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The work contained in this thesis is my own work unless otherwise stated.

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Abstract

ABSTRACT GOES HERE

Acknowledgements

ANY ACKNOWLEDGEMENTS GO HERE

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Notation

\mathbf{X} is a matrix

y is a vector

Abbreviations

DAIN Deep Adaptive Input Normalization

RDAIN Robust Deep Adaptive Input Normalization

EDAIN Extended Deep Adaptive Input Normalization

EDAIN-KL Extended Deep Adaptive Input Normalization, optimised with
Kullback–Leibler divergence

BIN Bilinear Input Normalization

pdf probability density function

KL-divergence Kullbeck-Leibler divergence

PREPMIX-CAPS Preprocessing Mixture, optimised with Clustering and Parallel
Search

1 Introduction

The introduction section goes here¹.

¹Tip: write this section last.

2 Background

TODO: introduction to this chapter

2.1 Deep learning

TODO: write details

2.1.1 Sequence models

2.2 Data preprocessing

Origin pa

[Koval \(2018\)](#) does some data preprocessing for neural networks, and [Nawi et al. \(2013\)](#) also investigate the effect of data preprocessing on neural network. Also looked at effect on classification performance by [Singh and Singh \(2020\)](#). Moreover, been studied as early as 1997 by ([Sola and Sevilla, 1997](#)).

2.2.1 Static distribution transformations

2.2.2 Adaptive distribution transformations

DAIN

The Deep Adaptive Input Normalization (DAIN) method, proposed by [Passalis et al. \(2019\)](#).

RDAIN

We have [Passalis et al. \(2021\)](#)

BiN

We have [Tran et al. \(2021\)](#)

2.3 Normalizing flows

TODO: write details

3 Methods

TODO: introduction to this chapter

3.1 EDAIN

My first contribution is the Extended Deep Adaptive Input Normalization (EDAIN) layer. This adaptive preprocessing layer is inspired by the likes of (Passalis et al., 2019) and (Tran et al., 2021) but unlike the aforementioned methods, the EDAIN layer also supports normalizing the data in a *global-aware* fashion, whereas the DAIN, Robust Deep Adaptive Input Normalization (RDAIN) and Bilinear Input Normalization (BIN) layers are all *local-aware*. Additionally, the EDAIN layer extends the other layers with two new operations: An outlier removal operation that is designed to reduce the negative impact of high-tail observations, as well as a power-transform operation that is designed to transform skewed data to be more normal.

3.1.1 Notation

Let $\{\mathbf{X}^{(i)} \in \mathbb{R}^{d \times T}; i = 1, \dots, N\}$ denote a set of N multivariate time-series, each composed of T d -dimensional feature vectors. We also let $\mathbf{x}_t^{(i)} \in \mathbb{R}^d$, where $t = 1, \dots, T$, denote the t th feature vector at time-step t in the time-series. When talking about applying operations on feature vectors of the form $\mathbf{x}_t^{(i)}$, the time index and data index might be dropped for notational clarity, giving $\mathbf{x} \in \mathbb{R}^d$. Furthermore, the vector operations $\oplus, \ominus, \odot, \oslash$ refer to the element-wise application of addition, subtraction, multiplication and division, respectively.

Something something vector function with vector input and vector output, is denoted with bold letter such as $\mathbf{f}(\mathbf{x})$, and functions applied elementwise is denoted $f(x)$.

3.1.2 Architecture

An overview of the layer's architecture is shown in figure fig. 3.1. Given some input time-series $\mathbf{X}^{(i)} \in \mathbb{R}^{d \times T}$, each temporal segment $\mathbf{x}_t^{(i)}$ is passed through an adaptive outlier removal layer, followed by an adaptive shift and scale operation, and then finally passed through an adaptive power transformation layer. The architecture also has two modes, *local-aware* and *global-aware*. In global-aware mode, the EDAIN layer aims to normalize each input such that the resulting distribution of all the samples in the dataset resemble

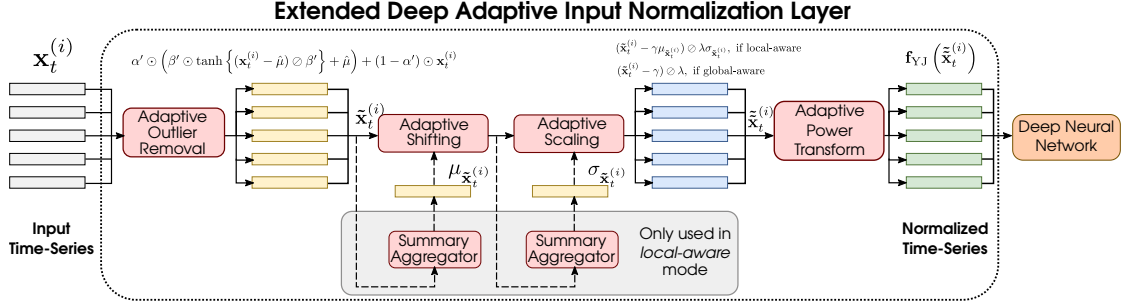


Figure 3.1: An overview of the architecture of the proposed EDAIN normalization layer.

