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Shape and Time Distortion Loss for Training Deep Time Series Forecasting Models

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Shape and Time Distortion Loss for Training Deep Time Series Forecasting Models

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Abstract

This paper addresses the problem of time series forecasting for non-stationary signals and multiple future steps prediction. To handle this challenging task, we introduce DILATE (DIstortion Loss including shApe and TimE), a new objective function for training deep neural networks. DILATE aims at accurately predicting sudden changes, and explicitly incorporates two terms supporting precise shape and temporal change detection. We introduce a differentiable loss function suitable for training deep neural nets, and provide a custom back-prop implementation for speeding up optimization. We also introduce a variant of DILATE, which provides a smooth generalization of temporally-constrained Dynamic Time Warping (DTW). Experiments carried out on various non-stationary datasets reveal the very good behaviour of DILATE compared to models trained with the standard Mean Squared Error (MSE) loss function, and also to DTW and variants. DILATE is also agnostic to the choice of the model, and we highlight its benefit for training fully connected networks as well as specialized recurrent architectures, showing its capacity to improve over state-of-the-art trajectory forecasting approaches.

1 Introduction

Time series forecasting [6] consists in analyzing the dynamics and correlations between historical data for predicting future behavior. In one-step prediction problems [39, 30], future prediction reduces to a single scalar value. This is in sharp contrast with multi-step time series prediction [49, 2, 48], which consists in predicting a complete trajectory of future data at a rather long temporal extent. Multi-step forecasting thus requires to accurately describe time series evolution.

This work focuses on multi-step forecasting problems for non-stationary signals, *i.e.* when future data cannot only be inferred from the past periodicity, and when abrupt changes of regime can occur. This includes important and diverse application fields, *e.g.* regulating electricity consumption [63, 36], predicting sharp discontinuities in renewable energy production [23] or in traffic flow [35, 34], electrocardiogram (ECG) analysis [9], stock markets prediction [14], *etc.*

Deep learning is an appealing solution for this multi-step and non-stationary prediction problem, due to the ability of deep neural networks to model complex nonlinear time dependencies. Many approaches have recently been proposed, mostly relying on the design of specific one-step ahead

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Overview

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Motivation

- Addresses the problem of time series forecasting for non-stationary, non-linear signals and multiple future steps prediction.

- Multi-step forecasting from non-stationary signals tend to **require more than just past periodicity** and includes the need to handle **abrupt regime shifts**.

- Important in the fields of:
  - Regulating electricity consumption [36, 63]
  - Predicting sharp discontinuities in renewable energy production [23]
  - Traffic flow [34, 35]
  - Electrocardiogram (ECG) analysis [9]
  - Stock markets prediction [14]
  - … *etc*

- **Little research has been published** on loss functions for shape and time localization.

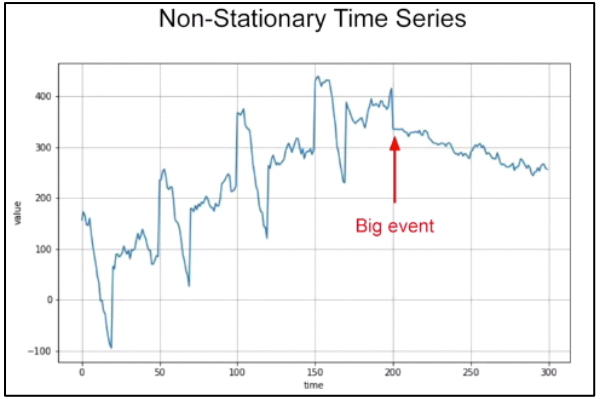


Figure source: https://morioh.com/p/c9290f02e74f

Problem description – introduction

- Time series forecasting include two main categories:
  - Time series with **linear and stationary dynamics** (or non-stationary made stationary by differencing)
  - Time series with **non-linear and non-stationary dynamics**

- The first category is mainly handled by traditional **State Space Models (SSMs)** [17] like the linear auto-regressive model, ARIMA [6], Exponential Smoothing [27] and is a well researched topic.

