NEURAL INFORMATION PROCESSING SYSTEMS

TEXAS
The University of Texas at Austin

CARD: CLASSIFICATION AND REGRESSION DIFFUSION MODELS

XIZEWEN HAN*, HUANGJIE ZHENG* & MINGYUAN ZHOU
Department of Statistics and Data Sciences & McCombs School of Business, The University of Texas at Austin

NeurIPS 2022

Modeling $P(y \mid x)$ instead of $\mathbb{E}(y \mid x)$

How do we model $P(y \mid x)$, the *conditional distribution* of a continuous or categorical response variable y given its covariates x, if we are interested in more than a point estimate of the conditional mean $\mathbb{E}(y \mid x)$?

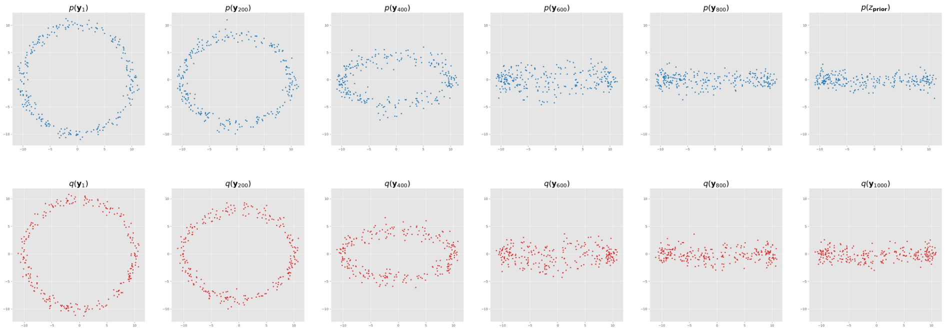
Potential scenarios:

- Uncertainty estimation plays an important role for the problem in hand
- $P(y \mid x)$ is multi-modal, *e.g.*, when there are missing covariates in x

Modeling $P(y \mid x)$ instead of $\mathbb{E}(y \mid x)$

- CARD

reverse diffusion process
$p_\theta(y_{t-1} \mid y_t, x)$



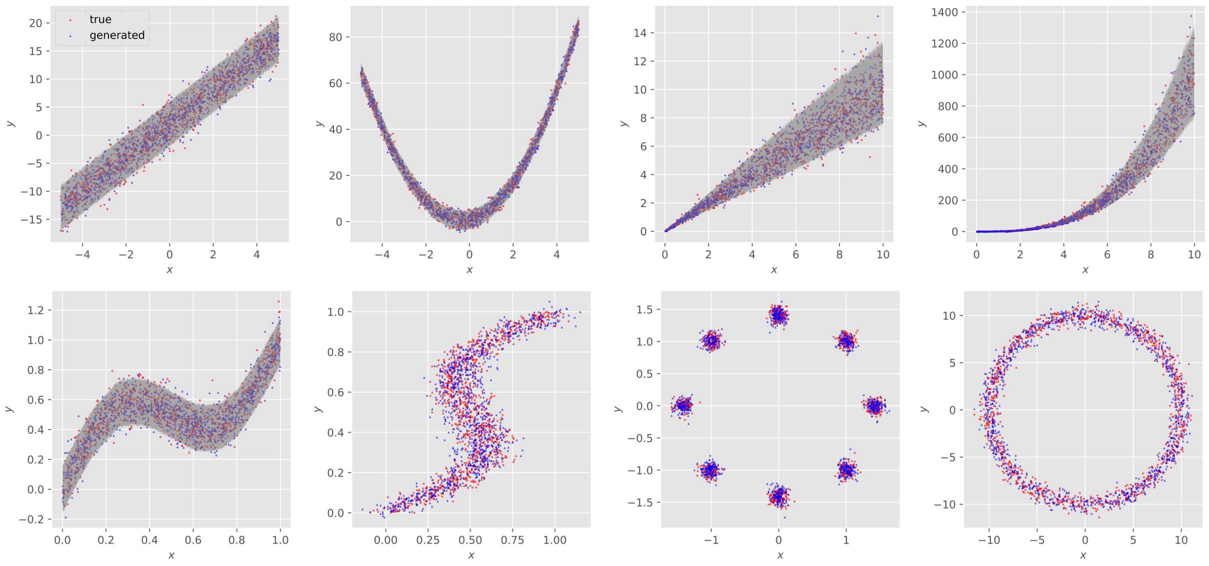
$\cancel{\boldsymbol{y}_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})}$