a unimodal normal distribution, that is a “global normalization”. In local-aware mode, the EDAIN layer’s normalization operations also depend on summary statistics of each input sample $\mathbf{X}^{(i)}$, and the goal is to transform all the data into a common normalized representation space, independent of where in the “global distribution” the sample originated from. This mode is most suitable for multi-modal input data, as samples from different modes can all be transformed into one common normalized unimodal distribution. On the other hand, the global-aware mode is most suitable if all the data comes from a similar data generation mechanism, and works best if the input data has few modes.

In local-aware mode, the EDAIN architecture is similar to the DAIN architecture proposed by [Passalis et al.](#), but it extends it with both a global-aware mode as well as an adaptive outlier removal sublayer and an adaptive power transform sublayer.

Outlier removal

Handling outliers and extreme values in the dataset can increase predictive performance if done correctly (citation needed). Two common ways of doing this are omission and winsorization ([Nyitrai and Virág, 2019](#)). With the former, observations that are deemed to be extreme are simply removed during training. With the latter, all the data is still used, but observations lying outside a certain number of standard deviation from the mean, or below or above certain percentiles, are *clamped down* to be closer to the mean or median of the data. For example, if winsorizing data using 3 standard deviation, all values less than $\mu - 3\sigma$ are set to be exactly $\mu - 3\sigma$. Similarly, the values above $\mu + 3\sigma$ are *clamped* to this value. Winsorization can also be done using percentiles, where common boundaries are the first and fifth percentiles ([Nyitrai and Virág, 2019](#)). However, the type of winsorization, as well as the number of standard deviation or percentiles to use, might depend on the dataset. Additionally, it might not be necessary to winsorize the data at all if the outliers turn out to not negatively affect performance. All this introduces more hyperparameters to tune during modelling. The outlier removal operation presented here aims to automatically determine both whether winsorization is necessary for a particular feature, and determine the threshold at which to apply

winsorization.

For input vector $\mathbf{x}_t^{(i)} \in \mathbb{R}^d$, the adaptive outlier removal operation is defined as:

$$\mathbf{h}_1(\mathbf{x}_t^{(i)}) = \underbrace{\boldsymbol{\alpha}' \odot \left(\boldsymbol{\beta}' \odot \tanh \left\{ (\mathbf{x}_t^{(i)} - \hat{\boldsymbol{\mu}}) \oslash \boldsymbol{\beta}' \right\} + \hat{\boldsymbol{\mu}} \right)}_{\text{smooth adaptive centred winsorization}} + \underbrace{(1 - \boldsymbol{\alpha}') \odot \mathbf{x}}_{\text{residual connection}}, \quad (3.1)$$

where $\boldsymbol{\alpha}' \in [0, 1]^d$ is a parameter controlling how much winsorization to apply to each feature, and $\boldsymbol{\beta}' \in [\beta_{\min}, \infty)^d$ controls the winsorization threshold for each feature, that is, the maximum absolute value of the output, thus controlling the range of the output. The effect of the two parameters is illustrated in fig. 3.2. The unknown parameters of the model are $\boldsymbol{\alpha} \in \mathbb{R}^d$ and $\boldsymbol{\beta} \in \mathbb{R}^d$, and they are transformed into the constrained parameters $\boldsymbol{\alpha}'$ and $\boldsymbol{\beta}'$, as used in eq. (3.1) through the following element-wise mappings:

$$\boldsymbol{\alpha}' = \frac{e^{\boldsymbol{\alpha}}}{1 \oplus e^{\boldsymbol{\alpha}}} \quad \boldsymbol{\beta}' = \beta_{\min} \oplus e^{\boldsymbol{\beta}}, \quad (3.2)$$

where $\beta_{\min} \in \mathbb{R}$ is a hyperparameter that can be tuned, but a suitable value is $\beta_{\min} = 1$.

The $\hat{\boldsymbol{\mu}} \in \mathbb{R}^d$ parameter in eq. (3.1) is an estimate of the mean of the data, and is used to ensure the winsorization is centred. When setting the EDAIN layer in *local-aware* mode, it is simply the mean of the current batch of data points, \mathcal{B} :

$$\hat{\mu}_k = \frac{1}{|\mathcal{B}|T} \sum_{i \in \mathcal{B}} \sum_{j=1}^T x_{j,k}^{(i)}, \quad k = 1, \dots, d \quad (3.3)$$

while if using the *global-aware* mode, it is iteratively updated using a cumulative moving average estimate at each forward pass of the layer. This is to better approximate the global mean of the data.

