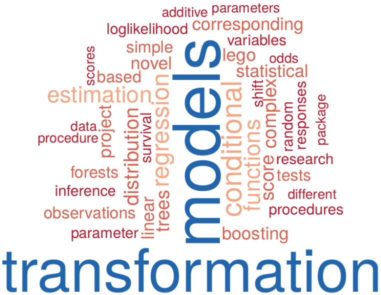
Ensembling deep transformation models

Advances in statistical modeling with neural networks

Lucas Kook, Andrea Goetschi, Philipp FM Baumann,
Torsten Hothorn, Beate Sick



CMStatistics 2022
December 16, 2022

Kook_Lucas
LucasKook

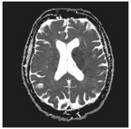
Setup

Available data:

Tabular

5.0	3.6	1.4
5.4	3.9	1.7
4.6	3.4	1.4
5.0	3.4	1.5
4.4	2.9	1.4
4.9	3.1	1.5
5.4	3.7	1.5
4.8	3.4	1.6
4.8	3.0	1.4

Image



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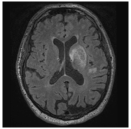

Text

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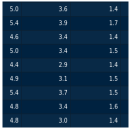

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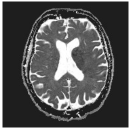

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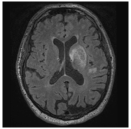
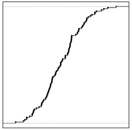


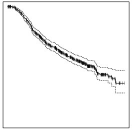
Text

Response:

Continuous



Survival



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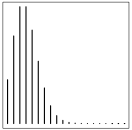
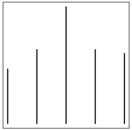


Ordinal



How do changes in the predictors propagate to the **distribution** of the response?

Setup

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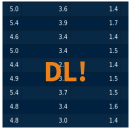

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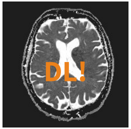

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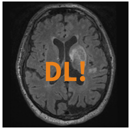

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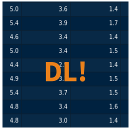

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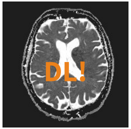

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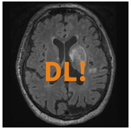

Text

$\longrightarrow$

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Continuous

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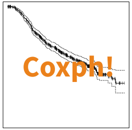

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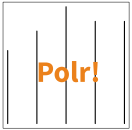

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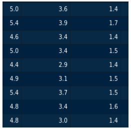

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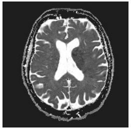

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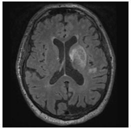
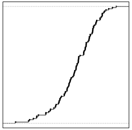


Text

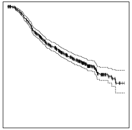
How can we handle non-tabular data?

Response:

Continuous



Survival



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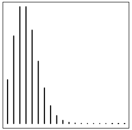

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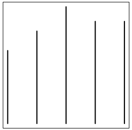


How can we cover all response types?

A bird's eye view on regression

$$F_{Y|\boldsymbol{X}=\boldsymbol{x}}(\cdot) := \mathbb{P}(Y \leq \cdot \mid \boldsymbol{X} = \boldsymbol{x})$$

- Normal linear regression

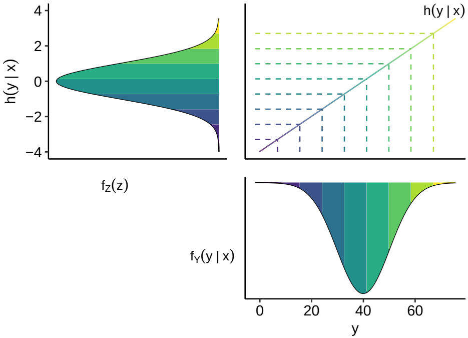
$$F_{Y|\boldsymbol{X}=\boldsymbol{x}}(y) = \Phi(\sigma^{-1}(y - \alpha + \boldsymbol{x}^\top \beta))$$

- Proportional odds logistic regression

$$F_{Y|\boldsymbol{X}=\boldsymbol{x}}(y_k) = \operatorname{expit}(\vartheta_k + \boldsymbol{x}^\top \beta)$$

- Cox proportional hazards model

$$F_{Y|\boldsymbol{X}=\boldsymbol{x}}(y) = 1 - \exp(-\exp(\log \Lambda_0(y) + \boldsymbol{x}^\top \beta))$$



