Zero-Shot Forecasting and Neural Operators
Master Lab

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Abstract

A

1. Structure

- abstract
- a brief introduction (Nadia)
- a discussion of related work (Decoder Only, Statistical models like ARIMA, (briefly FIM-l and DeepONet with reference to chapter conceptual aspects) ... do more research...) (Nadia)
- An explanation of the main conceptual aspects (e.g. DeepONets, random function generation and maybe zero-shot learning) is expected. (Arwin)
- In an experimental section, give details for reproducibility of your work (e.g. hyperparameters, training objectives, hardware, runtime...). (Jan)
- A results section could include a description of the tasks and your findings (use tables and figures to present your results).
- Finish the report with a short concluding section.

- Note that you are encouraged to further improve and explore the models for each task! (Jan)

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[*]Equal contribution [1]Department of XXX, University of YYY, Location, Country [2]Company Name, Location, Country. Correspondence to: Firstname1 Lastname1 <first1.last1@xxx.edu>, Firstname2 Lastname2 <first2.last2@www.uk>.

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```

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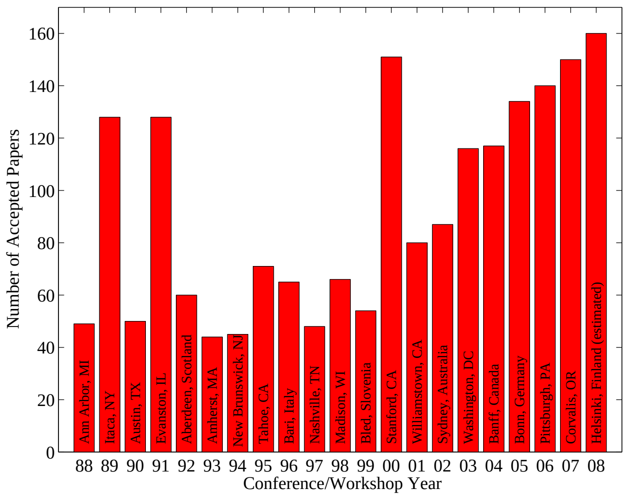

Figure 1. Historical locations and number of accepted papers for International Machine Learning Conferences (ICML 1993 – ICML 2008) and International Workshops on Machine Learning (ML 1988 – ML 1992). At the time this figure was produced, the number of accepted papers for ICML 2008 was unknown and instead estimated.

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Label all distinct components of each figure. If the figure takes the form of a graph, then give a name for each axis and include a legend that briefly describes each curve. Do not include a title inside the figure; instead, the caption should serve this function.

Number figures sequentially, placing the figure number and caption *after* the graphics, with at least 0.1 inches of space before the caption and 0.1 inches after it, as in Figure 1. The figure caption should be set in 9 point type and centered unless it runs two or more lines, in which case it should be flush left. You may float figures to the top or bottom of a column, and you may set wide figures across both columns (use the environment `figure*` in LaTeX). Always place two-column figures at the top or bottom of the page.

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Algorithm 1 Bubble Sort

Input: data x_i, size m
repeat
  Initialize $noChange = true$.
  for $i = 1$ **to** $m - 1$ **do**
    if $x_i > x_{i+1}$ **then**
      Swap x_i and x_{i+1}
      $noChange = false$
    end if
  end for
until $noChange$ is $true$

Table 1. Classification accuracies for naive Bayes and flexible Bayes on various data sets.

Data set	Naive	Flexible	Better?
Breast	95.9± 0.2	96.7± 0.2	$\surd$
Cleveland	83.3± 0.6	80.0± 0.6	$\times$
Glass2	61.9± 1.4	83.8± 0.7	$\surd$
Credit	74.8± 0.5	78.3± 0.6	
Horse	73.3± 0.9	69.7± 1.0	$\times$
Meta	67.1± 0.6	76.5± 0.5	$\surd$
Pima	75.1± 0.6	73.9± 0.5	
Vehicle	44.9± 0.6	61.5± 0.4	$\surd$

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Tables contain textual material, whereas figures contain graphical material. Specify the contents of each row and column in the table's topmost row. Again, you may float tables to a column's top or bottom, and set wide tables across both columns. Place two-column tables at the top or bottom of the page.

3.9. Theorems and such

The preferred way is to number definitions, propositions, lemmas, etc. consecutively, within sections, as shown below.

Definition 3.1. A function $f : X \to Y$ is injective if for any $x, y \in X$ different, $f(x) \neq f(y)$.