Scale and shift

Depending on the dataset, one might want to aim for a *global normalization*, in which case a *global-aware* scale and shift operation is most suitable. If the dataset has many different modes, with significantly different distribution characteristics, a *local normalization* based on the specific mode each data point comes from is more suitable, in which case a *local-aware* scale and shift operation works best. This gives two different approaches and scaling and shifting the data in an adaptive fashion.

Global-aware In global-aware mode, the adaptive shift and scale layer, combined, simply performs the operation

$$\mathbf{h}_3(\mathbf{h}_2(\mathbf{x}_t^{(i)})) := (\mathbf{x}_t^{(i)} - \boldsymbol{\gamma}) \oslash \boldsymbol{\lambda}, \quad (3.4)$$

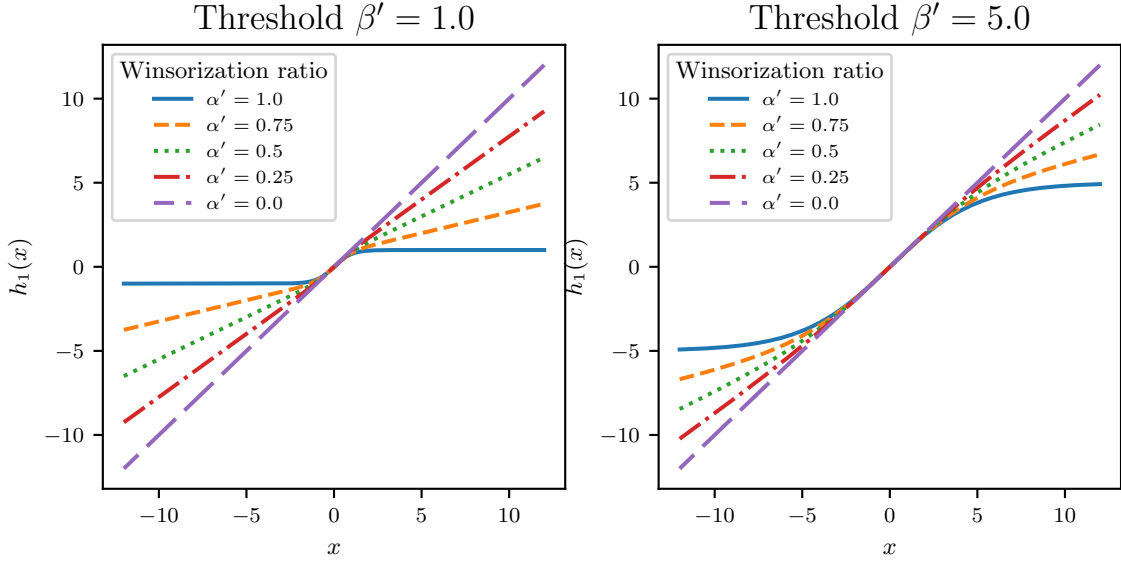


Figure 3.2: Plot of the adaptive outlier removal operation for different combinations of parameter values for α' and β' .

with input $\mathbf{x} \in \mathbb{R}^d$ and unknown parameters $\boldsymbol{\gamma} \in \mathbb{R}^d$ and $\boldsymbol{\lambda} \in (0, \infty)^d$. This makes the scale-and-shift layer a generalised version of Z-score scaling, or standard scaling, as setting

$$\boldsymbol{\gamma} := \frac{1}{NT} \sum_{i=1}^N \sum_{t=1}^T \mathbf{x}_t^{(i)} \quad (3.5)$$

and

$$\boldsymbol{\lambda} := \frac{1}{NT} \sum_{i=1}^N \sum_{t=1}^T \left(\mathbf{x}_t^{(i)} - \boldsymbol{\gamma} \right)^2 \quad (3.6)$$

makes the operation in eq. (3.4) equivalent to Z-score scaling. This *global-aware* mode is useful if the distribution is similar across batches and constitute a global unimodal distribution that should be centred, as the operation can generalise Z-score scaling.

Local-aware Some datasets might have multiple modes arising from significantly different data generation mechanisms. Attempting to scale and shift each batch to a global mean and standard deviation might hurt performance in such cases. Instead, [Passalis et al.](#) propose basing the scale and shift on a *summary representation* of each data point, allowing each sample to be normalized according the specific mode of the data it might have come from. This gives

$$\mathbf{h}_3(\mathbf{h}_2(\mathbf{x}_t^{(i)})) := (\mathbf{x}_t^{(i)} - [\boldsymbol{\gamma} \odot \boldsymbol{\mu}_{\mathbf{x}}]) \odot [\boldsymbol{\lambda} \odot \boldsymbol{\sigma}_{\mathbf{x}}], \quad (3.7)$$

where the summary representations $\sigma_{\mathbf{x}}$ and $\mu_{\mathbf{x}}$ are computed through reduction of the temporal dimension for each observation:

$$\mu_{\mathbf{x}}^{(i)} = \frac{1}{T} \sum_{t=1}^T \mathbf{x}_t^{(i)} \in \mathbb{R}^d \quad (3.8)$$

$$\sigma_{\mathbf{x}}^{(i)} = \sqrt{\frac{1}{T} \sum_{t=1}^T \left(\mathbf{x}_t^{(i)} - \mu_{\mathbf{x}}^{(i)} \right)^2} \in \mathbb{R}^d. \quad (3.9)$$

With this mode, it is difficult for the layer to generalise Z-score scaling, but it allows discarding mode information such that highly multimodal distributions appear unimodal.

