SubTab: Subsetting Features of Tabular Data for Self-Supervised Representation Learning

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NEURAL INFORMATION PROCESSING SYSTEMS

Abstract

Problem Statement

- Self-supervised learning in tabular data is understudied:
  - Lack of effective data augmentation methods
  - Lack of specialized architectures for tabular data

SubTab

- Introduces effective methods for tabular data
- Achieves 98.31%, the state of the art (SOTA), on MNIST data in tabular format and surpasses existing baselines on three other real-world datasets by a significant margin.
- Makes a simple MLP-based model perform on par with CNN-based SOTA models

Two key methods

- Reconstruction of all features from the subset of features
- Aggregating the embeddings of the subsets

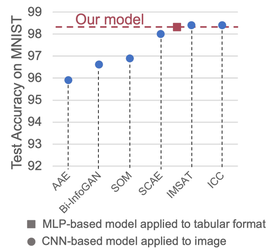


Figure-1: Comparing MLP-based SubTab to CNN-based SOTA models

Methodology

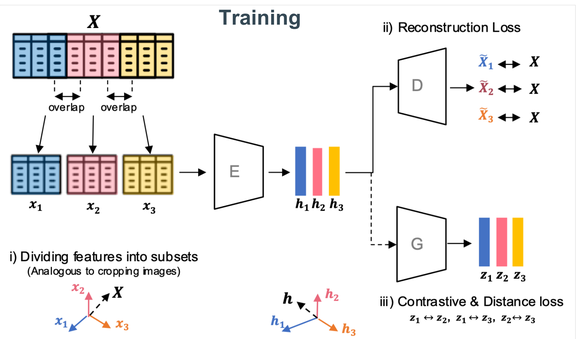


Figure-2: SubTab framework during training

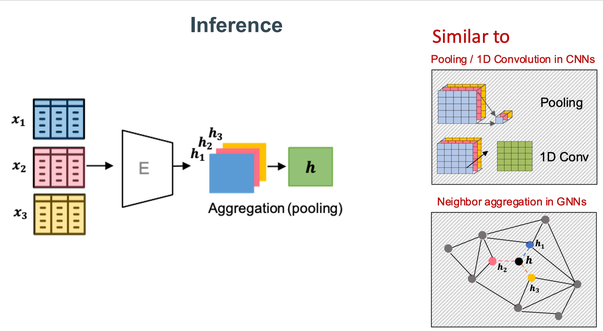


Figure-3: SubTab framework at test time

Results

Comparing SubTab to self-supervised and autoencoder baselines

Type	Models	MNIST	Income	Blog	Obesity	TCGA
Supervised baseline	Logistic Regression	92.60±0.03	84.68±0.05	84.15±0.12	62.35±4.02	36.98± 1.25
	Random Forest	96.96±0.06	84.62±0.07	83.61±0.15	67.45±2.23	61.62± 1.02
	XGBoost	98.02±0.086	86.11±0.20	84.29±0.23	64.05±4.52	72.61±1.31
Autoencoder baseline	AE	92.77±0.32	84.67±0.07	84.06±0.24	61.96±3.28	55.16±0.75
	AE w/ Dropout (p=0.2)	94.31±0.28	85.00±0.10	84.18±0.20	62.74±4.38	56.87±2.26
Self-supervised	DAE (RF)	96.30±0.14 (S)	84.37±0.36 (G)	84.12±0.29 (G)	56.43±5.79 (G)	54.31±1.39 (G)
	CAE (NC)	96.39±0.20 (S)	84.24±0.18 (G)	84.3±0.31 (G)	62.26±5.01 (G)	54.20±1.17 (G)
	VIME-self	95.23±0.17 (S)	84.43±0.08 (G)	84.11±0.27 (G)	66.45±4.54 (G)	55.11±1.37 (G)
	SubTab with:					
	Base model (No noise)	97.26±0.2	85.31±0.08	84.29±0.26	68.01±3.07	57.02±1.50
	+Noise	97.47±0.18 (S)	85.34±0.07 (G)	84.47±0.15 (G)	**71.13±4.08 (G)**	**58.25±1.36 (G)**
	+Distance loss	97.52±0.14 (S)	**85.35±0.06** (G)	**84.64±0.19** (G)	69.25±4.19 (G)	58.15±1.56 (G)
	+LatentDim=512	**97.86±0.07 (S)**	-	-	-	-

Table 1: Accuracy scores for all models for various datasets. The abbreviations in the table; **NC:** Neighbour columns used, **RF:** Random features used, **G:** Gaussian noise used, **S:** Swap noise used.

Ablation studies

I. Effects of loss terms, aggregation type etc.

Table 2: Ablation study using MNIST with 4 subsets with 75% overlap. Abbreviations are; **RL:** Reconstruction Loss, **CL:** Contrastive Loss, **DL:** Distance Loss, **SF:** Shuffled Features, **LD:** Latent Dim, **Agg:** Aggregating embeddings.

