Using Random Effects to Account for High-Cardinality Categorical Features and Repeated Measures in Deep Neural Networks

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Outline

- Motivation
- Linear Mixed Models
- Our approach: LMMNN
- Results
- Convergence
- Extensions

High cardinality categorical features

- Using EMR of hospital patients to predict hospital readmission, the feature **disease** could take 1 out of thousands of values (Lin et. al., 2019)
- Using the CelebA facial images dataset to develop a computer vision model to localize facial features, several images from the same **person** (a.k.a *repeated measures*), over 10K identities (Liu et. al., 2015)
- Predicting the price of a Airbnb rental, ~40K **hosts** in NYC alone (Kalehbasti et al., 2019)

Current solutions

- One-hot encoding (OHE) → q levels to q additional binary features
- Entity embeddings → reduce dimensionality from q to d with a *learned* $D_{q \times d}$ dictionary
- Ignore!
- Other (Hancock and Khoshgoftaar, 2020):
  - Clustering (expert knowledge, "other" strategy, clustering algos)
  - Feature Hashing
  - Supervised numerical encoding

TL;DR

Table 4: Real data features summary table

Dataset	n	q	p	Categorical	y	Input Type	DNN
UKB PA	96K	350	15	job	PA	Tabular	MLP
Drugs	215K	3.6K	10K	drug	rating	Text	LSTM
CelebA	202K	10K	218x178x3	identity	noseX-Y	Images	CNN
Airbnb	50K	40K	196	host	log(price)	Tabular	MLP

Table 5: Real data 5-CV mean test MSEs and standard errors in parentheses.

Dataset	Ignore	OHE	Embeddings	MeNets	LMMNN
UKB PA	**0.812 (.008)**	0.816 (.009)	0.817 (.010)	**0.811 (.009)**	**0.809 (.008)**
Drugs	2.74 (.032)	2.77 (.005)	2.72 (.051)	2.81 (.031)	**2.66 (.006)**
CelebA noseX	**1.68 (.05)**	–	3.6 (.3)	7.6 (.3)	**1.54 (.07)**
CelebA noseY	1.64 (.09)	–	2.5 (.2)	12.3 (1.1)	**1.39 (.04)**
Airbnb	0.156 (.002)	–	0.158 (.003)	0.153 (.003)	**0.142 (.002)**

Linear Mixed Models (LMM) (I)

$$\boxed{y} = \boxed{X\beta} + \boxed{Zb} + \boxed{\varepsilon}$$

$y \in R^n$	$n \times p$ “fixed” features matrix	$\beta \in R^p$ “fixed” effects	$n \times q$ “random” features matrix	$b \in R^q$ “random” effects (RE) $\sim N(0, D_{q\times q})$	$\varepsilon \in R^n$ $\sim N(0, \sigma_e^2 I_n)$

Random Intercepts model:

- single categorical (RE) feature of q levels
- $D = \sigma_b^2 I_q$
- Z is a binary matrix
- s.t. $y_{ij} = \beta_0 + \beta_1 x_{ij,1} + \cdots + \beta_1 x_{ij,p-1} + b_j + \varepsilon_{ij}, i = 1, \dots, n_i, j = 1, \dots, q$

Linear Mixed Models (LMM) (II)

- Marginal distribution of y:

$$y \sim N(X\beta, V(\psi))$$

where ψ are *variance components* to estimate and $V(\psi) = ZDZ' + \sigma_e^2 I_n$

- Log-likelihood of β, ψ:

$$l(\beta, \psi) = -\frac{1}{2}(y - X\beta)'V(\psi)^{-1}(y - X\beta) - \frac{1}{2}\log|V(\psi)| - \frac{n}{2}\log 2\pi$$

- Get $\hat{\beta}, \hat{\psi}$ via MLE/REML
- Predict (BLUP) $\hat{b} = DZ'V\left(\hat{\psi}\right)^{-1}(y - X\hat{\beta})$ (avoid inversion for random intercepts...)
- Predict $\hat{y}_{te} = X_{te}\hat{\beta} + \mathrm{Z}_{te}\hat{b}$ or $\hat{y}_{te} = X_{te}\hat{\beta}$ for unknown levels

Random effects: what for

By treating high-cardinality categorical features as RE in DNN, we hope to:

- Model the correlation between clustered observations better (faces of the same person!)
- Scale to higher q (only 2 additional params to estimate for random intercepts, many DNN ignore such features altogether)
- Ultimately leading to better prediction performance (e.g. MSE)
- Bonus: scale non-linear MM as well!