Power transform

Many real-world datasets exhibit significant skewness, which is often treated using power transformations (citation needed). The most common transformation is the Box-Cox transformation, but this is only valid for positive values, so it is not applicable to most real-world datasets (Box and Cox, 1964). An alternative is a transformation proposed by Yeo and Johnson who proposed to following transformation:

$$f_{\text{YJ}}(x) = \begin{cases} \frac{(x+1)^{\lambda^{(\text{YJ})}} - 1}{\lambda^{(\text{YJ})}}, & \text{if } \lambda^{(\text{YJ})} \neq 0, x \geq 0; \\ \log(x+1), & \text{if } \lambda^{(\text{YJ})} = 0, x \geq 0; \\ \frac{(1-x)^{2-\lambda^{(\text{YJ})}} - 1}{\lambda^{(\text{YJ})} - 2}, & \text{if } \lambda^{(\text{YJ})} \neq 2, x < 0; \\ -\log(1-x), & \text{if } \lambda^{(\text{YJ})} = 2, x < 0. \end{cases} \quad (3.10)$$

Like the Box-Cox transformation, transformation f_{YJ} only has one unknown parameter, $\lambda^{(\text{YJ})}$, but it works for any $x \in \mathbb{R}$, not just positive values (Yeo and Johnson, 2000). The power transform layer simply applies the transformation in eq. (3.10) along each dimension of the input, that is for each $i = 1, \dots, N$ and $t = 1, \dots, T$,

$$\left[\mathbf{h}_4 \left(\mathbf{x}_t^{(i)} \right) \right]_j := f_{\text{YJ}}(x_{t,j}^{(i)}), \quad j = 1, \dots, d. \quad (3.11)$$

The unknown parameters is the vector $\boldsymbol{\lambda}^{(\text{YJ})} \in \mathbb{R}^d$.

3.1.3 Optimisation through back-propagation

To optimise the unknown parameters $(\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\lambda}, \boldsymbol{\lambda}^{(\text{YJ})})$, the deep neural network is augmented by prepending the EDAIN layer, as shown in fig. 3.1. Then the input data is fed into the augmented model in batches, as when training a neural network, and after each forward pass of the model, the weights are updated through gradient descent while training the neural network. As observed by Passalis et al., the model convergence is unstable if the same learning rate $\eta \in \mathbb{R}$ that is used for training the deep neural

network is also used for training all the sublayers of the EDAIN layer. Therefore, separate learning rate modifiers η_{out} , η_{shift} , η_{scale} and η_{pow} for the outlier removal, shift, scale and power transform sublayers are introduced as additional hyperparameters and the weight updates happen according to the equation:

$$\Delta(\alpha, \beta, \gamma, \lambda, \lambda^{(\text{YJ})}) = -\eta \left(\eta_{\text{out}} \frac{\partial \mathcal{L}}{\partial \alpha}, \eta_{\text{out}} \frac{\partial \mathcal{L}}{\partial \beta}, \eta_{\text{shift}} \frac{\partial \mathcal{L}}{\partial \gamma}, \eta_{\text{scale}} \frac{\partial \mathcal{L}}{\partial \lambda}, \eta_{\text{pow}} \frac{\partial \mathcal{L}}{\partial \lambda^{(\text{YJ})}} \right). \quad (3.12)$$

3.2 EDAIN-KL

TODO: introduction something something alterative inspired by normalizing flow, and mention bijectors.

3.2.1 Architecture

The Extended Deep Adaptive Input Normalization, optimised with Kullback–Leibler divergence (EDAIN-KL) layer has a very similar architecture to the EDAIN layer, described in section 3.1, but the outlier removal transformation has been simplified to ensure its inverse is tractable. Additionally, the layer no longer supports local-aware mode, as this would make the inverse intractable. The EDAIN-KL transformations are:

$$\text{(Outlier removal)} \quad \mathbf{h}_1(\mathbf{x}_t^{(i)}) = \beta' \odot \tanh \left\{ (\mathbf{x}_t^{(i)} - \hat{\mu}) \oslash \beta' \right\} + \hat{\mu} \quad (3.13)$$

