On Embeddings for Numerical Features in Tabular Deep Learning

Overview

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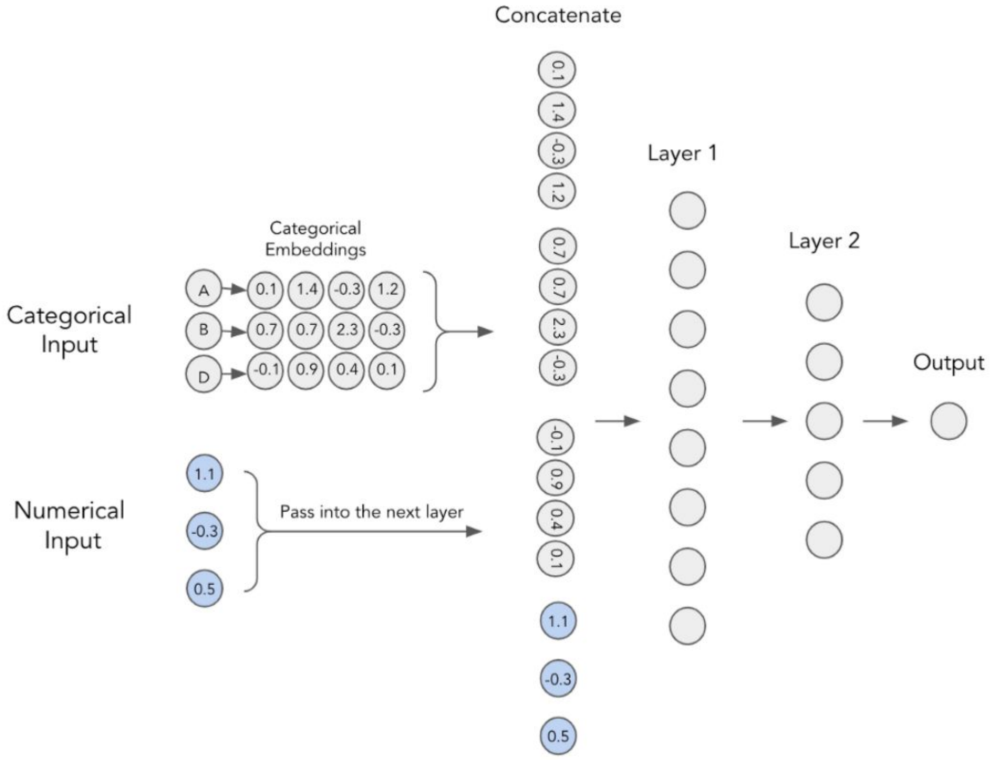
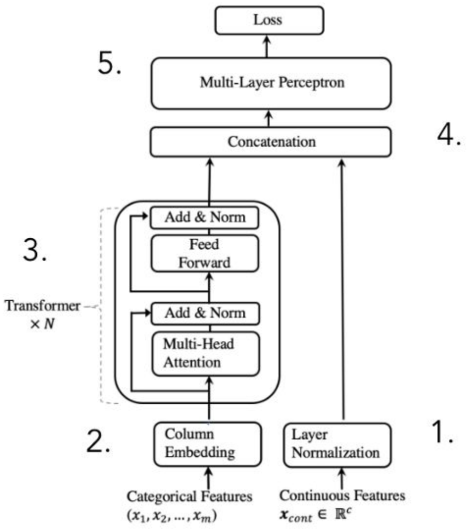
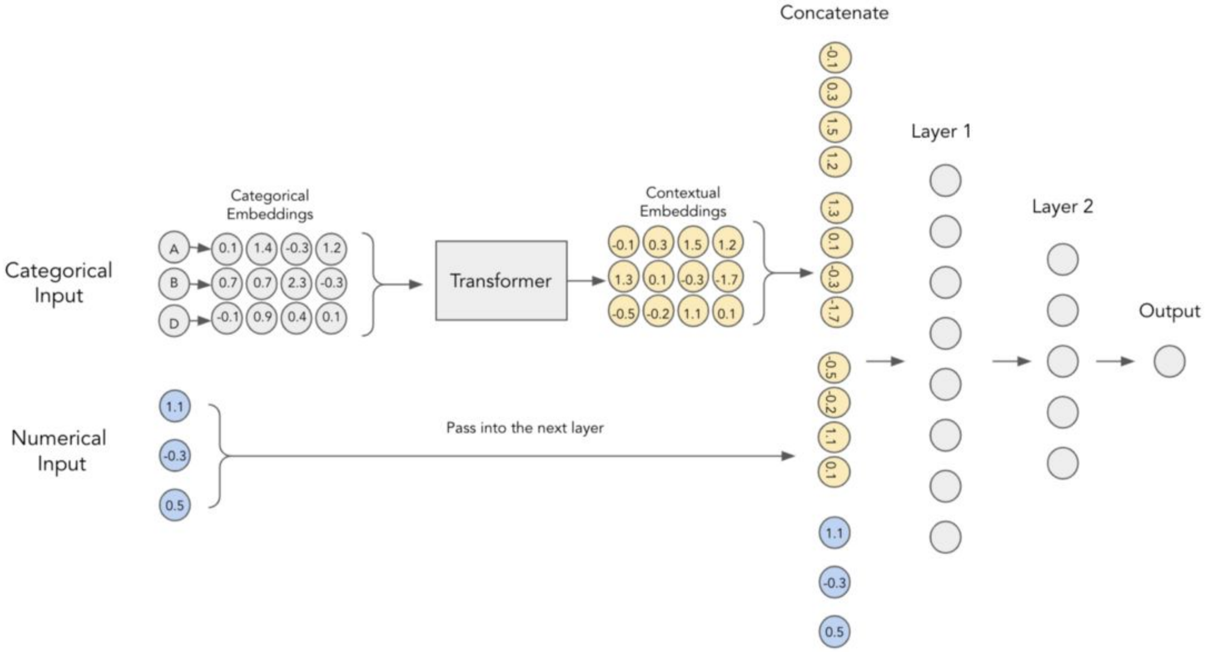
MLP in tabular data