- For the second category where linear SSMs are inadequate, **deep learning has become a popular tool to forecast non-stationary and multivariate time series.**
- Research in this area has focused on:
  - Leveraging attention mechanisms [30, 39, 50, 12]
  - Tensor factorizations [60, 58, 46]
  - Combining Deep Learning and State Space Models (SSMs) to model uncertainty [45, 44, 40, 56]

Problem description – examined paper

- The examined paper focuses on **deterministic multi-step forecasting:**

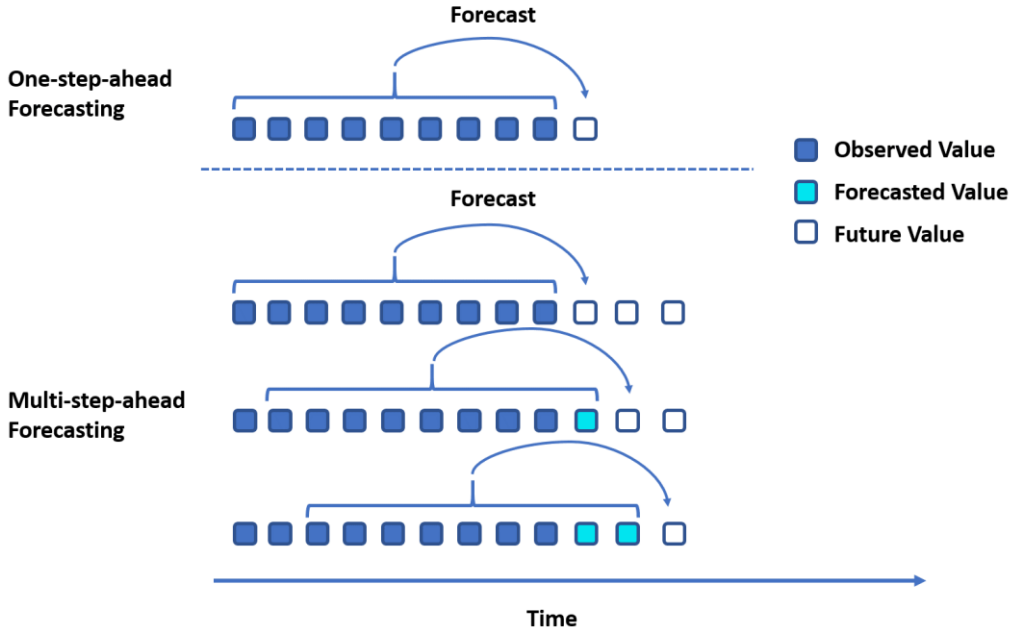
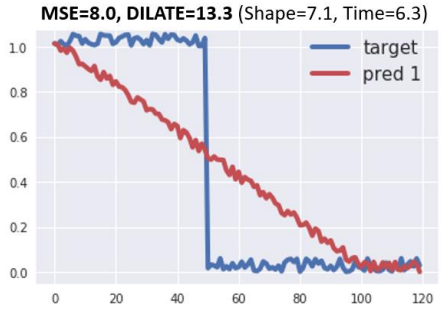
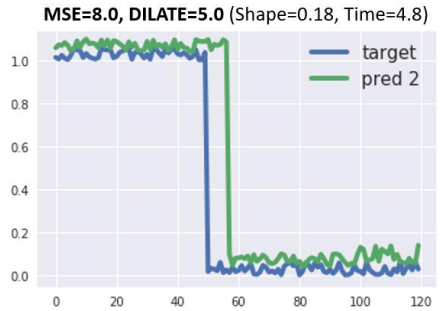


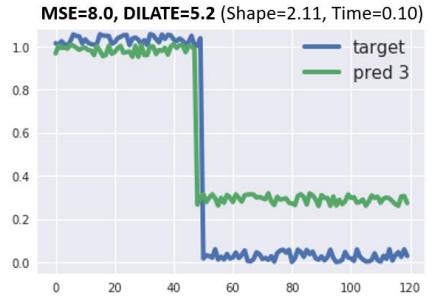
Figure source: https://github.com/sassoftware/python-dlpy/issues/101

