4	-	5	.1000±.0023
"	Δ_5	-	6	.1162±.0023
"	Δ_8	-	9	.1365±.0016
"	Δ_9	-	10	.1385±.0014

High: .0752~.1385

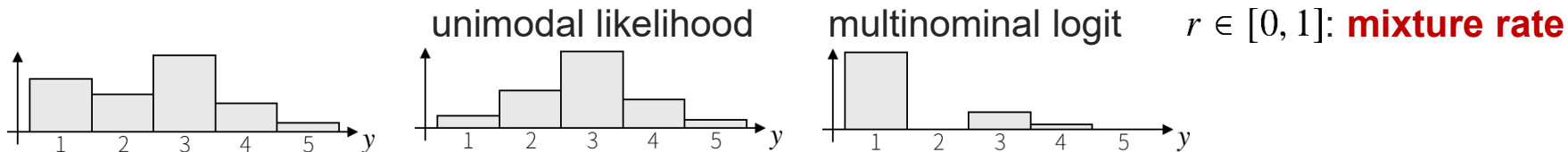
High: .0752~.1385

Low: .0000~.0105

- P. A. Gutierrez et al., “Ordinal regression methods: survey and experimental study,” *TKDE*, 2015.

We propose a **mixture-based AUL model** for modeling “low unimodality deviation” data :

$$P_{\text{AUL},y}(g_1(x), g_2(x); r) \equiv (1 - r)P_{\text{sm},y}(\hat{g}_1(x)) + rP_{\text{sm},y}(g_2(x)) \text{ with } g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}^K,$$



Theorem (simplified)

1. **AUL model can represent any unimodal CPD:**

$$\{P_{\text{AUL},y}(g_1(\cdot), g_2(\cdot); r) \mid g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}^K\} \supseteq \{p : \mathbb{R}^d \rightarrow \hat{\Delta}_{K-1}\}$$

It can represent only unimodal or close to be unimodal CPD.

2. **Unimodality deviation of AUL model is bounded from above by $\sqrt{2}r$:**

$$D_H((P_{\text{AUL},y}(g_1(x), g_2(x); r))_{y \in [K]}, \hat{\Delta}_{K-1}) \leq \sqrt{2}r \text{ for any } g_1, g_2, x$$

3. **Representation ability of AUL model is non-decreasing in r :**

$$\{P_{\text{AUL},y}(g_1(\cdot), g_2(\cdot); r_1) \mid g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}^K\} \subseteq \{P_{\text{AUL},y}(g_1(\cdot), g_2(\cdot); r_2) \mid g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}^K\} \text{ if } r_1 \leq r_2$$

Setting:

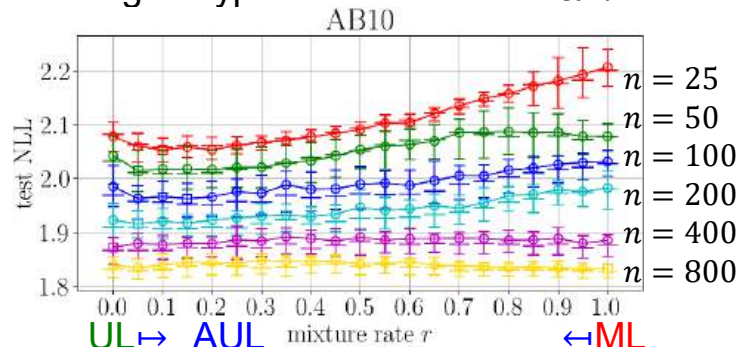
- **21 real-world ordinal datasets** used in a survey (Gutierrez+,15)
- **100 trials, training data size: 25, 50, ..., 800**, validation/test data size: 100/remaining
- Estimate CPD $(\Pr(y|x))_{y \in [K]}$ by **multinomial logit (ML)** ($r = 1$), **unimodal likelihood (UL)** ($r = 0$), **approximately UL (AUL)** ($r \in \{0.05, 0.1, \dots, 0.95\}$) models with a neural network
- Evaluate **negative log likelihood (NLL)**; **mean zero-one & absolute error (MZE & MAE)**
 $\mathbb{E}[\ell(f(x), y)], \ell(j, k) = \mathbb{I}(j \neq k), |j - k|$ for a classifier $f(x) = \operatorname{argmin}_{k \in [K]} \sum_{y=1}^K \ell(k, y) P_y(g(x))$

Result (NLL):

Tab.3: **Number of wins** over 21 datasets in Bonferroni correction with significance level 0.05 of U-test.