RL	CL	Noise	DL	SF	LD	Agg	Test Accuracy
+	-	-	-	-	128	+	97.13
-	+	-	-	-	128	+	97.11
+	+	-	-	-	128	+	97.26
+	+	Zero-out	-	-	128	+	97.25
+	+	Gaussian	-	-	128	+	97.25
+	+	Swap	-	-	128	+	97.47
+	+	Swap	+	-	128	+	97.52
+	+	Swap	+	+	128	+	97.2
+	+	Swap	+	-	512	-	95.92
+	+	Swap	+	-	512	+	**97.86**

II. Shallow vs Deep Architecture

Model	MNIST	Income	Blog	Obesity	TCGA
Deep SubTab	97.86±0.07	85.35±0.06	84.64±0.19	**71.13±4.08**	58.25± 1.36
Shallow SubTab	**98.31±0.06**	85.34±0.03	84.64±0.09	66.88±5.35	**61.41±1.11**

Table 3: Comparing shallow and deep SubTab architectures.

Experiments

I. Measuring information content of the joint embedding for the base model

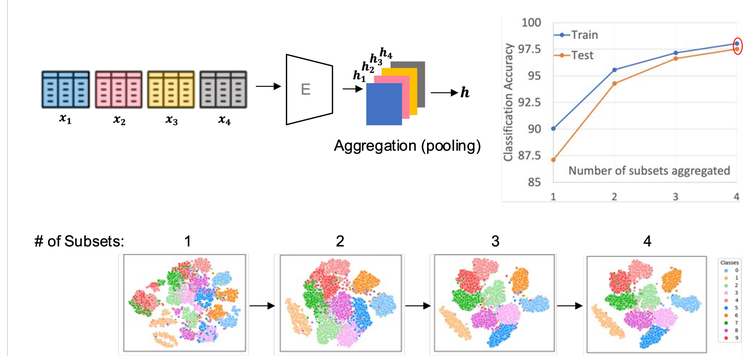


Figure-4: Once the model is trained on MNIST, which is divided into 4 subsets with 75% overlap between them, the information content of the joint embedding is measured by adding subsets one by one sequentially. As shown in t-SNE plots and classification accuracy, the quality of embedding improves as we add more and more subsets to obtain joint embedding.

GitHub: https://github.com/AstraZeneca/SubTab

II. Slicing MNIST to seven subsets with 0% overlap

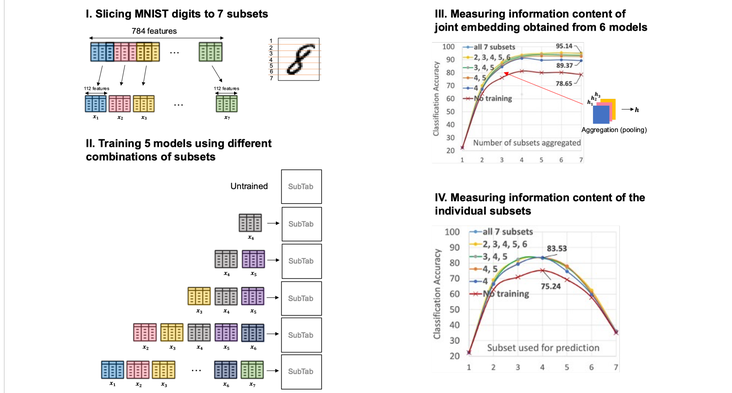
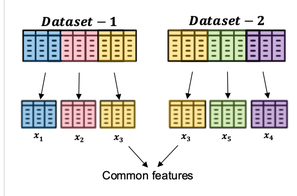


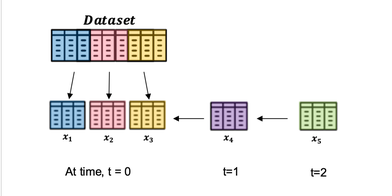
Figure-5: Measuring the information content of the joint embedding under missing data during training and/or test time (shown in step III above) as well as that of individual subsets (shown in step IV above)

Applications

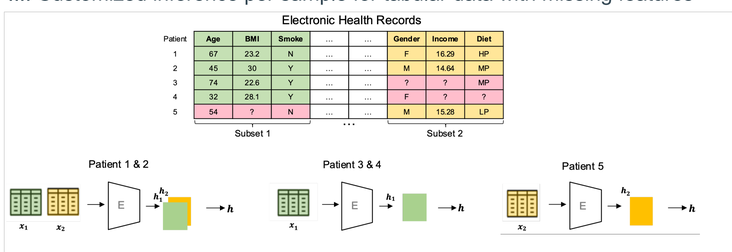
I. Transfer learning



II. Integrating new features over time



III. Customized inference per sample for tabular data with missing features



IV. Applying concepts in SubTab to other modalities, e.g. Sub**Img**