$$\text{(shift)} \quad \mathbf{h}_2(\mathbf{x}_t^{(i)}) = \mathbf{x}_t^{(i)} \oplus \gamma \quad (3.14)$$

$$\text{(scale)} \quad \mathbf{h}_3(\mathbf{x}_t^{(i)}) = \mathbf{x}_t^{(i)} \odot \lambda \quad (3.15)$$

$$\text{(power transform)} \quad \mathbf{h}_4(\mathbf{x}_t^{(i)}) = \left[f_{\text{YJ}}^{\lambda_1}(x_{t,0}^{(i)}) \quad f_{\text{YJ}}^{\lambda_2}(x_{t,1}^{(i)}) \quad \cdots \quad f_{\text{YJ}}^{\lambda_d}(x_{t,d}^{(i)}) \right], \quad (3.16)$$

where $f_{\text{YJ}}^{\lambda_i}(\cdot)$ is defined in eq. (3.10).

3.2.2 Optimisation through Kullback-Leibler divergence

This optimisation method is inspired by normalizing flow, of which [Kobyzev et al.](#) provide a great overview of.

Brief background on normalizing flow

Consider a random variable $\mathbf{Z} \in \mathbb{R}^d$ with a known and analytic expression for the probability density function (pdf) $p_{\mathbf{Z}} : \mathbb{R}^d \rightarrow \mathbb{R}$, which we call the *base distribution*. The idea behind normalizing flows is defining an arbitrarily complicated parametrised bijector $\mathbf{g}_{\theta} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ —an invertible function—and transforming the simple base distribution into a new arbitrarily complicated probability distribution: $\mathbf{Y} = \mathbf{g}_{\theta}(\mathbf{Z})$. The

pdf of the transformed distribution can then be computed using the change of variable formula (Kobyzev et al., 2021):

$$\begin{aligned} p_{\mathbf{Y}}(\mathbf{y}) &= p_{\mathbf{Z}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y})) \cdot |\det \mathbf{J}_{\mathbf{Y} \rightarrow \mathbf{Z}}(\mathbf{y})| \\ &= p_{\mathbf{Z}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y})) \cdot |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y}))|^{-1}, \end{aligned} \quad (3.17)$$

where $\mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}$ is the Jacobian matrix for the forward mapping $\mathbf{Y} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{Z})$. Taking logs on both sides, it follows that

$$\log p_{\mathbf{Y}}(\mathbf{y}) = \log p_{\mathbf{Z}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y})) - \log |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y}))|. \quad (3.18)$$

One common application of normalizing flows is density estimation (Kobyzev et al., 2021); Given a dataset $\mathcal{D} = \{\mathbf{y}^{(i)}\}_{i=1}^N$ with samples from some unknown complicated distribution, we want to estimate its unknown pdf, $p_{\mathcal{D}}$. This can be done with likelihood-based estimation, where we assume the data points come from parametrised distribution $\mathbf{Y} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{Z})$ and optimise $\boldsymbol{\theta}$ to maximise the data log-likelihood:

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^N \log p_{\mathbf{Y}}(\mathbf{y}^{(i)}|\boldsymbol{\theta}) \quad (3.19)$$

$$\stackrel{\text{eq. (3.18)}}{=} \sum_{i=1}^N \log p_{\mathbf{Z}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y}^{(i)})) - \log |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}(\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\mathbf{y}^{(i)}))|. \quad (3.20)$$

This is equivalent to minimising the Kullback-Leibler divergence (KL-divergence) between the empirical distribution \mathcal{D} and the transformed distribution $\mathbf{Y} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{Z})$:

$$\arg \max_{\boldsymbol{\theta}} \log p(\mathcal{D}|\boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^N \log p_{\mathbf{Y}}(\mathbf{y}^{(i)}|\boldsymbol{\theta}) \quad (3.21)$$

$$= \frac{1}{N} \sum_{i=1}^N \log p_{\mathcal{D}}(\mathbf{y}^{(i)}) + \arg \max_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^N \log p_{\mathbf{Y}}(\mathbf{y}^{(i)}|\boldsymbol{\theta}) \quad (3.22)$$

$$= \arg \min_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^N \log p_{\mathcal{D}}(\mathbf{y}^{(i)}) - \frac{1}{N} \sum_{i=1}^N \log p_{\mathbf{Y}}(\mathbf{y}^{(i)}|\boldsymbol{\theta}) \quad (3.23)$$

$$= \arg \min_{\boldsymbol{\theta}} \sum_{i=1}^N p_{\mathcal{D}}(\mathbf{y}^{(i)}) \log p_{\mathcal{D}}(\mathbf{y}^{(i)}) \quad (3.24)$$

$$- \sum_{i=1}^N p_{\mathcal{D}}(\mathbf{y}^{(i)}) \log p_{\mathbf{Y}}(\mathbf{y}^{(i)}|\boldsymbol{\theta}) \quad (3.25)$$

$$= \arg \min_{\boldsymbol{\theta}} D_{\text{KL}}(\mathcal{D} \parallel (\mathbf{Y} | \boldsymbol{\theta})). \quad (3.26)$$

When training an normalizing flow model, we adjust $\boldsymbol{\theta}$ to minimize the above KL-divergence.