NLL	$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL vs ML	18,0	19,0	14,0	7,3	0,10	1,14
AUL vs UL	14,0	12,0	8,0	5,0	3,1	7,1

Fig.1: Typical behaviors in r & n



• P. A. Gutierrez et al., “Ordinal regression methods: survey and experimental study,” *TKDE*, 2015.

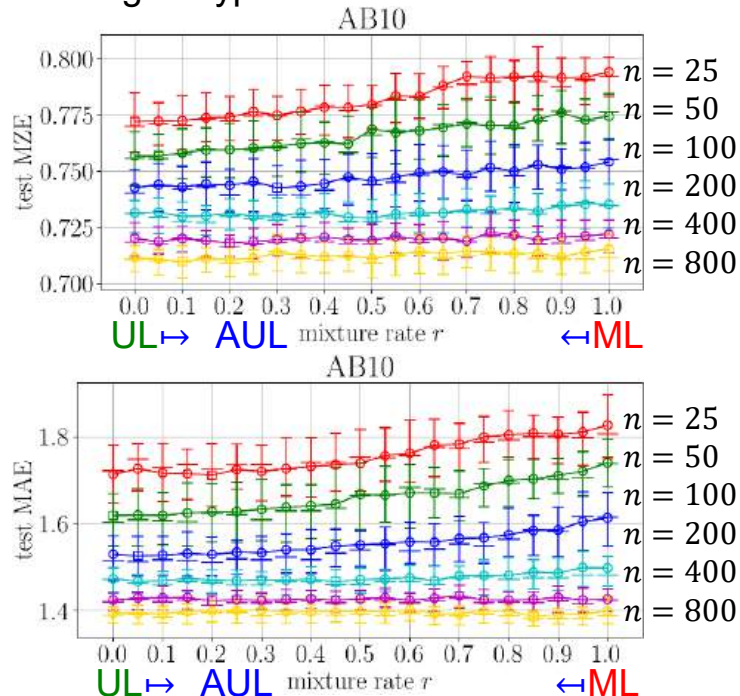
Result (MZE & MAE):

Tab.4: **Number of wins** over 21 datasets in Bonferroni correction with significance level 0.05 of U-test.

MZE	$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL vs ML	19,0	17,0	10,0	1,3	1,3	4,5
AUL vs UL	6,0	7,0	10,0	11,0	8,0	6,0
MAE	$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL vs ML	20,0	16,0	10,0	3,2	0,5	1,5
AUL vs UL	3,0	4,0	2,0	5,0	4,0	7,0

Regarding NLL, MZE & MAE,
AUL model was better than UL model,
and better than ML model for small n .

Fig.2: Typical behaviors in r & n



We verified that **many ordinal data would have “low unimodality deviation”**.

Tab.2: **mean±std of MUD & evaluation for uniform random data** (for comparison in same K)

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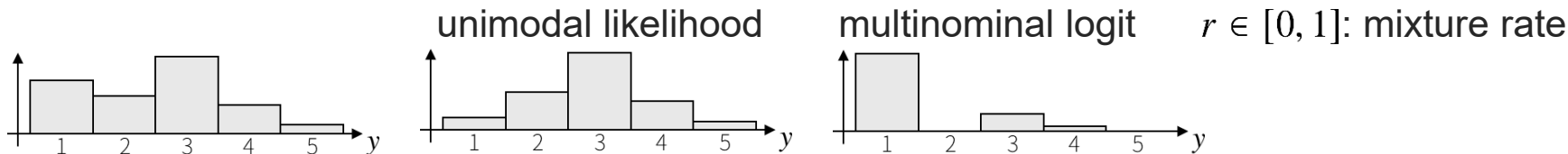
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High: .0752~.1385