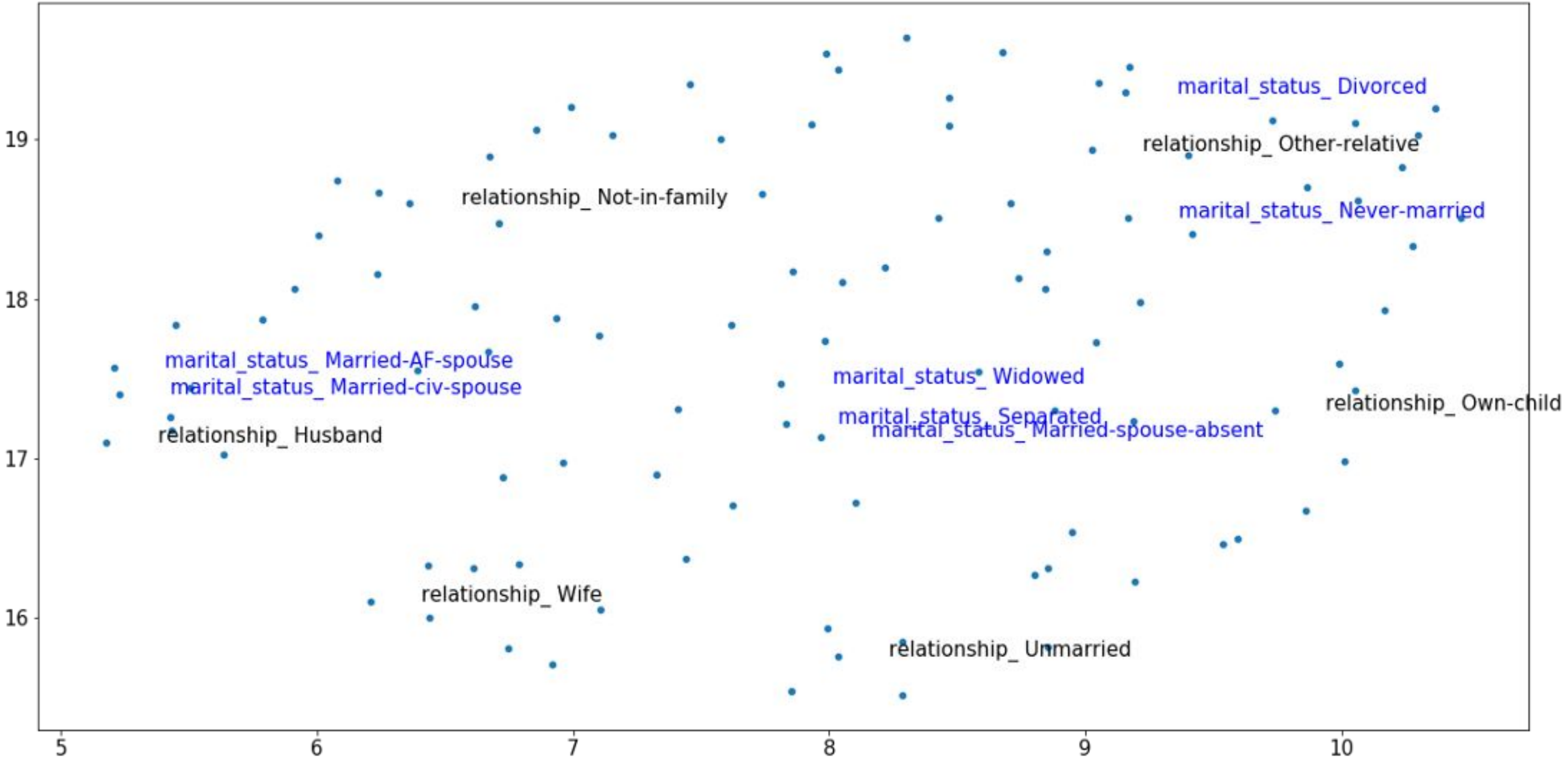


Contextual Embeddings in tabular data





Contextual Embeddings in tabular data



Purposes

- research of embedding schemes for numerical features in tabular DL
- test new solution on public benchmarks
- achieve the new state-of-the-art of tabular DL

PLE for numerical features (MLP)