Using Definition 3.1 we immediate get the following result:

Proposition 3.2. *If f is injective mapping a set X to another set Y, the cardinality of Y is at least as large as that of X*

Proof. Left as an exercise to the reader. □

Lemma 3.3 stated next will prove to be useful.

Lemma 3.3. *For any $f : X \to Y$ and $g : Y \to Z$ injective functions, $f \circ g$ is injective.*

Theorem 3.4. *If $f : X \to Y$ is bijective, the cardinality of X and Y are the same.*

An easy corollary of Theorem 3.4 is the following:

Corollary 3.5. *If $f : X \to Y$ is bijective, the cardinality of X is at least as large as that of Y.*

Assumption 3.6. The set X is finite.

Remark 3.7. According to some, it is only the finite case (cf. Assumption 3.6) that is interesting.

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Use an unnumbered first-level section heading for the references, and use a hanging indent style, with the first line of the reference flush against the left margin and subsequent lines indented by 10 points. The references at the end of this document give examples for journal articles, conference publications, book chapters, books, edited volumes, technical reports, and dissertations.

Alphabetize references by the surnames of the first authors, with single author entries preceding multiple author entries. Order references for the same authors by year of publication, with the earliest first. Make sure that each reference includes all relevant information (e.g., page numbers).

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The above statement can be used verbatim in such cases, but we encourage authors to think about whether there is content which does warrant further discussion, as this statement will be apparent if the paper is later flagged for ethics review.

4. Problem Definition

The goal of our project was to create a model which forecasts the future points of a time-series in a zero-shot manner. Concretely we want to build a model, that takes in k previous windows of length L of a time-series and then predicts the next $k+1$ window of length L. The model should also work in a zero-shot manner, meaning it should work without requiring any fine-tuning on the specific data it will be used on. To accomplish this we constructed a synthetic training dataset, build to cover a wide range of different time-series for the model to learn in order to facilitate the zero-shot use of the model. Our model consists of two separate networks, one for encoding the k windows and a second one for predicting the window $k+1$ from the encodings.

5. Methods

In this section we will look at the two main architectures that our model is based on. We will first look at DeepONet (**?**) in Section 5.1 and afterwards at FIM and FIM-l (**?**) in Section 7.1.

5.1. DeepONet

Deep operator network (DeepONet)(**?**) is a neural network architecture designed to learn nonlinear operators more accurately and efficiently than standard fully-connected networks. DeepONet consists of two sub-networks, a branch net and a trunk net. The branch net takes in m fixed values of the input function $f(t)$ and encodes them while the trunk net takes in the time point/location t^* for the output function we want to predict and encodes it. Both networks return a p-dimensional encoding and to obtain the output function value at our time point t^*, the scalar product between both encodings is calculated.

5.2. FIM-l

6. Model architecture

Next, we proceed with a detailed description of the architectures for both the FIM-l and FIM models. The FIM-l model serves as an operator, aiming to learn the underlying function from noisy samples, while the FIM model is designed as a forecasting framework. Our description closely follows the original implementations of both architectures, as outlined in (**?**).

6.1. FIM-ℓ

The primary aim of the FIM-ℓ model is to learn the underlying function $f(\tau)$ that has been augmented by noise to generate the observed time series (y_i, τ_i). The model should allow querying interpolated values of the underlying function $f(\tau)$ at arbitrary time points, including those not present in the observed data. We can therefore think of FIM-ℓ as a learned *neural interpolation operator* that maps the observed data into a continuous function space. To achieve this, we will leverage the ideas and architecture proposed by DeepONet (**?**). Given our noisy input sequence $(y_1, \tau_1), \ldots, (y_l, \tau_l)$, with observation values $y_i \in \mathbb{R}$ and ordered observation times $\tau_i \in \mathbb{R}^+$, as well as query points t_i, we define two feedforward neural network (FFN) embedding networks, ϕ_0^θ and ϕ_1^θ, to transform both the observed values and time points into an embedded representation:

$$\hat{y_i} = \phi_0^\theta(y_i), \quad \hat{t_i} = \phi_1^\theta(t_i).$$

We then proceed by concatenating both components to obtain the individual observation embeddings:

$$\mathbf{y_i^\theta} = \text{Concat}(\hat{y_i}, \hat{t_i}).$$

Following the work of DeepONet, we define a *branch net*-equivalent network consisting of a transformer-encoder network (**?**), denoted as ψ_0^θ, and a multilayer perceptron (MLP), denoted as ϕ_3^θ. Together, these form

$$\mathbf{u}^\theta = \phi_3^\theta\big(\psi_0^\theta(\mathbf{y_1^\theta}, \ldots, \mathbf{y_l^\theta})\big).$$