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We proposed a **mixture-based approximately unimodal likelihood (AUL) model**:

$$P_{\text{AUL},y}(g_1(x), g_2(x); r) \equiv (1 - r)P_{\text{sm},y}(\hat{g}_1(x)) + rP_{\text{sm},y}(g_2(x)) \text{ with } g_1, g_2 : \mathbb{R}^d \rightarrow \mathbb{R}^K,$$



AUL model gave good prediction for ordinal data when training data size was small.

Thank you for listening!

Contact: ryoya.yamasaki@r.hit-u.ac.jp

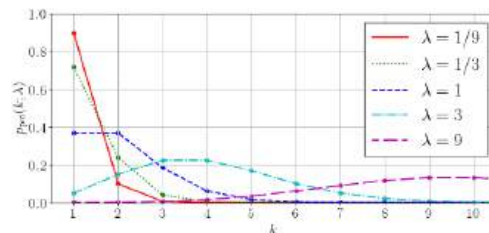
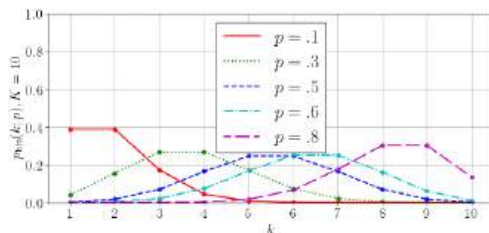
APPENDIX

We define “representation ability” of a likelihood model as a functional of the CPD that that likelihood model can represent (see also (Yamasaki,22)):

For likelihood model $(P_y(\mathbf{g}(x)))_{y \in [K]}$, $\mathbf{g} \in G$, representation ability is $\left\{ (P_y(\mathbf{g}(x)))_{y \in [K]} \mid \mathbf{g} \in G \right\}$.

(da Costa+,05) inspired by shape of binomial and Poisson distributions and developed

$$p_{\text{bin}}(y, \frac{1}{1+e^{-g(x)}}) \text{ with } p_{\text{bin}}(k, p) = \binom{K-1}{k-1} p^{k-1} (1-p)^{K-k} \quad \frac{p_{\text{poi}}(y, e^{g(x)})}{\sum_{k=1}^K p_{\text{poi}}(k, e^{g(x)})} \text{ with } p_{\text{poi}}(k, \lambda) = \frac{\lambda^{k-1} e^{-\lambda}}{(k-1)!}$$

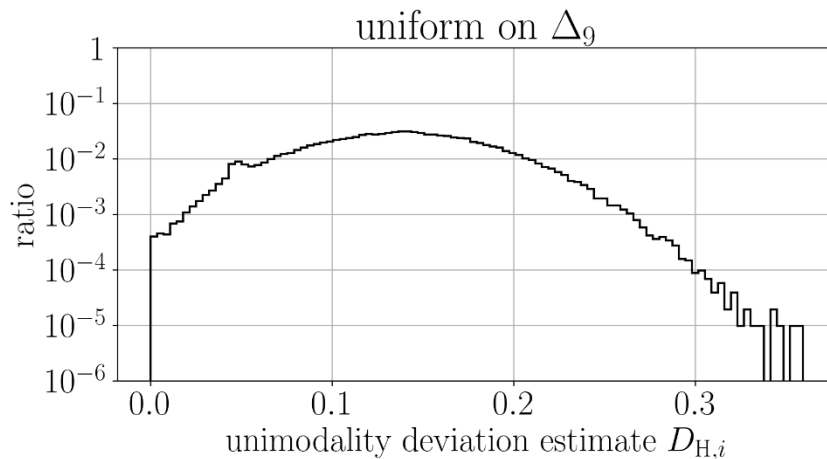
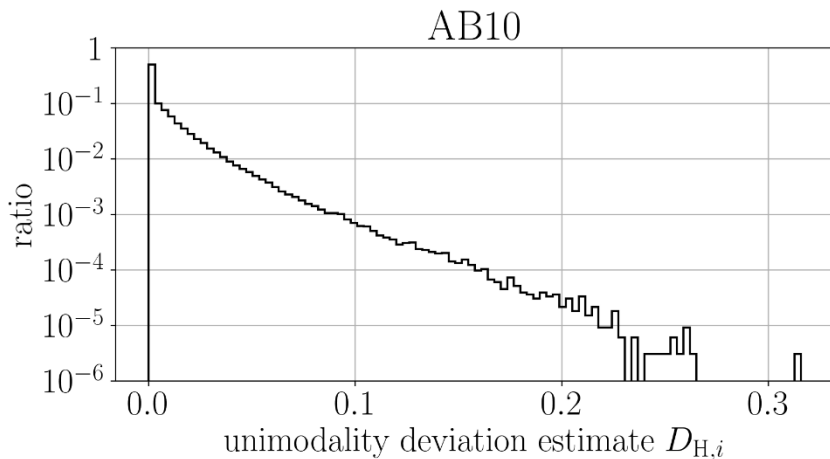