This requires computing all the terms in eq. (3.20), which requires analytic and differentiable expressions for the inverse transformation $\mathbf{g}_\theta^{-1}(\cdot)$, the pdf of the base distribution $p_{\mathbf{Z}}(\cdot)$ and the log determinant of the Jacobian matrix for \mathbf{g}_θ^{-1} , $\log |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}|$. Using a result stated in [Kobyzev et al.](#), the following can be shown:

Theorem 3.2.1. Let $\mathbf{g}_1, \dots, \mathbf{g}_n : \mathbb{R}^d \rightarrow \mathbb{R}^d$ all be bijective functions, and consider the composition of these functions, $\mathbf{g} = \mathbf{g}_n \circ \mathbf{g}_{n-1} \cdots \circ \mathbf{g}_1$. Then, \mathbf{g} is a bijective function with inverse

$$\mathbf{g}^{-1} = \mathbf{g}_1^{-1} \circ \cdots \circ \mathbf{g}_{n-1}^{-1} \circ \mathbf{g}_n^{-1}, \quad (3.27)$$

and the log of the absolute value of the determinant of the Jacobian is given by

$$\log |\det \mathbf{J}_{\mathbf{g}^{-1}}(\cdot)| = \sum_{i=1}^N \log |\det \mathbf{J}_{\mathbf{g}_i^{-1}}(\cdot)|. \quad (3.28)$$

Similarly,

$$\log |\det \mathbf{J}_{\mathbf{g}}(\cdot)| = \sum_{i=1}^N \log |\det \mathbf{J}_{\mathbf{g}_i}(\cdot)|. \quad (3.29)$$

Application to EDAIN-KL

Like with the EDAIN layer, we want to compose the outlier removal, shift, scale and power transform transformations into one operation, which we do by defining

$$\mathbf{g}_\theta = \mathbf{h}_1^{-1} \circ \mathbf{h}_2^{-1} \circ \mathbf{h}_3^{-1} \circ \mathbf{h}_4^{-1}, \quad (3.30)$$

where $\theta = (\beta, \gamma, \lambda, \lambda^{(YJ)})$. Notice that we apply all the operations in reverse order, compared to the EDAIN layer. This is because we will use \mathbf{g}_θ to transform our base distribution \mathbf{Z} into a distribution that is as close to our dataset \mathcal{D} as possible. Then, when we want to normalize the dataset, we apply

$$\mathbf{g}_\theta^{-1} = h_4 \circ h_3 \circ h_2 \circ h_1 \quad (3.31)$$

to each sample. It can be shown that all the transformations defined in eqs. (3.13) to (3.16) are invertible. Using theorem 3.2.1, it follows that \mathbf{g}_θ , as defined in eq. (3.30), is bijective and that its inverse is given by eq. (3.31). As we will see in later in section 3.2.2, the inverse transformation in eq. (3.31) has a tractable and differentiable expression, so \mathbf{g}_θ can be used as a normalizing flow bijection.

Making the input data as Gaussian as possible usually increases performance of deep sequence models (citation needed), so a suitable base distribution is the standard multivariate Gaussian distribution

$$\mathbf{Z} \sim \mathcal{N}(0, \mathbf{I}_d), \quad (3.32)$$

whose pdf has a tractable and differentiable expression, so it is suitable for our needs.

We have that both $p_{\mathbf{Z}}(\cdot)$ and $\mathbf{g}_{\boldsymbol{\theta}}^{-1}(\cdot)$ have analytic expressions and are differentiable, so we have almost everything that we need in order to use eq. (3.20) to optimise $\boldsymbol{\theta}$. The only part remaining is an expression for the log of the determinant of the Jacobian of the forward transformation given by $\mathbf{g}_{\boldsymbol{\theta}}^{-1}$, which we will derive in the next section. Once we have that, $\boldsymbol{\theta}$ can be optimised using back-propagation as described in TODO, using the negation of eq. (3.20) as the loss function $\mathcal{L}(\boldsymbol{\theta})$.