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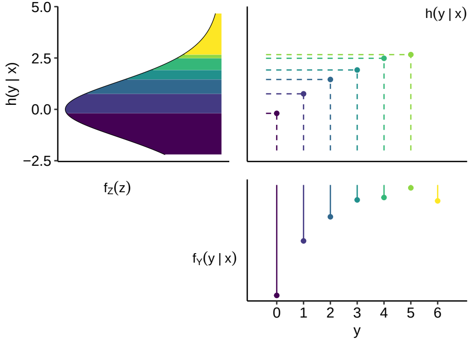

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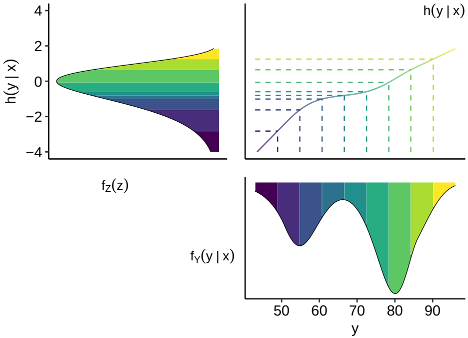

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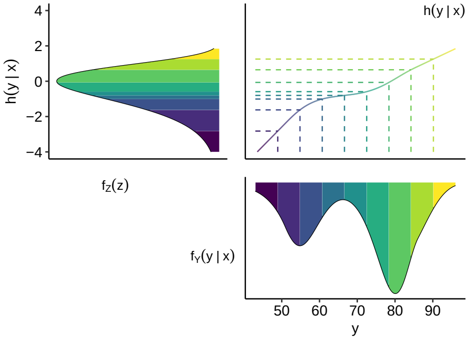
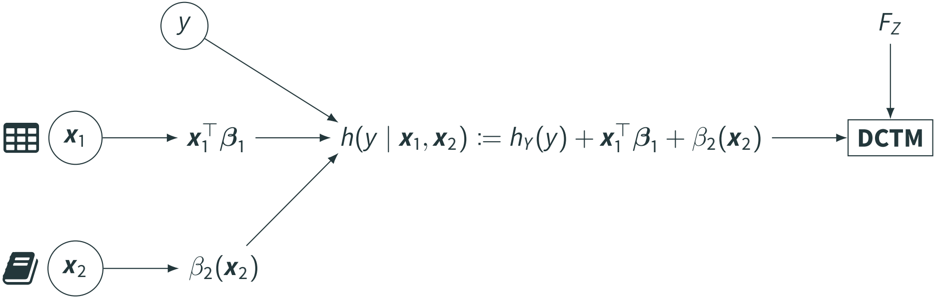
- And many more ...



Transformation models

$$F_{Y|\boldsymbol{X}=\boldsymbol{x}}(y) = F_Z(h_Y(y) + \boldsymbol{x}^\top \boldsymbol{\beta})$$

Example: Parametrization of an additive transformation function

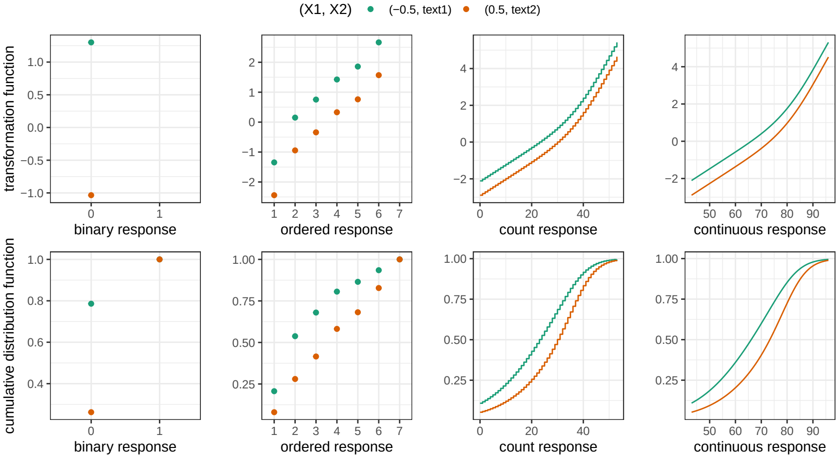


DCTM: Deep conditional transformation model : Tabular data : Text data

10.48550/arXiv.2211.13665

Example: Parametrization of an additive transformation function

$$h(y \mid \boldsymbol{x}_1, \boldsymbol{x}_2) := h_Y(y) + \boldsymbol{x}_1^\top \beta_1 + \beta_2(\boldsymbol{x}_2)$$



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DCTMs are not enough

Individual deep learning models may make **unreliable predictions**

Common criticism:

- No uncertainty quantification
- Small sample sizes
- Stochastic fitting procedure