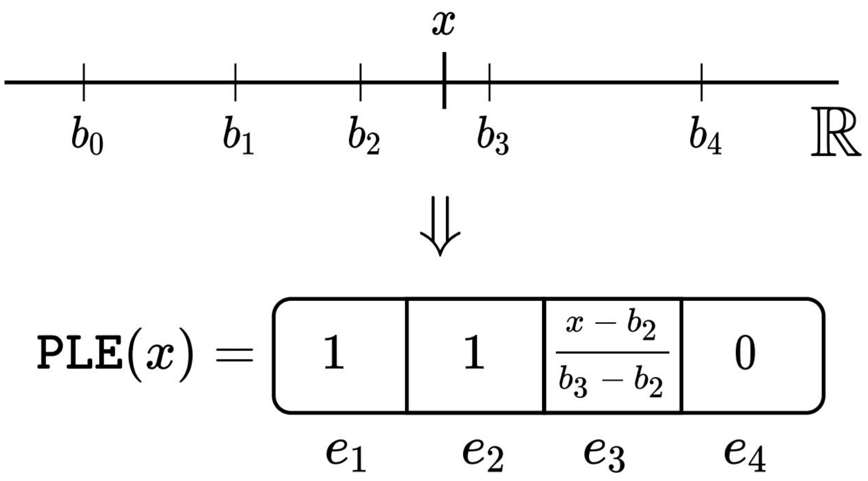
1. Binarization

$$B_t^i = [b_{t-1}^i, b_t^i)$$

2. Embedding

$$\texttt{PLE}(x) = [e_1, \ \dots, \ e_T] \in \mathbb{R}^T$$

$$e_t = \begin{cases} 0, & x < b_{t-1} \ \texttt{AND} \ t > 1 \\ 1, & x \geq b_t \ \texttt{AND} \ t < T \\ \frac{x - b_{t-1}}{b_t - b_{t-1}}, & \text{otherwise} \end{cases}$$