Derivations of inverse log determinant Jacobians

Recall that the EDAIN-KL architecture is just a bijector that is composed of 4 other bijective functions. Using the result in theorem 3.2.1, we get

$$\log |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}(\cdot)| = \sum_{i=1}^4 \log |\det \mathbf{J}_{h_i^{-1}}(\cdot)|. \quad (3.33)$$

Considering the transformations in eqs. (3.13) to (3.16), we notice that all the transformation happen element-wise, so for $i \in \{1, 2, 3, 4\}$, we have $\frac{\partial h_i^{-1}(x_j)}{\partial x_k} = 0$ for $k \neq j$. Therefore, the Jacobians are diagonal matrices, so the determinant is just the product of the diagonal entries, giving

$$\log |\det \mathbf{J}_{\mathbf{Z} \rightarrow \mathbf{Y}}(\mathbf{x})| = \sum_{i=1}^4 \log \left| \prod_{j=1}^d \frac{\partial h_i^{-1}(x_j)}{\partial x_j} \right| \quad (3.34)$$

$$= \sum_{i=1}^4 \sum_{j=1}^d \log \left| \frac{\partial h_i^{-1}(x_j)}{\partial x_j} \right|. \quad (3.35)$$

We now proceed to deriving the derivatives appearing on the right-hand side for h_1^{-1} , h_2^{-1} , h_3^{-1} , and h_4^{-1} .

Shift We first consider $h_2(x_j; \gamma_j) = x_j + \gamma_j$. Its inverse is $h_2^{-1}(z_j; \gamma_j) = z_j - \gamma_j$, and it follows that

$$\log \left| \frac{\partial h_2^{-1}(z_j; \gamma_j)}{\partial z_j} \right| = \log 1 = 0. \quad (3.36)$$

Scale We now consider $h_3(x_j; \lambda_j) = x_j \cdot \lambda_j$, whose inverse is $h_3^{-1}(z_j; \lambda_j) = \frac{z_j}{\lambda_j}$. It follows that

$$\log \left| \frac{\partial h_3^{-1}(z_j; \lambda_j)}{\partial z_j} \right| = \log \left| \frac{1}{\lambda_j} \right| = -\log |\lambda_j|. \quad (3.37)$$

Outlier removal We now consider $h_1(x_j; \beta'_j) = \beta'_j \tanh \left\{ \frac{(x_j - \hat{\mu}_j)}{\beta'_j} \right\} + \hat{\mu}_j$. Its inverse is

$$h_1^{-1}(z_j; \beta'_j) = \beta'_j \tanh^{-1} \left\{ \frac{z_j - \hat{\mu}_j}{\beta'_j} \right\} + \hat{\mu}_j. \quad (3.38)$$

It follows that

$$\log \left| \frac{\partial h_1^{-1}(z_j; \beta'_j)}{\partial z_j} \right| = \log \left| \frac{1}{1 - \left(\frac{z_j - \hat{\mu}_j}{\beta'_j} \right)^2} \right| = -\log \left| 1 - \left(\frac{z_j - \hat{\mu}_j}{\beta'_j} \right)^2 \right|. \quad (3.39)$$

Power transform By considering the expression in eq. (3.16), it can be shown that for fixed λ , negative inputs are always mapped to negative values and vice versa, making the Yeo-Johnson transformation invertible. Additionally, in $\mathbf{h}_4(\cdot)$ the Yeo-Johnson transformation is applied element-wise, so we get

$$\mathbf{h}_4^{-1}(\mathbf{z}) = \left[\left[f_{\text{YJ}}^{\lambda_1} \right]^{-1}(z_1) \quad \left[f_{\text{YJ}}^{\lambda_2} \right]^{-1}(z_2) \quad \cdots \quad \left[f_{\text{YJ}}^{\lambda_d} \right]^{-1}(z_d) \right], \quad (3.40)$$

where it can be shown that the inverse Yeo-Johnson transformation for a single element is given by

$$\left[f_{\text{YJ}}^{\lambda} \right]^{-1}(z) = \begin{cases} (z\lambda + 1)^{1/\lambda} - 1, & \text{if } \lambda \neq 0, z \geq 0; \\ e^z - 1, & \text{if } \lambda = 0, z \geq 0; \\ 1 - \{1 - z(2 - \lambda)\}^{1/(2-\lambda)}, & \text{if } \lambda \neq 2, z < 0; \\ 1 - e^{-z}, & \text{if } \lambda = 2, z < 0. \end{cases} \quad (3.41)$$

The derivative with respect to z then becomes

$$\frac{\partial \left[f_{\text{YJ}}^{\lambda} \right]^{-1}(z)}{\partial z} = \begin{cases} (z\lambda + 1)^{(1-\lambda)/\lambda}, & \text{if } \lambda \neq 0, z \geq 0; \\ e^z, & \text{if } \lambda = 0, z \geq 0; \\ \{1 - z(2 - \lambda)\}^{(\lambda-1)/(2-\lambda)}, & \text{if } \lambda \neq 2, z < 0; \\ e^{-z}, & \text{if } \lambda = 2, z < 0. \end{cases} \quad (3.42)$$

It follows that

$$\log \left| \frac{\partial \left[f_{\text{YJ}}^{\lambda} \right]^{-1}(z)}{\partial z} \right| = \begin{cases} \frac{1-\lambda}{\lambda} \log(z\lambda + 1), & \text{if } \lambda \neq 0, z \geq 0; \\ z, & \text{if } \lambda = 0, z \geq 0; \\ \frac{\lambda-1}{2-\lambda} \log \{1 - z(2 - \lambda)\}, & \text{if } \lambda \neq 2, z < 0; \\ -z, & \text{if } \lambda = 2, z < 0, \end{cases} \quad (3.43)$$

which we use as the expression for $\log \left| \frac{\partial h_4^{-1}(z_j; \lambda^{(\text{YJ})})}{\partial z_j} \right|$ for $z = z_1, \dots, z_d$.