Problem description – examined paper

- Deep learning approaches to tackle multi-step forecasting for non-stationary time series mostly rely on **recursively applied single-step architectures** or on **direct multi-step models** such as **Seq2Seq** [55].
- Most of these proposed models rely on Mean Squared Error (**MSE**) as the loss function for training.
- This paper argues that **MSE is inadequate in the context of non-stationary time series**, as it **does not capture** the distinct regime shifts **(shape)** nor temporal aspects **(time).** This is illustrated with the following figures, all having equal MSE=8:







- To rectify this, the authors introduces a new objective function for training: **DILATE**

Related work

- **Research suggests direct multi-step models are to be preferred.**
  - Seq2Seq RNN models which has been used for machine translation [44, 31, 60, 57, 19]
  - WaveNET for audio generation [53]
  - CNNs with dilation for time series forecasting [5]
- **These models, however, rely mainly on MSE and its variants as loss functions.**

- Some work exist on incorporating shape and temporal localization as a **metric.**
  - Shape is considered by Dynamic Time Warping (DTW) [43]
  - Time can be considered by Change Point Detection [8, 33], or Hausdorff distance [22, 51]
- These however are **non-differentiable and therefore useless** for training deep neural nets.

- Recently, **some attempts have been made** to include these aspects to the loss function.
  - A smooth approximation of DTW enables focus on the shape loss [13, 37, 1], **however, ignores temporal localization.**
  - A differentiable timing error loss function based on DTW has been proposed [41], however only applicable for binary time series.
- Therefore, **the paper specifically focus on both shape and temporal localization.**

Methodology – general method

- Define a set of N input time series:

$$\mathcal{A} = \{\mathbf{x}_i\}_{i \in \{1:N\}}$$

- For each input sample of length *n*, predict a k-step ahead forecast by a neural network forecasting model:

$$\mathbf{x}_i = (\mathbf{x}_i^1, ..., \mathbf{x}_i^n) \in \mathbb{R}^{p \times n} \longrightarrow \hat{\mathbf{y}}_i = (\hat{\mathbf{y}}_i^1, ..., \hat{\mathbf{y}}_i^k) \in \mathbb{R}^{d \times k}$$

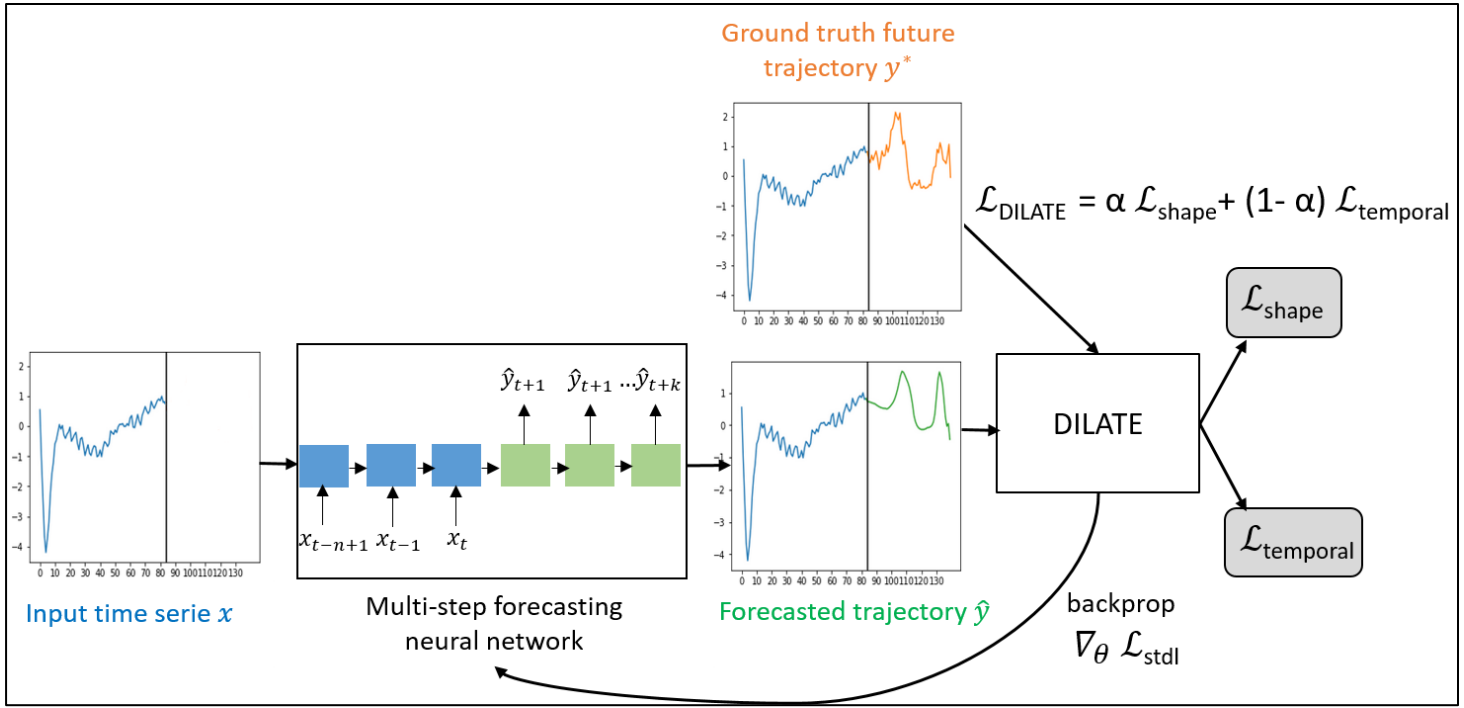
- Compare predicted forecast with actual future trajectory by the DILATE objective function:

$$\overset{*}{\mathbf{y}}_i = (\overset{*}{\mathbf{y}}_i{}^1, ..., \overset{*}{\mathbf{y}}_i{}^k)$$

$$\mathcal{L}_{DILATE}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) = \alpha \, \mathcal{L}_{shape}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) + (1 - \alpha) \, \mathcal{L}_{temporal}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i)$$

Methodology – general method

- The described method is summarised by the following picture:



Methodology – loss function

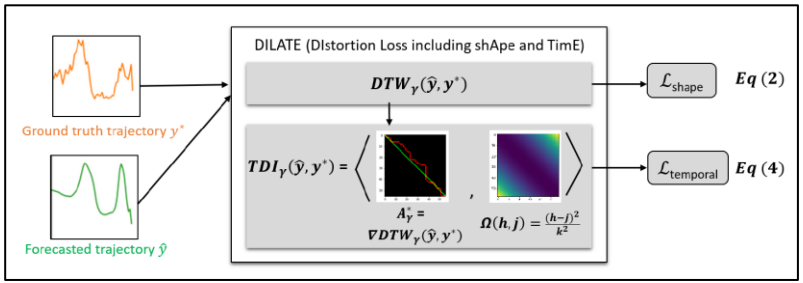
- A modified DTW function made differentiable to account for shape loss:

$$\mathcal{L}_{shape}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) = DTW_\gamma(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) := -\gamma \log \left(\sum_{\mathbf{A} \in \mathcal{A}_{k,k}} \exp \left(-\frac{\left\langle \mathbf{A}, \mathbf{\Delta}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) \right\rangle}{\gamma} \right) \right)$$

- Smoothed temporal loss based on Time Distortion Index (TDI) for temporal misalignment, derived from the DTW function.

$$\mathcal{L}_{temporal}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) := \left\langle \mathbf{A}^*_\gamma, \mathbf{\Omega} \right\rangle = \frac{1}{Z} \sum_{\mathbf{A} \in \mathcal{A}_{k,k}} \langle \mathbf{A}, \mathbf{\Omega} \rangle \exp^{-\frac{\left\langle \mathbf{A}, \mathbf{\Delta}(\hat{\mathbf{y}}_i, \overset{*}{\mathbf{y}}_i) \right\rangle}{\gamma}}$$

- **Key takeaway: Modified DTW and TDI functions made differentiable to account for shape and temporal loss**.