(Iannario+,11) developed a mixture of (da Costa+,05)'s binomial-based and uniform models,
 (Beckham+,17) developed scaling-extension of (da Costa+,05),
 (Yamasaki,22) developed various models with higher representation ability.

- J. F. P. da Costa+, "Classification of ordinal data using neural networks," *ECML*, 2005.
- M. Iannario+, "Cub models: statistical methods and empirical evidence," in *Modern Analysis of Customer Surveys*, 2011.
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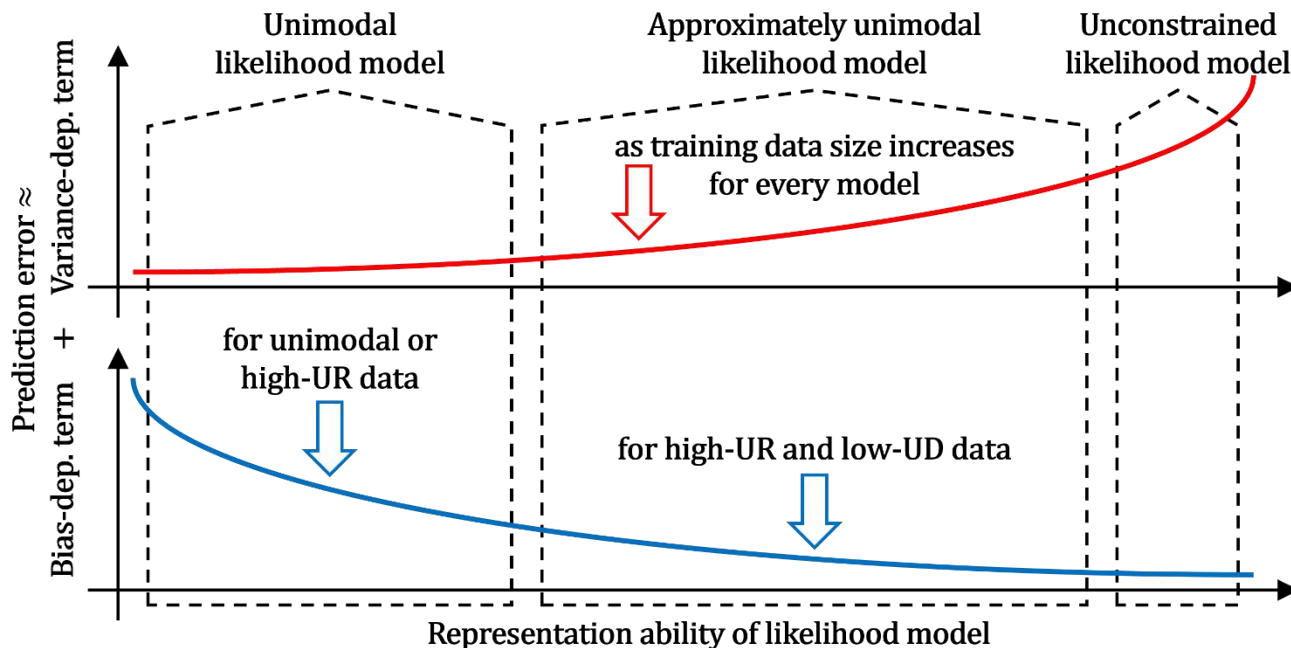
Low Unimodality Deviation