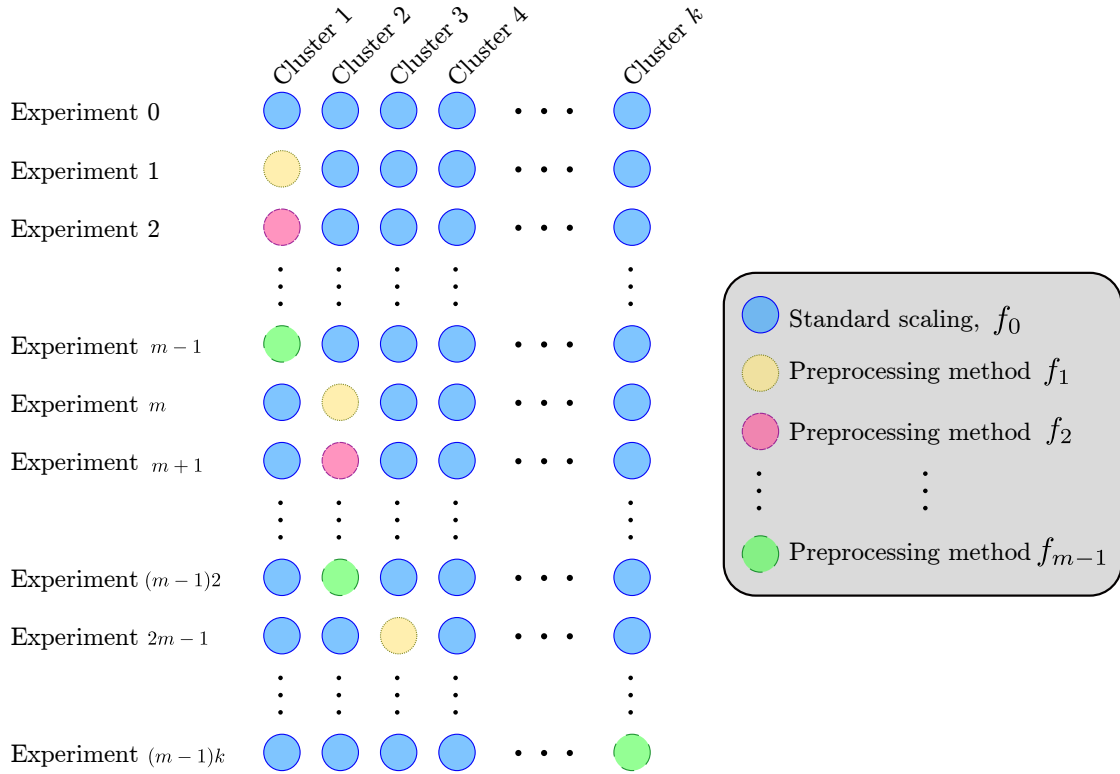


Figure 3.3: Illustration of “ablation studies” done for finding the optimal preprocessing method for each cluster, as part of the PREPMIX-CAPS routine.

3.3 PREPMIX-CAPS

TODO: introduction to this method, and overview of how all the below subsections tie together in the final method

3.3.1 Clustering the predictor variables

3.3.2 Determining the optimal preprocessing method for each cluster

In fig. 3.3, see overview.

Optimisations

4 Results

TODO: introduction to this chapter

4.1 Evaluation methodology

Small introduction

4.1.1 Sequence model architecture

4.1.2 Fitting the models

Mention scheduling, early stopping, optimizer used, learning rate etc.

4.1.3 Tuning adaptive preprocessing model hyperparameters

Details on the tuning for all the methods presented

4.1.4 Evaluation metrics

4.1.5 Cross-validation

4.2 Simulation study

Small introduction, including motivation

4.2.1 Multivariate time-series data generation algorithm

4.2.2 Negative effects of irregularly-distributed data

4.2.3 Preprocessing method experiments

4.3 American Express default prediction dataset

4.3.1 Description

4.3.2 Preprocessing method experiments

5 Discussion

TODO: introduction to this chapter

5.1 EDAIN

5.2 EDAIN-KL

5.3 PREPMIX-CAPS

6 Conclusion

6.1 Summary

Conclusion goes here.

6.2 Main contributions

6.3 Future work

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