Finally, to generate a sequence-length-agnostic embedding, we take $\mathbf{u}^\theta$ from the branch network and feed it into a Multi-Head Attention () summary block λ_0^θ, where $\mathbf{u}^\theta$ serves as the *keys* and *values*, and a *learnable* vector q_{θ^*} is used as the *query*. The attention calculation is defined as

$$\mathbf{h}^\theta = \text{softmax}\left(\frac{q_{\theta^*} K^\top}{\sqrt{d_k}}\right) V = \lambda_0^\theta(\mathbf{u}^\theta),$$

where $K = \mathbf{u}^\theta$ are the keys, $V = \mathbf{u}^\theta$ are the values, and d_k is the dimensionality of the keys.

Next, we define our *trunk net*-equivalent network. We begin by introducing a separate embedding network, ϕ_4^θ, for the query points t. Additionally, we define another MLP, ϕ_5^θ. The final trunk net output, $\mathbf{t}^\theta$, is then obtained as

$$\mathbf{t}^\theta = (\phi_5^\theta \circ \phi_4^\theta)(t).$$

To finally obtain the interpolated values of the learned underlying function at the query points t, we define a final MLP, ϕ_7^θ, such that

$$\mathbf{y}(t) = \phi_7^\theta\big(\text{Concat}(\mathbf{h}^\theta, \mathbf{t}^\theta)\big),$$

where $\mathbf{y}(t)$ represents the learned underlying function given our noisy observation values.

6.2. FIM

We now proceed by utilizing the learned representations $\mathbf{h}^\theta$ of each local function window to predict the values of the time series at arbitrary points within the next, previously unseen window. Starting from the beginning, we receive a noisy time sequence $(y_1, \tau_1), \ldots, (y_l, \tau_l)$. We then split these values into $K = 5$ windows, such that for window S_j, we have

$$S_{ji} = (y_{\alpha+i}, \tau_{\alpha+i}), \quad \alpha = \sum_{l=1}^{j-1} w_l,$$

where w_l is the number of observations in window $l \leq K-1$. Additionally, for each of these windows, we construct their local scale characteristics $s_l \in \mathbb{R}^9$ (??), which are fed into an embedding layer σ_0^ω, defined as

$$\hat{s_l} = \sigma_0^\omega(s_l).$$

We then pass each window of observations into the pretrained embedding layers of the FIM-ℓ model. Specifically, we define:

$$\mathbf{y}_i^j = \text{Concat}\big(\phi_0^\theta((S_{ji})_1), \phi_1^\theta((S_{ji})_2)\big), \quad \text{j} \leq K-1, i \leq w_j.$$

We proceed by passing these $\mathbf{y}^j$ into the branch network of the FIM-ℓ, resulting in

$$\mathbf{h}_j = (\lambda_0^\theta \circ \phi_3^\theta \circ \psi_0^\theta)\big(\mathbf{y}_1^j, \ldots, \mathbf{y}_{w_j}^j\big).$$

After extracting the local embeddings for each of the $K-1$ windows, we proceed to reconstruct the K-th window. To achieve this, we first concatenate each local-scale embedding $\hat{s}_j$ with the observation embeddings and feed them into a Transformer encoder block ψ_1^ω. This is again followed by an attention-based summary network λ_1^ω, which generates the final embedding for the K-th window

$$\mathbf{h}_K^* = (\eta_0^\omega \circ \lambda_1^\omega \circ \psi_1^\omega)\Big((\mathbf{h}_1, \hat{s}_1), \ldots, \eta_0^\omega(\mathbf{h}_{K-1}, \hat{s}_{K-1})\Big).$$

Due to the concatenation of the observation and scale embeddings, the feature dimension is now doubled compared to the original embedding size. However, the frozen projection network of FIM-ℓ expects inputs in the original embedding dimension. To address this, we utilize an extractor network η_0^σ, which transforms the output of the summary network λ_1^ω back to the dimension expected by the FIM-ℓ projection layer.

To generate the final predictions for the K-th window, we utilize the embedding and trunk networks of the pretrained FIM-ℓ to predict the function values at the query points t. This is expressed as

$$\mathbf{y}(t) = \phi_7^\theta\big(\text{Concat}(\mathbf{h}_K^*, (\phi_5^\theta \circ \phi_4^\theta)(t))\big).$$

7. Model Training

In this section, we provide the necessary information to ensure the reproducibility of our work. Specifically, we outline the detailed structure of the aforementioned MLPs and discuss all relevant hyperparameters for both the model and the optimization algorithms.