Our approach (LMMNN*) (I)

$y = X\beta + Zb + \varepsilon$

$$y = \boxed{f(X)} + \boxed{g(Z)b} + \varepsilon$$

“fixed” part: output of (any) regression DNN

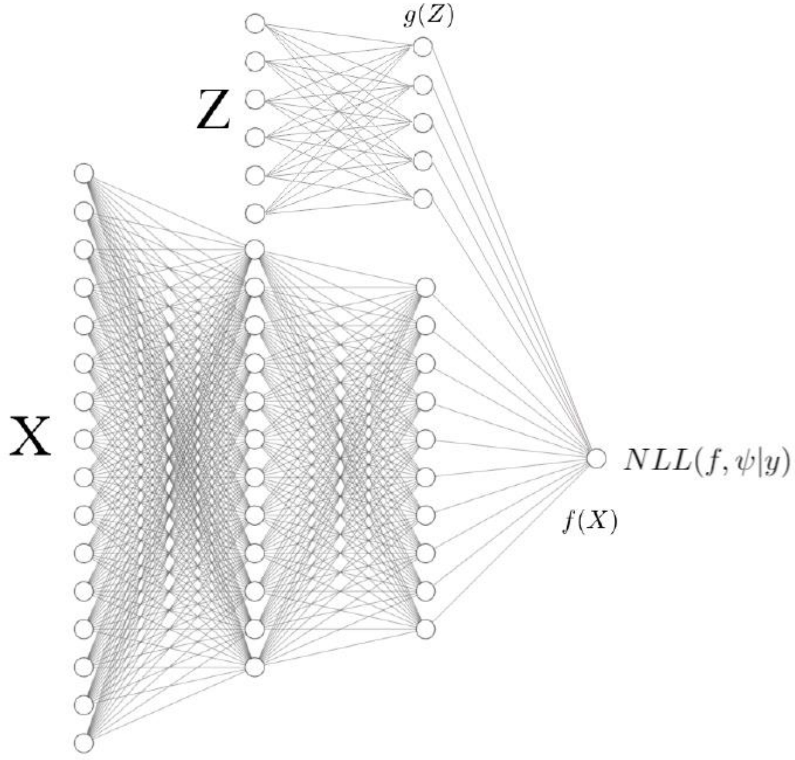
“random” part: output of NN / embeddings, many times $g(Z) = Z$

$b \in R^d$ “random” effects (RE) $\sim N(0, D_{d\times d})$

$\varepsilon \in R^n \sim N(0, \sigma_e^2 I_n)$

*In this work we focus on the random intercepts model for high-cardinality categorical features in a regression setting first, see extensions later.

Our approach (LMMNN) (II)



Our approach (LMMNN) (III)

- Marginal distribution of y:

$$y \sim N(f(X), V(g,\psi))$$

where ψ are *variance components* to estimate and $V(g,\psi) = g(Z)Dg(Z)' + \sigma_e^2 I_n$

- *Negative* log-likelihood (NLL) of f, g, ψ is a natural loss function at each gradient descent iteration on mini-batch ξ of size m:

$$\mathrm{NLL}_\xi(f,g,\psi) = \frac{1}{2}\left(y_\xi - f(X_\xi)\right)' V(g,\psi)_\xi^{-1}\left(y_\xi - f(X_\xi)\right) + \frac{1}{2}\log\left|V(g,\psi)_\xi\right| + \frac{m}{2}\log 2\pi$$

- Get $\hat{f}, \hat{g}, \hat{\psi}$ via DNN optimization (mini-batch SGD, auto-differentiation)
- Predict (BLUP) $\hat{b} = DZ'V\left(\hat{g},\hat{\psi}\right)^{-1}(y - \hat{f}(X))$ (avoid inversion for random intercepts…)
- Predict $\hat{y}_{te} = \hat{f}(X_{te}) + \hat{g}(Z_{te})\hat{b}$ or $\hat{y}_{te} = \hat{f}(X_{te})$for unknown levels

Other approaches

- MeNets (Xiong et. al., 2019)

$$y = f(X)\beta + f(Z)b + \varepsilon$$

- DeepGLMM (Tran et. al., 2020)

$$g(\mu_{it}) = f\left(x_{it}^{(1)}, \omega, \beta^{(1)}\right) + (\beta^{(2)} + \alpha_i)' x_{it}^{(2)}$$

Results: Simulated data (I)