$\boldsymbol{y}_T \sim \mathcal{N}(f_\phi(\boldsymbol{x}), \boldsymbol{I})$

forward diffusion process
$q(y_t \mid y_{t-1}, x)$

$$\mathcal{L}_{\boldsymbol{\epsilon}} = \left|\left|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\left(\boldsymbol{x}, \sqrt{\bar\alpha_t}\boldsymbol{y}_0 + \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon} + (1-\sqrt{\bar\alpha_t}) f_\phi(\boldsymbol{x}), f_\phi(\boldsymbol{x}), t\right)\right|\right|^2$$

Regression



Regression toy example scatter plots.
(**Top**) left to right: linear regression, quadratic regression, log-log linear regression, log-log cubic regression;
(**Bottom**) left to right: sinusoidal regression, inverse sinusoidal regression, 8 Gaussians, full circle.

Regression

Dataset	RMSE ↓ PBP	MC Dropout	Deep Ensembles	GCDS	CARD (ours)
Boston	2.89 ± 0.74	3.06 ± 0.96	3.17 ± 1.05	2.75 ± 0.58	$\mathbf{2.61 \pm 0.63}$
Concrete	5.55 ± 0.46	5.09 ± 0.60	4.91 ± 0.47	5.39 ± 0.55	$\mathbf{4.77 \pm 0.46}$
Energy	1.58 ± 0.21	1.70 ± 0.22	2.02 ± 0.32	0.64 ± 0.09	$\mathbf{0.52 \pm 0.07}$
Kin8nm[1]	9.42 ± 0.29	7.10 ± 0.26	8.65 ± 0.47	8.88 ± 0.42	$\mathbf{6.32 \pm 0.18}$
Naval[2]	0.41 ± 0.08	0.08 ± 0.03	0.09 ± 0.01	0.14 ± 0.05	$\mathbf{0.02 \pm 0.00}$
Power	4.10 ± 0.15	4.04 ± 0.14	4.02 ± 0.15	4.11 ± 0.16	$\mathbf{3.93 \pm 0.17}$
Protein	4.65 ± 0.02	4.16 ± 0.12	4.45 ± 0.02	4.50 ± 0.02	$\mathbf{3.73 \pm 0.01}$
Wine	0.64 ± 0.04	$\mathbf{0.62 \pm 0.04}$	0.63 ± 0.04	0.66 ± 0.04	0.63 ± 0.04
Yacht	0.88 ± 0.22	0.84 ± 0.27	1.19 ± 0.49	0.79 ± 0.26	$\mathbf{0.65 \pm 0.25}$
Year	8.86± NA	8.77± NA	8.79± NA	9.20± NA	**8.70**± NA
# best	0	1	0	0	**9**

Dataset	NLL ↓ PBP	MC Dropout	Deep Ensembles	GCDS	CARD (ours)
Boston	2.53 ± 0.27	2.46 ± 0.12	2.35 ± 0.16	18.66 ± 8.92	$\mathbf{2.35 \pm 0.12}$
Concrete	3.19 ± 0.05	3.21 ± 0.18	$\mathbf{2.93 \pm 0.12}$	13.64 ± 6.88	2.96 ± 0.09
Energy	2.05 ± 0.05	1.50 ± 0.11	1.40 ± 0.27	1.46 ± 0.72	$\mathbf{1.04 \pm 0.06}$
Kin8nm	-0.83 ± 0.02	-1.14 ± 0.05	-1.06 ± 0.02	-0.38 ± 0.36	$\mathbf{-1.32 \pm 0.02}$
Naval	-3.97 ± 0.10	-4.45 ± 0.38	-5.94 ± 0.10	-5.06 ± 0.48	$\mathbf{-7.54 \pm 0.05}$
Power	2.92 ± 0.02	2.90 ± 0.03	2.89 ± 0.02	2.83 ± 0.06	$\mathbf{2.82 \pm 0.02}$
Protein	3.05 ± 0.00	2.80 ± 0.08	2.89 ± 0.02	2.81 ± 0.09	$\mathbf{2.49 \pm 0.03}$
Wine	1.03 ± 0.03	0.93 ± 0.06	0.96 ± 0.06	6.52 ± 21.86	$\mathbf{0.92 \pm 0.05}$
Yacht	1.58 ± 0.08	1.73 ± 0.22	1.11 ± 0.18	$\mathbf{0.61 \pm 0.34}$	0.90 ± 0.08
Year	3.69± NA	3.42± NA	3.44± NA	3.43± NA	**3.34**± NA
# best	0	0	1	1	**8**