We also evaluated distribution of unimodality deviation $D_H \left((\Pr(y|x))_{y \in [K]}, \hat{\Delta}_{K-1} \right)$ as well.

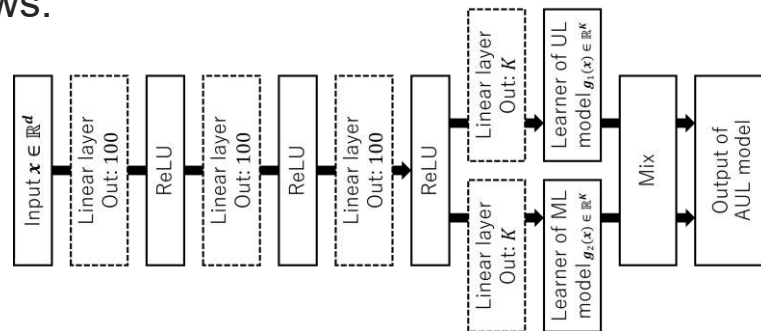
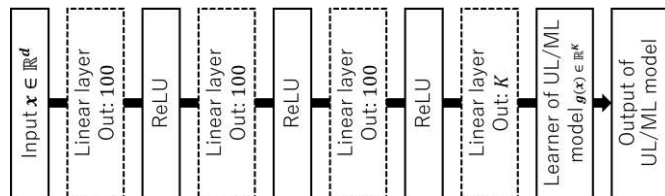


Regarding distribution, many real-world ordinal data would have “low unimodality deviation”.

From bias-variance tradeoff, we expect that likelihood models with good representation of data and smaller representation ability will give good prediction performance with small-size training data.

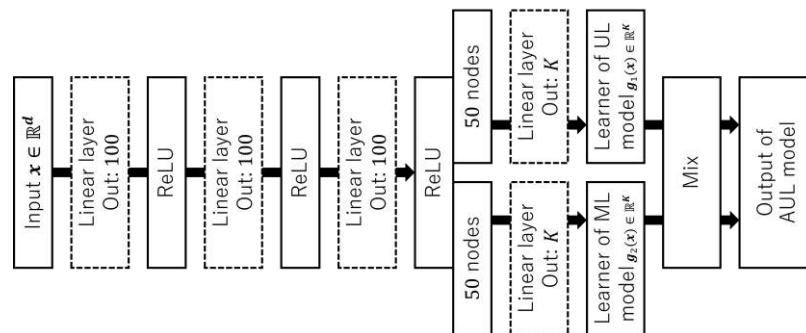
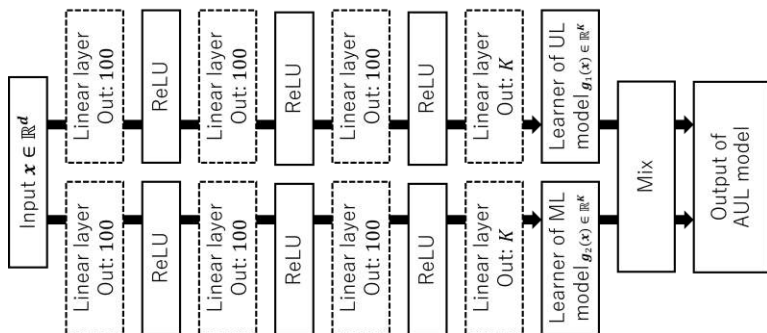


UL/ML and AUL models are implemented as follows:



Those models have different numbers of parameters.