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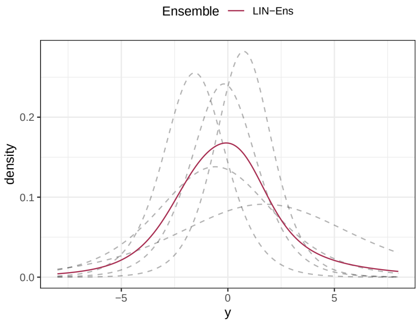
Deep ensembles improve prediction

1. Fit M instances of the same model
2. Average their M predictions



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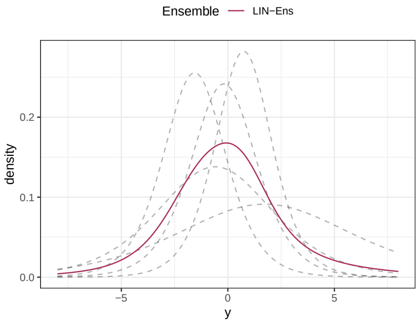
Deep ensembles lose additivity and interpretability!



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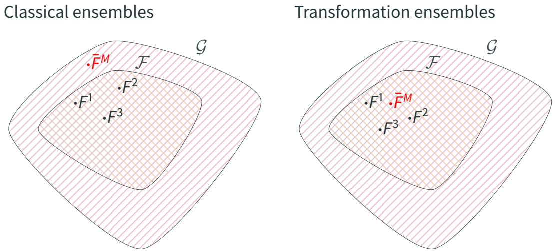
Transformation ensembles

Transformation ensembles average the **transformation function** instead

$$\bar{F}^M_{Y|\boldsymbol{X}=\boldsymbol{x}}(\cdot) := F_Z\left(\sum_{m=1}^{M} h^m_Y(\cdot) + \beta^m(\boldsymbol{x})\right)$$

10.48550/arXiv.2205.12729

- Remain partially **interpretable**



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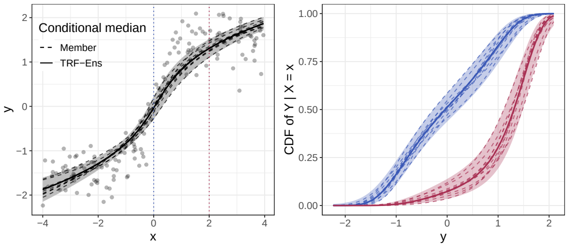
10.48550/arXiv.2205.12729

- Remain partially **interpretable**
- Quantify **algorithmic uncertainty**



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- Remain partially **interpretable**
- Quantify **algorithmic uncertainty**
- Perform **on par** with deep ensembles

Deep Interpretable Ensembles

Lucas Kook[1,2], Andrea Götschi[1], Philipp F. M. Baumann[3], Torsten Hothorn[1], Beate Sick[1,2]

Fit transformation ensembles in R with ‘deeptrafo’

1. Model formula

```
fm <- vote_count ~ 0 + s(budget, df = 6) +  popularity + deep(texts)
```

Fit transformation ensembles in R with ‘deeptrafo’

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2. Neural network

```r
embd_mod <- function(x) x |>
  layer_embedding(input_dim = nr_words, output_dim = embedding_size) |>
  layer_lstm(units = 50, return_sequences = TRUE) |>
  layer_lstm(units = 50, return_sequences = FALSE) |> layer_dropout(rate = 0.1) |>
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```

4. Fit ensemble

```
ens <- ensemble(m, n_ensemble = 3, epochs = 50, batch_size = 64)
```

Example: Movie ratings

Prediction for a single movie from the test data

- Budget: 2.7×10^8 \$
- Popularity: 57.93
- Overview: “superman returns discover 5 absence allowed lex luthor walk free closest abandoned moved luthor plots ultimate revenge millions killed change planet forever ridding steel ”

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Test NLL:

```
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## members1 members2 members3     mean  ensemble
##     8.24     8.28     8.16     8.23     8.11
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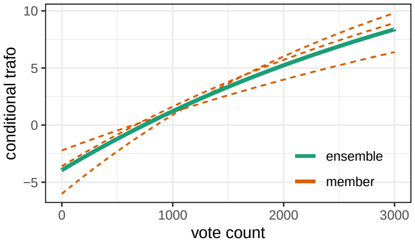

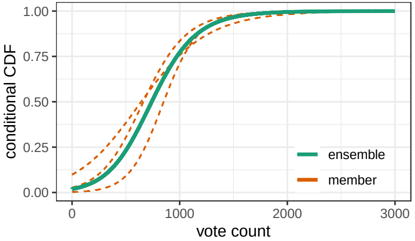

Acknowledgements

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zh aw School of Engineering

Swiss National Science Foundation

NOVARTIS