Methodology – training networks

- Direct computation of the previous equations is intractable due to the cardinal of $\mathcal{A}_{k,k}$ growing exponentially with *k*. Therefore, **a custom implementation is devised.**

- Custom shape loss is computation:
  - Forward pass: A **Bellman Dynamic Programming** approach [13]
  - Backward pass: **Recursion**, implemented in Pytorch [13]

- Custom temporal loss computation:
  - Forward pass: **Bellman Dynamic Programming** (same as above)
  - Backward pass: **Custom Dynamic Programming** implementation in Pytorch for computing the Hessian of the DTW function [37].

- The final time complexity turns out to be O(k^2).
  - (k being number of steps in a k-step ahead prediction)

Experimental results - setup

- **Experiments done on 3 non-stationary time series data sets from different domains.**
  - Synthetic (k = 20) consisting of 500 generated time series
  - ECG5000 (k = 56) from UCR Time Series Classification Archive [10]
  - Traffic (k = 24) from California Department of Transportation

- **Performance is evaluated in three different ways.**
  - Evaluation of DILATE against networks trained on MSE and the smooth DTW function used in previous research (which only accounts for shape) [13, 37].
  - Evaluation by comparing forecast results using external metrics: Ramp score (shape) and Hausdorff distance (time).
  - Evaluation against state-of-the-art models trained on MSE.

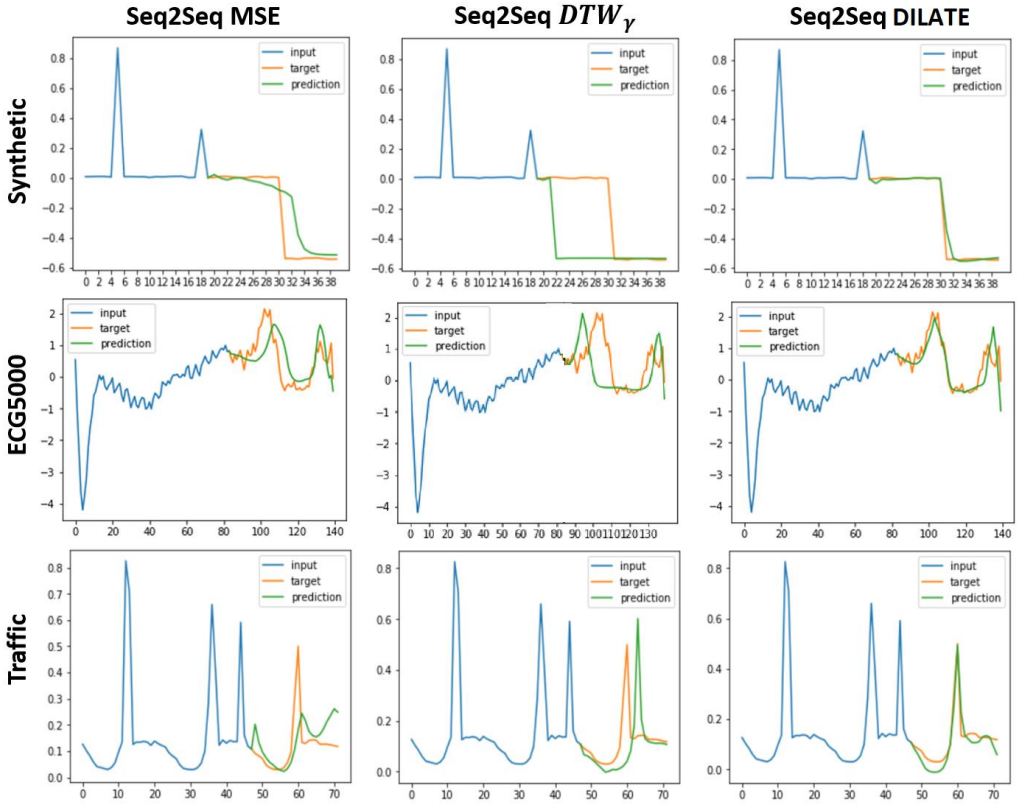
Experimental results – evaluation of loss function