We also tried different implementation of AUL model:



Setting of Experiment

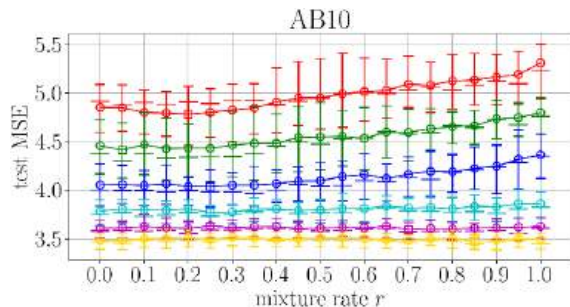
We trained every model by Adam optimization with the NLL as the objective function, mini-batch size 16, and ascending learning rate $10^{2t/300-4}$ at t -th epoch for 300 epochs.

At the end of each epoch, we evaluated the errors, NLL, MZE, MAE, and MSE, with validation data of the size 100.

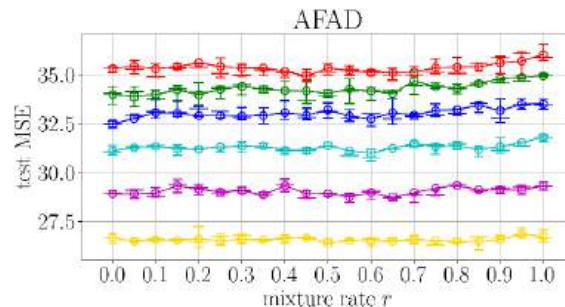
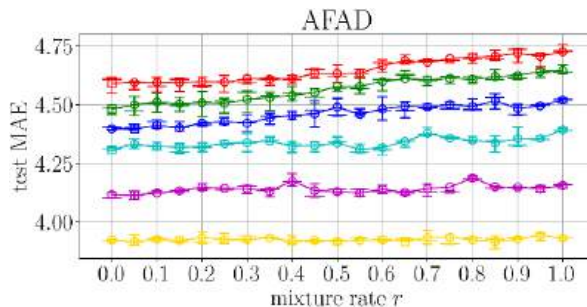
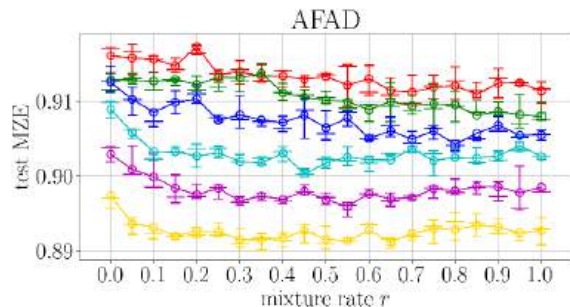
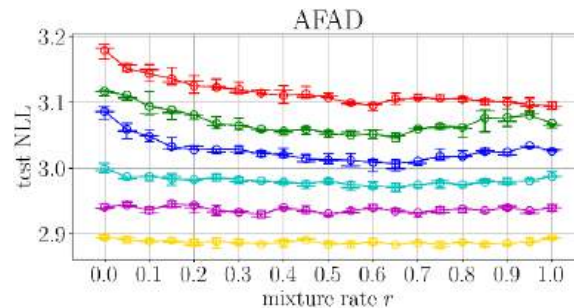
We then adopted a model at the epoch when the validation error got minimum (and simultaneously selected the mixture rate r), and calculated the error with remaining test data of the size $(n_{\text{tot}} - n - 100)$ for that model.

Result of Experiment

We also evaluate mean squares error (MSE).



We also experimented face-age estimation with $n = 1250, 2500, 5000, 10000, 20000, 40000$.