PLE (peicewise linear encoding)

PLE for numerical features (Transformer)

1. Binarization

$$B_t^i = [b_{t-1}^i, b_t^i)$$

2. Embedding

$$\texttt{PLE}(x) = [e_1, \ \ldots, \ e_T] \in \mathbb{R}^T$$

$$e_t = \begin{cases} 0, & x < b_{t-1} \ \texttt{AND} \ t > 1 \\ 1, & x \geq b_t \ \texttt{AND} \ t < T \\ \frac{x - b_{t-1}}{b_t - b_{t-1}}, & \text{otherwise} \end{cases}$$

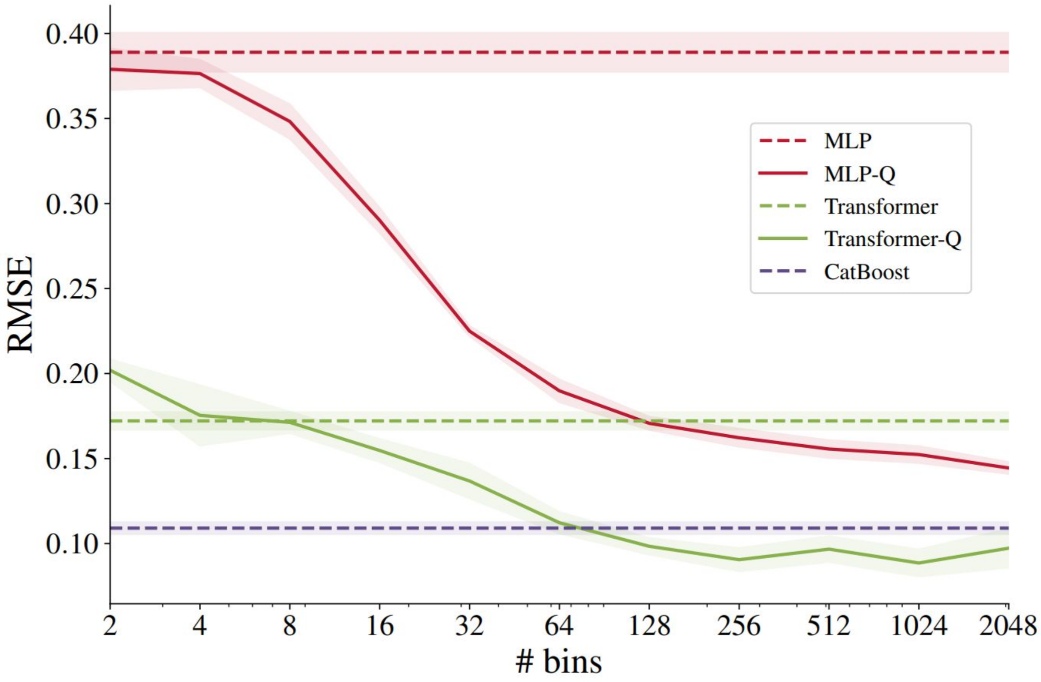
3. Positional Encoding

- Weighted embedding

$$f_i(x) = v_0 + \sum_{t=1}^{T} e_t \cdot v_t = \texttt{Linear}(\texttt{PLE}(x))$$

Embeddings for numerical features (benchmark)

Synthetic GBDT-friendly dataset



Periodic Activation Functions for numerical features

$$f_i(x) = \texttt{Periodic}(x) = \texttt{concat}[\sin(v),\ \cos(v)],$$
$$v = [2\pi c_1 x,\ \ldots,\ 2\pi c_k x]$$

(c_i are trainable parameters initialized from N(0, σ))

Binarization

- obtaining bins from quantiles

$$b_t = \mathrm{Q}_{\frac{t}{T}}\left(\{x_i^{j(num)}\}_{j \in J_{train}}\right)$$

- building target-aware bins

$$b_0^i = \min_{j \in J_{train}} x_i^j \qquad b_T^i = \max_{j \in J_{train}} x_i^j$$