7.1. FIM-ℓ Training

The implementation of our previously defined FIM-ℓ architecture is described in 7.1. Here, we use d_{model} to denote the embedding dimension. In our setting, we set $d_{\text{model}} = 256$ and $n_{\text{heads}} = 4$. Since *LeakyReLU* is shift-invariant, the bias term in the linear layer can be omitted if it is followed by a *LayerNorm*, as the *LayerNorm* neutralizes any bias introduced by the preceding layer. We train the model with a batch size of 128, using the *AdamW* optimizer with the following hyperparameters: β-values $(\beta_1, \beta_2) = (0.9, 0.999)$, $\epsilon = 10^{-8}$, and a weight decay of 0.01. Additionally, we employ an *Inverse Square Root Learning Rate* (*InverseSquareRootLR*)(**?**) scheduling strategy, with 100 warm-up steps, an initial learning rate of 10^{-4}, and a minimum learning rate of 10^{-5}.
To save memory and computational resources, we utilize the PyTorch *Automatic Mixed Precision* package, which trains the model in mixed precision. Specifically, it selects half-precision data types (*bfloat16* in our case) for operations it deems suitable. This approach enables the model to leverage the highly optimized NVIDIA Tensor Cores, maximizing performance during matrix operations.
For our loss computations, we use the standard *Mean Squared Error* (MSE) between the predicted outputs of the model and the precomputed ground truth. Before performing the optimizer update step, we apply gradient clipping to ensure that the gradient norm does not exceed the length of a unit vector. This stabilizes training by limiting the size of each gradient step during optimization.
We then provide the model with the noisy observation sequence, observation time points, query points, and the branch mask. The branch mask is then utilized by both the Transformer encoder ψ_0^θ and the summary network λ_0^θ as the padding mask.

Component	Details
Branch Embedding ϕ_0^θ	Linear(1, d_{model})
Branch Embedding ϕ_1^θ	Linear(1, d_{model})
Trunk Embedding ϕ_4^θ	Linear(1, d_{model})
Branch Encoder Input	Concatenate embeddings of y and t
Branch Encoder ψ_0^θ	Transformer Encoder (6 layers, $2d_{\text{model}}$, n_{heads})
Branch MLP ϕ_3^θ	Linear($2d_{\text{model}} \to d_{\text{model}}$), LeakyReLU, LayerNorm
Learnable Query	Parameter tensor of shape (1, d_{model})
Branch Attention λ_0^θ	Multihead Attention (d_{model}, heads=1)
Trunk MLP ϕ_5^θ	4x Linear($d_{\text{model}} \to d_{\text{model}}$), LeakyReLU, LayerNorm
Combine Outputs	Concatenate outputs of Branch Attention and Trunk MLP
Final Projection ϕ_7^θ	5x Linear ($2d_{\text{model}} \to 1$), LeakyReLU, LayerNorm

Table 2. FIM-ℓ architecture implementation

7.2. FIM Training

The implementation of the FIM network that we defined is detailed in Table 7.2. We set $d_{\text{model}} = 256$ and $n_{\text{heads}} = 8$. Regarding the optimizer and learning rate strategy, we use the same settings as described previously, along with automatic mixed precision training. The loss function remains the *Mean Squared Error* (MSE), and the gradients are clipped to ensure their norm does not exceed the length of a unit vector. We again provide the model with the noisy observation sequence, observation time points, query points, and the branch mask. However, instead of treating a single window as one data point, each example now comprises all local windows of the global function.

Component	Details
Pretrained FIM-ℓ	$n_{\text{heads-fim-}\ell}$, d_{model} (Frozen)
Local Scale Embedding σ_0^ω	Linear(9, d_{model})
Combine Outputs	Concatenate outputs of Pretrained FIM-ℓ and Local Scale Embedding
Transformer Encoder ψ_1^ω	8 layers, $2d_{\text{model}}$, n_{heads}
Learnable Query	Parameter tensor of shape (1, $2d_{\text{model}}$)
Summary Attention λ_1^ω	Multihead Attention ($2d_{\text{model}}$, n_{heads})
Extractor Network η_0^ω	Sequential: Linear($2d_{\text{model}}$, $4d_{\text{model}}$) LeakyReLU, LayerNorm Linear($4d_{\text{model}}$, $2d_{\text{model}}$) LeakyReLU, Linear($2d_{\text{model}}$, d_{model})
Trunk Embedding ϕ_4^θ	Reused from FIM-ℓ (Frozen)
Trunk MLP ϕ_5^θ	Reused from FIM-ℓ (Frozen)
Combine Outputs	Concatenate outputs of Trunk Network and Summary Network
Final Projection ϕ_7^θ	Reused from FIM-ℓ (Frozen): 5x Linear ($2d_{\text{model}} \to 1$), LeakyReLU, LayerNorm

Table 3. FIM Architecture Overview

8. Experiments

In this section, we discuss additional experiments conducted on the model's architecture and the construction of the loss function to achieve higher prediction accuracy. The impact of each of these approaches will be presented later in Section **??**.