Dataset	QICE ↓ PBP	MC Dropout	Deep Ensembles	GCDS	CARD (ours)
Boston	3.50 ± 0.88	3.82 ± 0.82	$\mathbf{3.37 \pm 0.00}$	11.73 ± 1.05	3.45 ± 0.83
Concrete	2.52 ± 0.60	4.17 ± 1.06	2.68 ± 0.64	10.49 ± 1.01	$\mathbf{2.30 \pm 0.66}$
Energy	6.54 ± 0.90	5.22 ± 1.02	$\mathbf{3.62 \pm 0.58}$	7.41 ± 2.19	4.91 ± 0.94
Kin8nm	1.31 ± 0.25	1.50 ± 0.32	1.17 ± 0.22	7.73 ± 0.80	$\mathbf{0.92 \pm 0.25}$
Naval	4.06 ± 1.25	12.50 ± 1.95	6.64 ± 0.60	5.76 ± 2.25	$\mathbf{0.80 \pm 0.21}$
Power	$\mathbf{0.82 \pm 0.19}$	1.32 ± 0.37	1.09 ± 0.26	1.77 ± 0.33	0.92 ± 0.21
Protein	1.69 ± 0.09	2.82 ± 0.41	2.17 ± 0.16	2.33 ± 0.18	$\mathbf{0.71 \pm 0.11}$
Wine	$\mathbf{2.22 \pm 0.64}$	2.79 ± 0.56	2.37 ± 0.63	3.13 ± 0.79	3.39 ± 0.69
Yacht	6.93 ± 1.74	10.33 ± 1.34	7.22 ± 1.41	$\mathbf{5.01 \pm 1.02}$	8.03 ± 1.17
Year	2.96± NA	2.43± NA	2.56± NA	1.61± NA	**0.53**± NA
# best	2	0	2	1	**5**

Evaluation metric tables of UCI regression tasks.
(**Top to Bottom**) RMSE, NLL, and QICE.

QICE: the mean absolute error between the proportion of true data contained by each quantile interval of the generated y samples and the optimal proportion $1/M$.

$$\text{QICE} := \frac{1}{M}\sum_{m=1}^{M}\left|r_m - \frac{1}{M}\right|, \text{ where } r_m = \frac{1}{N}\sum_{n=1}^{N}\mathbb{1}_{y_n \geq \hat{y}_n^{\text{low}_m}} \cdot \mathbb{1}_{y_n \leq \hat{y}_n^{\text{high}_m}}.$$

Classification

By assuming the categorical response variables to come from real continuous spaces, we can apply the same modeling framework in training and inference for regression and classification:

Algorithm 1 Training (Regression)

Pre-train $f_\phi(\boldsymbol{x})$ that predicts $\mathbb{E}(\boldsymbol{y} \mid \boldsymbol{x})$ with MSE
repeat
  Draw $y_0 \sim q(\boldsymbol{y}_0 \mid \boldsymbol{x})$
  Draw $t \sim \text{Uniform}(\{1 \dots T\})$
  Draw $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
  Compute noise estimation loss

$$\mathcal{L}_{\boldsymbol{\epsilon}} = \Big|\Big|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\big(\boldsymbol{x}, \sqrt{\bar{\alpha}_t}\boldsymbol{y}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} + (1-\sqrt{\bar{\alpha}_t})f_\phi(\boldsymbol{x}), f_\phi(\boldsymbol{x}), t\big)\Big|\Big|^2$$

  Take numerical optimization step on:

$$\nabla_\theta \mathcal{L}_{\boldsymbol{\epsilon}}$$

until Convergence

Algorithm 2 Inference (Regression)