Benchmark datasets

- Gesture Phase Prediction (GE)
- Churn Modeling (CH)
- Eye Movements (EY)
- California Housing (CA)
- House 16H (HO)
- Adult (AD)
- Otto Group Product Classification (OT)
- Higgs (the version with 98K samples available at the OpenML repository (Vanschoren et al., 2014))
- Facebook Comments (FA)
- Santander Customer Transaction Prediction (SA)
- Covertype (CO)
- Microsoft (MI)

Benchmark datasets

Name	Embedding function (f_i)
L	Linear
LR	ReLU ∘ Linear
LRLR	ReLU ∘ Linear ∘ ReLU ∘ Linear
Q	PLE_q
Q−L	Linear ∘ PLE_q
Q−LR	ReLU ∘ Linear ∘ PLE_q
Q−LRLR	ReLU ∘ Linear ∘ ReLU ∘ Linear ∘ PLE_q
T	PLE_t
T−L	Linear ∘ PLE_t
T−LR	ReLU ∘ Linear ∘ PLE_t
T−LRLR	ReLU ∘ Linear ∘ ReLU ∘ Linear ∘ PLE_t
P	Periodic
PL	Linear ∘ Periodic
PLR	ReLU ∘ Linear ∘ Periodic
PLRLR	ReLU ∘ Linear ∘ ReLU ∘ Linear ∘ Periodic
AutoDis	Linear ∘ SoftMax ∘ Linear_{-} ∘ LReLU ∘ Linear_{-}

PLE_q - PLE quantiles

PLE_t - PLE target aware bins

Benchmark datasets (PLE)

	GE ↑	CH ↑	EY ↑	CA ↓	HO ↓	AD ↑	OT ↑	HI ↑	FB ↓	SA ↑	CO ↑	MI ↓
MLP	0.632	0.856	0.615	0.495	3.204	0.854	0.818	0.720	5.686	0.912	0.964	**0.747**
MLP-Q	**0.653**	0.854	0.604	0.464	**3.163**	0.859	0.816	0.721	5.766	0.922	0.968	0.750
MLP-T	**0.647**	**0.861**	0.682	0.447	**3.149**	0.864	**0.821**	0.720	5.577	0.923	0.967	0.749
MLP-Q-LR	**0.646**	0.857	**0.693**	0.455	**3.184**	0.863	0.811	0.720	**5.394**	0.923	**0.969**	**0.747**
MLP-T-LR	0.640	**0.861**	**0.685**	**0.439**	3.207	**0.868**	0.818	**0.724**	**5.508**	**0.924**	**0.968**	0.747
Transformer-L	0.632	0.860	0.731	0.465	3.239	0.858	**0.817**	0.725	**5.602**	0.924	0.971	**0.746**
Transformer-Q-L	**0.659**	0.856	0.753	0.451	3.319	0.867	0.812	**0.729**	5.741	**0.924**	**0.973**	0.747
Transformer-T-L	**0.663**	**0.861**	**0.775**	0.454	**3.197**	**0.871**	**0.817**	0.726	5.803	**0.924**	**0.974**	0.747
Transformer-Q-LR	**0.659**	0.857	**0.796**	0.448	3.270	0.867	0.812	0.723	5.683	0.923	0.972	0.748
Transformer-T-LR	**0.665**	0.860	**0.789**	**0.442**	**3.219**	0.870	**0.818**	**0.729**	5.699	**0.924**	0.973	0.747

Benchmark datasets (periodic activation functions)

	GE ↑	CH ↑	EY ↑	CA ↓	HO ↓	AD ↑	OT ↑	HI ↑	FB ↓	SA ↑	CO ↑	MI ↓
MLP	0.632	0.856	0.615	0.495	3.204	0.854	**0.818**	0.720	5.686	0.912	0.964	0.747
MLP-P	0.631	**0.860**	0.701	0.489	3.129	0.869	0.807	0.723	5.845	0.923	0.968	0.747
MLP-PL	0.641	**0.859**	0.866	**0.467**	3.113	0.868	**0.819**	0.727	**5.530**	0.924	**0.969**	0.746
MLP-PLR	**0.674**	**0.857**	**0.920**	**0.467**	**3.050**	**0.870**	**0.819**	**0.728**	**5.525**	**0.924**	**0.970**	**0.746**
Transformer-L	**0.632**	0.860	0.731	**0.465**	3.239	0.858	**0.817**	0.725	**5.602**	**0.924**	**0.971**	**0.746**
Transformer-PLR	**0.646**	**0.863**	**0.940**	**0.464**	**3.162**	**0.870**	0.814	**0.730**	5.760	**0.924**	**0.972**	**0.746**