- $y = (X_1 + \cdots + X_{10}) \cdot \cos(X_1 + \cdots + X_{10}) + 2 \cdot X_1 \cdot X_2 + g(Z)b + \varepsilon$
- $X_l \sim U(-1, 1); l = 1, \ldots, 10$
- $\sigma_e^2 = 1$
- $q \in \{100, 1{,}000, 10{,}000\}; \sigma_b^2 \in \{0.1, 1.0, 10.0\}$
- $n = 100{,}000, 80/20\%$ train/test split
- 5 repetitions
- Base DNN: 4-layers MLP with [100, 50, 25, 12, 1] neurons, 25% Dropout, ReLU activation

Results: Simulated data (II)

Table 1: Simulated model with $g(Z) = Z$, mean test MSEs and standard errors in parentheses. Bold results are non-inferior to the best result in a paired t-test.

σ_b^2	q	Ignore	OHE	Embeddings	lme4	MeNets	LMMNN
0.1	10^2	1.25 (.012)	1.20 (.010)	1.18 (.006)	2.92 (.017)	1.15 (.013)	**1.14 (.010)**
	10^3	1.23 (.009)	1.31 (.008)	1.24 (.004)	2.96 (.022)	1.40 (.065)	**1.14 (.009)**
	10^4	1.22 (.004)	1.54 (.008)	1.56 (.007)	2.97 (.014)	1.51 (.133)	**1.17 (.010)**
1	10^2	2.17 (.041)	1.23 (.008)	1.21 (.010)	2.93 (.013)	1.22 (.022)	**1.09 (.010)**
	10^3	2.16 (.015)	1.39 (.015)	1.32 (.014)	2.94 (.013)	1.42 (.091)	**1.14 (.006)**
	10^4	2.14 (.013)	1.68 (.013)	1.68 (.013)	3.17 (.021)	1.66 (.056)	**1.27 (.014)**
10	10^2	10.45 (.38)	1.56 (.044)	1.57 (.039)	2.92 (.012)	1.86 (.156)	**1.10 (.013)**
	10^3	11.37 (.11)	1.75 (.022)	1.72 (.041)	2.95 (.024)	2.19 (.143)	**1.12 (.015)**
	10^4	11.31 (.04)	2.34 (.027)	2.20 (.033)	3.37 (.020)	3.29 (.423)	**1.32 (.007)**

Results: Simulated data (III)

Table 3: Simulated model with $\boxed{g(Z) = ZW}$, mean test MSEs and standard errors in parentheses.