- Evaluation against other loss functions. **DILTAE outperforms in most cases.**

		Fully connected network (MLP)			Recurrent neural network (Seq2Seq)		
Dataset	Eval	MSE	DTW_γ [13]	DILATE (ours)	MSE	DTW_γ [13]	DILATE (ours)
Synth	MSE	**1.65 ± 0.14**	4.82 ± 0.40	**1.67± 0.184**	**1.10 ± 0.17**	2.31 ± 0.45	**1.21 ± 0.13**
	DTW	38.6 ± 1.28	**27.3 ± 1.37**	32.1 ± 5.33	**24.6 ± 1.20**	**22.7 ± 3.55**	**23.1 ± 2.44**
	TDI	15.3 ± 1.39	26.9 ± 4.16	**13.8 ± 0.712**	17.2 ± 1.22	20.0 ± 3.72	**14.8 ± 1.29**
ECG	MSE	**31.5 ± 1.39**	70.9 ± 37.2	37.2 ± 3.59	**21.2 ± 2.24**	75.1 ± 6.30	30.3 ± 4.10
	DTW	19.5 ± 0.159	18.4 ± 0.749	**17.7 ± 0.427**	17.8 ± 1.62	17.1 ± 0.650	**16.1 ± 0.156**
	TDI	**7.58 ± 0.192**	38.9 ± 8.76	**7.21 ± 0.886**	8.27 ± 1.03)	27.2 ± 11.1	**6.59 ± 0.786**
Traffic	MSE	**0.620 ± 0.010**	2.52 ± 0.230	1.93 ± 0.080	**0.890 ± 0.11**	2.22 ± 0.26	**1.00 ± 0.260**
	DTW	24.6 ± 0.180	**23.4 ± 5.40**	**23.1 ± 0.41**	24.6 ± 1.85	**22.6 ± 1.34**	**23.0 ± 1.62**
	TDI	**16.8 ± 0.799**	27.4 ± 5.01	**16.7 ± 0.508**	**15.4 ± 2.25**	22.3 ± 3.66	**14.4± 1.58**

Table 1: Forecasting results evaluated with MSE (×100), DTW (×100) and TDI (×10) metrics, averaged over 10 runs (mean ± standard deviation). For each experiment, best method(s) (Student t-test) in bold.

Experimental results – evaluation of loss function



Experimental results – comparison to state of art

- Comparison to state-of-the-art models trained by MSE.
  - LSTNet recursive prediction for multi-step [30]
  - Tensor-Train RNN trained for multi-step [60, 61]

- **Seq2Seq trained by DILATE outperforms the more complex models on shape and time metrics.** TT-RNN outperforms on MSE.

Eval loss		LSTNet-rec [30]	TT-RNN [60, 61]	Seq2Seq DILATE
Euclidian	MSE (x100)	1.74 ± 0.11	$\mathbf{0.837 \pm 0.106}$	1.00 ± 0.260
Shape	DTW (x100)	42.0 ± 2.2	25.9 ± 1.99	$\mathbf{23.0 \pm 1.62}$
	Ramp (x10)	9.00 ± 0.577	6.71 ± 0.546	$\mathbf{5.93 \pm 0.235}$
Time	TDI (x10)	25.7 ± 4.75	17.8 ± 1.73	$\mathbf{14.4 \pm 1.58}$
	Hausdorff	$\mathbf{2.34 \pm 1.41}$	$\mathbf{2.19 \pm 0.125}$	$\mathbf{2.13 \pm 0.514}$

Table 4: Comparison with state-of-the-art forecasting architectures trained with MSE on Traffic, averaged over 10 runs (mean $\pm$ standard deviation).

Conclusion

- The authors introduce **DILATE**, a **new differentiable loss function** that explicitly consider **shape and time localization** of non-stationary time series with sudden changes.

- DILATE is comparable to MSE and **outperforms on shape and time metrics**. DILATE also **compares favourably to state-of-the-art models**.

- Possibilities for future work:
  - **Extending the ideas to probabilistic forecasting,** for example in Bayesian deep learning [21]**.**
  - Adapt the training scheme for semi-supervised or weakly supervised [16, 42] contexts for full trajectory forecasting using only categorical labels.

- Bonus: Code is available on Github! https://github.com/vincent-leguen/DILATE

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