Benchmark datasets

	GE ↑	CH ↑	EY ↑	CA ↓	HO ↓	AD ↑	OT ↑	HI ↑	FB ↓	SA ↑	CO ↑	MI ↓	Avg. Rank
CatBoost	0.692	0.861	0.757	0.430	3.093	0.873	0.825	0.727	5.226	0.924	0.967	**0.741**	6.8 ± 4.9
XGBoost	0.683	0.859	0.738	0.434	3.152	**0.875**	0.827	0.726	5.338	0.919	0.969	0.742	9.0 ± 5.7
MLP	0.665	0.856	0.637	0.486	3.109	0.856	0.822	0.727	5.616	0.913	0.968	0.746	15.6 ± 2.4
MLP-LR	0.679	0.861	0.694	0.463	3.012	0.859	0.826	0.731	5.477	0.924	0.972	0.744	10.2 ± 4.4
MLP-Q-LR	0.682	0.859	0.732	0.433	3.080	0.867	0.818	0.724	**5.144**	0.924	0.974	0.745	10.7 ± 4.6
MLP-T-LR	0.673	0.861	0.729	0.435	3.099	0.870	0.821	0.727	5.409	0.924	0.973	0.746	10.3 ± 3.8
MLP-PLR	**0.700**	0.858	0.968	0.453	**2.975**	0.874	**0.830**	**0.734**	5.388	**0.924**	0.975	0.743	4.9 ± 4.8
ResNet	0.690	0.861	0.667	0.483	3.081	0.856	0.821	0.734	5.482	0.918	0.968	0.745	12.1 ± 4.7
ResNet-LR	0.672	0.862	0.735	0.450	2.992	0.859	0.822	0.733	5.415	0.923	0.971	0.743	9.8 ± 4.3
ResNet-Q-LR	0.674	0.859	0.794	0.427	3.066	0.868	0.815	0.729	5.309	0.923	0.976	0.746	9.2 ± 4.8
ResNet-T-LR	0.683	0.862	0.817	**0.425**	3.030	0.872	0.822	0.731	5.471	0.923	0.975	0.744	7.8 ± 3.6
ResNet-PLR	0.691	0.861	0.925	0.443	3.040	**0.874**	0.825	0.734	5.400	0.924	0.975	0.743	5.2 ± 2.3
Transformer-L	0.668	0.861	0.769	0.455	3.188	0.860	0.824	0.727	5.434	0.924	0.973	0.743	10.6 ± 3.3
Transformer-LR	0.666	0.861	0.776	0.446	3.193	0.861	0.824	0.733	5.430	0.924	0.973	0.743	9.4 ± 4.1
Transformer-Q-LR	0.690	0.857	0.842	**0.425**	3.143	0.868	0.818	0.726	5.471	**0.924**	0.975	0.744	8.5 ± 5.5
Transformer-T-LR	0.686	0.862	0.833	**0.423**	3.149	0.871	0.823	0.733	5.515	0.924	**0.976**	0.744	7.2 ± 4.6
Transformer-PLR	0.686	**0.864**	**0.977**	0.449	3.091	0.873	0.823	0.734	5.581	**0.924**	0.975	0.743	6.0 ± 4.5

Results

- MLP can benefit from embedding modules
- the simple LR module leads to modest, but consistent improvements when applied to MLP
- The piecewise linear encoding is often beneficial for both types of architectures (MLP and Transformer) and the profit can be significant
- For most datasets, embeddings for numerical features can provide noticeable improvements