8.1. Learned Positional Encoding for FIM-ℓ Embeddings

In this approach, we hypothesize that the model may benefit from additional positional encoding for the attention-based summary network λ_1^ω. We define

$$\mathbf{p} = \psi_1^\omega\Big((\mathbf{h}_1, \hat{s}_1), \ldots, \eta_0^\omega(\mathbf{h}_{K-1}, \hat{s}_{K-1})\Big), \quad \mathbf{p} \in \mathbb{R}^{(K-1)\times d_{\text{model}}}.$$

as the output from the FIM transformer encoder network. In our standard implementation, $\mathbf{p}$ is passed to the summary attention network λ_1^ω, which, by default, lacks a sense of order among these embeddings, aside from the local scale statistics of each window. We hypothesize that providing positional information may help this layer better identify the order of embeddings, enabling more informed predictions of the K-th embedding.
To address this, we introduce an additional parameter vector $\mathbf{z} \in \mathbb{R}^{(K-1)\times d_{\text{model}}}$, which serves as a learnable positional encoding. We add $\mathbf{z}$ elementwise to $\mathbf{p}$ before passing the result to λ_1^ω, as follows

$$\mathbf{h}_K^* = (\eta_0^\omega \circ \lambda_1^\omega)\Big(\mathbf{p} + \mathbf{z}\Big).$$

8.2. Similarity loss between FIM-ℓ ground truth and predicted embeddings.

Another strategy is the usage of the ground truth $\mathbf{h}_K$ for enabling more accurate predictions. The idea is to align the predicted $\mathbf{h}_K^*$ and the actual ground truth $\mathbf{h}_K$ such that they are as close as possible to each other. We can do this by adding an additional term to the model's loss function, which incentivizes it to form predictions $\mathbf{h}_K^*$ that are close to the FIM-ℓ predicted $\mathbf{h}_K$. A suitable metric for this is the *cosine similarity*, defined as

$$\text{CosSim}(\mathbf{a}, \mathbf{b}) = \frac{\mathbf{a}^T\mathbf{b}}{\|\mathbf{a}\|\|\mathbf{b}\|}, \quad \mathbf{a}, \mathbf{b} \in \mathbb{R}^n.$$

$$\forall \mathbf{a}, \mathbf{b} \in \mathbb{R}^n \setminus \{\mathbf{0}\}, \quad \text{CosSim}(\mathbf{a}, \mathbf{b}) \in [-1, 1].$$

Geometrically, the *cosine similarity* represents the cosine of the angle between two vectors. Specifically, $\text{CosSim}(\mathbf{a}, \mathbf{b}) = 0$ indicates orthogonality, while $\text{CosSim}(\mathbf{a}, \mathbf{b}) = 1$ and $\text{CosSim}(\mathbf{a}, \mathbf{b}) = -1$ correspond to vectors pointing in the same and opposite directions, respectively.
We now define our new loss function $\mathcal{L}(y, \hat{y}, \mathbf{h}_K^*, \mathbf{h}_K)$, which incorporates both prediction accuracy and alignment between the predicted and ground-truth representations. The loss function is given by

$$\mathcal{L}(y, \hat{y}, \mathbf{h}_K^*, \mathbf{h}_K) = \frac{1}{n}\sum_1^n (y_i - \hat{y}_i)^2 + \beta \cdot |\text{CosSim}(\mathbf{h}_K^*, \mathbf{h}_K) - 1|,$$

where y denotes the ground truth values of the target variable, and $\hat{y}$ represents the corresponding predicted values by the model. We choose $\beta \ll 1$ to ensure that the optimization does not focus too aggressively on aligning $\mathbf{h}_K^*$ and $\mathbf{h}_K$.

9. Results

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You can have as much text here as you want. The main body must be at most 8 pages long. For the final version, one more page can be added. If you want, you can use an appendix like this one.

The `\onecolumn` command above can be kept in place if you prefer a one-column appendix, or can be removed if you prefer a two-column appendix. Apart from this possible change, the style (font size, spacing, margins, page numbering, etc.) should be kept the same as the main body.