We also experimented **cumulative-logits (CL)**, **proportional-odds (PO) CL**, **POUL** models:

CL:

$$P_{cl,y}(g(x)) \equiv \begin{cases} \frac{1}{1+e^{-g_1(x)}} & \text{for } k = 1 \\ 1 - \frac{1}{1+e^{-g_{K-1}(x)}} & \text{for } k = K \\ \frac{1}{1+e^{-g_y(x)}} - \frac{1}{1+e^{-g_{y-1}(x)}} & \text{for other } k \end{cases}$$

POCL:

$$P_{cl,y}(g(x)) \text{ with } g(x) = (\hat{b}_1 - a(x), \dots, \hat{b}_{K-1} - a(x)),$$

$$\hat{b}_k = \begin{cases} b_1 & \text{for } k = 1 \\ \hat{b}_{k-1} + \{b_k\}^2 & \text{for } k \geq 2 \end{cases}$$

POUL:

$$P_{sm,y}(\hat{g}(x)) \text{ with } \hat{g}(x) = (-\{\hat{b}_1 - a(x)\}^2, \dots, -\{\hat{b}_K - a(x)\}^2)$$

NLL			$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs	ML	18,0	19,0	14,0	7,3	0,10	1,14
AUL	vs	UL	14,0	12,0	8,0	5,0	3,1	7,1
AUL	vs	CL	17,0	14,0	10,2	6,6	3,5	3,8
AUL	vs	POCL	16,1	19,0	16,1	14,4	12,7	7,4
AUL	vs	POUL	11,1	14,3	12,2	12,1	11,0	11,0

MZE			$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs	ML	19,0	17,0	10,0	1,3	1,3	4,5
AUL	vs	UL	6,0	7,0	10,0	11,0	8,0	6,0
AUL	vs	CL	16,0	8,0	5,0	3,1	2,1	2,3
AUL	vs	POCL	18,1	17,0	16,0	15,0	14,1	10,2
AUL	vs	POUL	4,1	6,0	10,0	14,0	17,0	14,0

POCL model is popular and often called “ordinal regression model”.

AUL model is better for small n .

MAE			$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs	ML	20,0	16,0	10,0	3,2	0,5	1,5
AUL	vs	UL	3,0	4,0	2,0	5,0	4,0	7,0
AUL	vs	CL	11,0	11,0	7,0	2,0	1,1	1,1
AUL	vs	POCL	6,0	8,0	12,0	8,0	9,1	6,2
AUL	vs	POUL	6,0	4,0	5,1	8,1	9,0	11,0

We also experimented unimodality-promoting regularization learning (UPRL) methods. Here, **ML'** is ML + UPRL; **AUL'** is AUL + UPRL.

NLL		$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs ML	18,0	19,0	14,0	7,3	0,10	1,14
AUL	vs UL	14,0	12,0	8,0	5,0	3,1	7,1
AUL	vs ML'	13,2	12,0	7,2	2,5	0,12	1,10
AUL	vs AUL'	0,6	0,2	0,2	0,0	0,0	0,0

AUL model is better than **ML'** for small n .
AUL' model is the best for small n .

MZE		$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs ML	19,0	17,0	10,0	1,3	1,3	4,5
AUL	vs UL	6,0	7,0	10,0	11,0	8,0	6,0
AUL	vs ML'	15,0	7,0	3,0	0,1	2,3	4,4
AUL	vs AUL'	0,2	0,0	1,0	1,0	0,0	1,1

MAE		$n=25$	$n=50$	$n=100$	$n=200$	$n=400$	$n=800$
AUL	vs ML	20,0	16,0	10,0	3,2	0,5	1,5
AUL	vs UL	3,0	4,0	2,0	5,0	4,0	7,0
AUL	vs ML'	14,0	8,0	3,0	0,1	0,3	4,5
AUL	vs AUL'	0,0	0,0	0,0	0,0	0,0	0,0

- S. Belharbi+, “Non-parametric uni-modality constraints for deep ordinal classification,” *arXiv preprint arXiv:1911.10720*, 2020.
- T. Albuquerque+, “Ordinal losses for classification of cervical cancer risk,” *PeerJ Computer Science*, vol. 7, p. e457, 2021.

THANK YOU.