$\boldsymbol{y}_T \sim \mathcal{N}(f_\phi(\boldsymbol{x}), \boldsymbol{I})$
for $t = T$ to 1 **do**
  Draw $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$if $t > 1$
  Calculate reparameterized $\hat{\boldsymbol{y}}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}\Big(\boldsymbol{y}_t - (1-\sqrt{\bar{\alpha}_t})f_\phi(\boldsymbol{x}) - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_\theta\big(\boldsymbol{x}, \boldsymbol{y}_t, f_\phi(\boldsymbol{x}), t\big)\Big)$
  Let $\boldsymbol{y}_{t-1} = \gamma_0\hat{\boldsymbol{y}}_0 + \gamma_1\boldsymbol{y}_t + \gamma_2 f_\phi(\boldsymbol{x}) + \sqrt{\tilde{\beta}_t}\boldsymbol{z}$ if $t > 1$, else set $\boldsymbol{y}_{t-1} = \hat{\boldsymbol{y}}_0$
end for
return $\boldsymbol{y}_0$

Adaptation for classification tasks:

1. For $\boldsymbol{y}_0$, replace the response variable with a one-hot encoded label vector;
2. For $f_\phi(\boldsymbol{x})$, replace the mean estimator with a classifier pre-trained with the cross-entropy objective, which outputs softmax probabilities of the class labels.

Classification

- Assess model prediction confidence ***at the instance level***

For each test instance, we sample N class prototype reconstructions by CARD, and perform the following computations:

1. We directly calculate the prediction interval width (PIW) between the 2.5^{th} and 97.5^{th} percentiles of the N reconstructed values for all classes, *i.e.*, with C different classes in total, we would obtain C PIWs for each instance;
2. We then convert the samples into probability space as a softmax form of a temperature-weighted Brier score, and apply paired two-sample t-test as an uncertainty estimation method: we obtain the 1^{st} and 2^{nd} most predicted classes for each instance, and test whether the difference in their mean predicted probability is statistically significant.

$$\Pr(y=k) = \frac{\exp(-(\boldsymbol{y}_0 - \mathbf{1}_C)_k^2/\tau)}{\sum_{i=1}^{C}\exp(-(\boldsymbol{y}_0 - \mathbf{1}_C)_i^2/\tau)}; \ \hat{y} = \arg\max_k \big(-(\boldsymbol{y}_0 - \mathbf{1}_C)_k^2\big).$$

Classification

Dataset	Accuracy	PIW Correct	PIW Incorrect	Acc. by PIW	Acc. by t-test Result Rejected	Acc. by t-test Result Not-Rejected (Count)
FashionMNIST						
overall	91.79%	0.67	3.20	89.36%	92.07%	55.84% (77)
most acc.	98.50%	0.39	2.08			
least acc.	74.80%	1.37	3.26			
CIFAR-10						
overall	90.95%	2.37	21.52	87.84%	91.25%	42.86% (63)
most acc.	96.00%	0.55	29.27			
least acc.	81.90%	5.48	21.45			
CIFAR-100						
overall	71.42%	0.59	3.91	60.53%	71.56%	35.90% (39)
most acc.	95.00%	0.16	1.92			
least acc.	44.00%	5.09	5.84			
ImageNet-100						
overall	82.34%	2.06	13.73	68.64%	82.90%	34.48% (58)
most acc.	98.00%	0.72	8.06			
least acc.	42.00%	6.79	14.15			
ImageNet (f_ϕ Accuracy 73.87%)						
overall	74.28%	0.65	3.11	69.22%	74.63%	24.93% (349)
most acc.	98.00%	0.27	2.80			
least acc.	8.00%	20.10	50.07			
ImageNet (f_ϕ Accuracy 76.13%)						
overall	76.20%	0.51	3.60	75.21%	76.30%	25.71% (105)
most acc.	98.00%	0.08	2.66			
least acc.	18.00%	1.87	3.26			
ImageNet (f_ϕ Accuracy 80.30%)						
overall	80.35%	1.42	5.13	74.08%	80.59%	27.63% (228)
most acc.	98.00%	0.49	2.34			
least acc.	8.00%	91.70	84.61			

PIW (multiplied by 100), accuracy by predicting with the narrowest PIW, and accuracy by t-test rejection status, for the FashionMNIST, CIFAR-10, CIFAR-100, ImageNet-100, and ImageNet classification tasks, over a single experimental run. We only report the PIW for all test instances, and within the most and least accurate classes.

- Paper: https://arxiv.org/abs/2206.07275
- Code: https://github.com/XzwHan/CARD