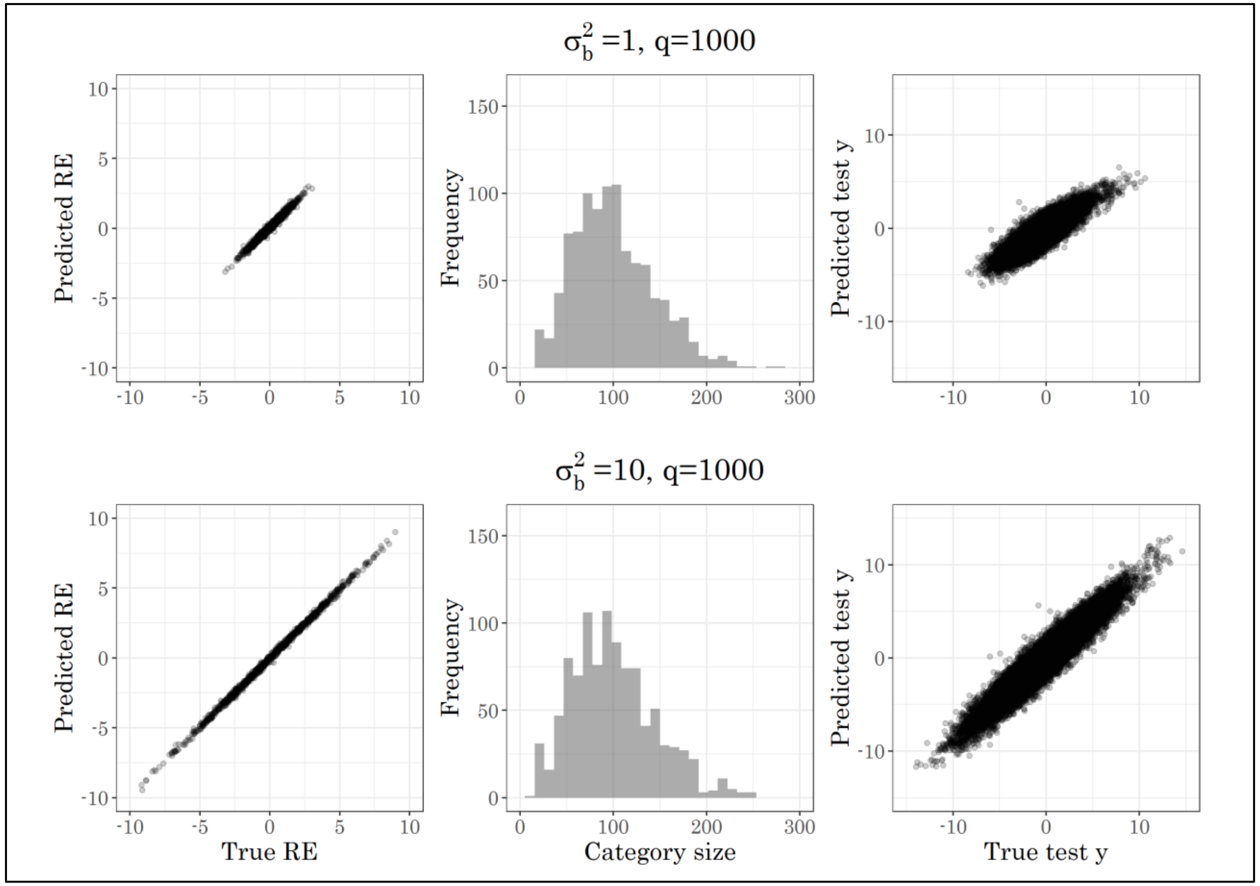
σ_b^2	q	Ignore	OHE	Embeddings	lme4	MeNets	LMMNN
0.1	10^2	1.42 (.039)	1.22 (.018)	1.19 (.024)	2.91 (.021)	1.25 (.084)	**1.13 (.013)**
	10^3	4.92 (.345)	1.49 (.033)	1.43 (.035)	2.95 (.020)	1.44 (.061)	**1.16 (.013)**
	10^4	35.1 (.456)	3.25 (.086)	3.39 (.116)	3.42 (.036)	7.35 (1.9)	**1.59 (.023)**
1	10^2	4.13 (.626)	1.32 (.025)	1.31 (.033)	2.88 (.023)	1.40 (.106)	**1.16 (.011)**
	10^3	35.6 (2.78)	2.49 (.151)	2.56 (.355)	2.96 (.045)	7.00 (1.9)	**1.19 (.028)**
	10^4	334 (18)	9.13 (2.29)	14.4 (2.89)	4.29 (.1)	143.3 (32)	**3.43 (.757)**
10	10^2	32.5 (6.86)	1.74 (.121)	2.43 (.317)	2.90 (.023)	12.0 (3.03)	**1.12 (.012)**
	10^3	324 (25)	8.94 (.79)	9.27 (.92)	2.96 (.031)	164 (18)	**1.20 (.020)**
	10^4	3337 (134)	60.1 (4.6)	91.1 (4.5)	**13.8 (1.2)**	2880 (463)	**13.3 (2.0)**

Results: Simulated data (IV)

Table 2: Simulated model, estimated variance components on average

		$g(Z) = Z$				$g(Z) = ZW$			
		lme4		LMMNN		lme4		LMMNN	
σ_b^2	q	$\hat{\sigma}_e^2$	$\hat{\sigma}_b^2$	$\hat{\sigma}_e^2$	$\hat{\sigma}_b^2$	$\hat{\sigma}_e^2$	$\hat{\sigma}_b^2$	$\hat{\sigma}_e^2$	$\hat{\sigma}_b^2$
0.1	10^2	2.92	0.09	1.12	0.10	2.92	0.49	1.09	0.15
	10^3	2.91	0.10	1.16	0.10	2.91	3.52	0.92	0.16
	10^4	2.90	0.10	1.17	0.17	2.91	33.8	0.19	0.16
1	10^2	2.90	1.01	1.12	1.00	2.91	2.44	1.07	0.41
	10^3	2.90	0.98	1.15	1.00	2.90	32.0	0.84	0.43
	10^4	2.90	0.99	1.26	1.02	2.92	336.6	0.19	0.35
10	10^2	2.90	10.13	1.04	9.24	2.89	32.9	1.06	2.21
	10^3	2.91	10.02	1.12	10.01	2.89	337.8	0.75	1.30
	10^4	2.91	10.01	1.34	9.72	2.90	3305.6	0.22	1.98

Results: Simulated data (V)



Results: Real data

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Convergence

- Main challenge in decomposing the full NLL gradient: $V(g,\psi)^{-1}$and $\log|V(g,\psi)|$ where V is $n \times n$ and only a $m \times m$ "part" of it is used in each mini-batch of size m
- For the simple random intercepts model with $g(Z) = Z$ we show in the paper how the full gradient can be written exactly as the sum of q sub-gradients where each batch consists of n_j level j observations:

$$\frac{\partial NLL}{\partial \psi} = \sum_{j=1}^{q}\left[-\frac{1}{2}\left(y_j - f(X_j)\right)' V_j^{-1}\frac{\partial V_j}{\partial \psi} V_j^{-1}\left(y_j - f(X_j)\right) + \frac{1}{2} tr\left(V_j^{-1}\frac{\partial V_j}{\partial \psi}\right)\right]$$

- This:
  - may not be realistic for some datasets as n_j could be large for some j
  - is not the case in general when $g(Z) \neq Z$
  - for other LMM scenarios, needs a block-diagonal $V(g,\psi)$ (see Extensions)
- For a more general structure of $V(g,\psi)$ see e.g. Chen et. al. 2020, but this is still WIP

Extensions

- A single high-cardinality categorical feature is just the start
- Many useful correlation structures D have already shown promising results (future work):
  - Multiple categorical features (see simulations)
  - Longitudinal data
  - Kriging over random fields, similar to GP
  - GLMM (e.g. classification setting)

Table 6: Simulated model with $g(Z) = Z$ and two categorical features, mean test MSEs and standard errors in parentheses.

σ^2_{b1}	σ^2_{b2}	q_1	q_2	Ignore	OHE	Embeddings	lme4	LMMNN
0.5	0.5	10^3	10^3	2.18 (.03)	1.45 (.02)	1.34 (.01)	2.97 (.03)	**1.13 (.01)**
		10^3	10^4	2.15 (.02)	1.70 (.01)	1.68 (.02)	3.12 (.03)	**1.23 (.01)**
		10^4	10^4	2.13 (.02)	1.83 (.02)	1.80 (.02)	3.23 (.03)	**1.30 (.00)**
0.5	5.0	10^3	10^3	6.73 (.04)	1.66 (.03)	1.57 (.02)	3.00 (.04)	**1.12 (.00)**
		10^3	10^4	6.75 (.04)	2.20 (.03)	2.01 (.03)	3.31 (.02)	**1.29 (.01)**
		10^4	10^3	6.50 (.05)	1.88 (.03)	1.92 (.04)	3.15 (.01)	**1.23 (.01)**
		10^4	10^4	6.68 (.12)	2.48 (.03)	2.16 (.02)	3.43 (.01)	**1.37 (.01)**
5.0	5.0	10^3	10^3	11.26 (.19)	1.83 (.02)	1.80 (.07)	2.97 (.02)	**1.14 (.02)**
		10^3	10^4	11.33 (.19)	2.36 (.03)	2.11 (.02)	3.32 (.02)	**1.30 (.01)**
		10^4	10^4	11.24 (.09)	3.02 (.03)	2.55 (.000)	3.69 (.02)	**1.49 (.02)**

Code

- Python 3.8, Tensorflow-Keras (Chollet, 2015)
- `lmmnn` package, key feature: `NLL` custom Keras loss layer
- All code in: https://github.com/gsimchoni/lmmnn

```python
# after importing all that is necessary for Keras
from lmmnn.layers import NLL

def cnn_lmmnn():
    input_layer = Input((IMG_HEIGHT, IMG_WIDTH, 3))
    y_true_input = Input(shape=(1, ),)
    Z_input = Input(shape=(1, ), dtype=tf.int64)
    x = Conv2D(64, (2, 2), activation='relu')(input_layer)
    x = MaxPool2D((2, 2))(x)
    x = Conv2D(32, (2, 2), activation='relu')(x)
    x = MaxPool2D((2, 2))(x)
    x = Conv2D(16, (2, 2), activation='relu')(x)
    x = MaxPool2D((2, 2))(x)
    x = Flatten()(x)
    x = Dense(100, activation='relu')(x)
    y_pred_output = Dense(1)(x)
    nll = NLL('intercepts', 1.0, [1.0])(
        y_true_input, y_pred_output, [Z_input]
    )
    return Model(
        inputs = [input_layer, y_true_input, Z_input],
        outputs=nll
    )

model = cnn_lmmnn()
model.compile(optimizer= 'adam')

history = model.fit(
    [X_train['images'], y_train, X_train[RE_feature]],
    None,
    validation_split = 0.1,
    batch_size = batch_size, epochs=epochs
)
```

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Thank you.