# Package 'fonfDNN'

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Title Hybrid deep tensor network for function-on-function regression with mixed predictors
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<b>Description</b> Functions for implementing deep tensor network for function-on-function regression with mixed predictors.
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air_data Air Quality Dataset from Lombardy, Italy (2023–2024)

# Description

Type Package

A real-world dataset containing daily air pollution measurements from the Lombardy region in Italy, covering the years 2023 and 2024. This dataset includes functional trajectories of various pollutants recorded over time across 1481 monitoring stations, and serves as the empirical application for the proposed hybrid deep tensor network (HDTN) model for function-on-function regression with mixed predictors.

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## Usage

```
data(air_data)
```

#### **Format**

A list with the following components:

- y A matrix of dimension n x M representing the functional response curves (daily mean  $PM_{2.5}$  concentrations), where n is the number of stations and M is the number of grid points.
- x A list of length 5, where each element is an n x M matrix corresponding to a functional predictor:
  - 1. Daily mean NO<sub>2</sub> concentration,
  - 2. Daily maximum 1-hour NO<sub>2</sub> concentration,
  - 3. Daily maximum 8-hour O<sub>3</sub> concentration,
  - 4. Daily maximum 1-hour O<sub>3</sub> concentration,
  - 5. Daily mean  $PM_{10}$  concentration.

xscl A matrix of dimension  $n \times 3$  containing scalar predictors:

## **Details**

This dataset is sourced from the ARPA Lombardy regional environmental monitoring agency and was accessed using the ARPALData package. It is used in the empirical section of the paper to demonstrate the effectiveness of the HDTN model in predicting fine particulate matter concentrations based on mixed-type predictors (functional and scalar).

## Value

A list containing the functional response and covariate data required to fit the HDTN model, including:

y Functional response ( $PM_{2.5}$  curves) x List of 5 functional covariate matrices xscl Matrix of scalar covariates

## Note

The dataset has been preprocessed and standardized for modeling purposes. Time series lengths and grid structures are aligned for all stations.

## References

Maranzano, M., and Algieri, C. (2024). ARPALData: An R package for retrieving and analyzing air quality and weather data from ARPA Lombardia (Italy). *Environmental and Ecological Statistics*, 31(2), 187-218.

# **Examples**

```
## NOTE: This example involves ultra high-dimensional functional data.
## Running the model may require a PC with at least 64 GB of RAM.
# data(air_data)
# y <- air_data$y</pre>
```

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```
# x <- air_data$x</pre>
# xscl <- air_data$xscl</pre>
# ntot <- dim(y)[1]
# ntrain <- 1000
# ntest <- ntot - ntrain</pre>
# train_ind <- sample(1:ntot, ntrain, replace = FALSE)</pre>
# Training sample
# y_train <- y[train_ind, ]</pre>
# y_test <- y[-train_ind, ]</pre>
# xscl_train <- xscl[train_ind, ]</pre>
# xscl_test <- xscl[-train_ind, ]</pre>
# Test sample
# x_train <- x_test <- vector("list", length = 5)</pre>
# for (j in 1:5) {
x_{\text{train}[[j]]} \leftarrow x[[j]][train_ind, ]
   x_test[[j]] <- x[[j]][-train_ind, ]</pre>
# }
# Train HDTN approach
# nfof_model <- fonf_fit(resp = y_train, func_cov = x_train, scalar_cov = xscl_train)</pre>
# Obtain predictions with conformal prediction intervals
# band <- fonf_predict(nfof_model,</pre>
                          func\_cov\_new = x\_test,
#
#
                          scalar_cov_new = xscl_test,
                                          = "conformal")
#
                          interval
```

dgp\_mixed

Simulate Mixed Functional–Scalar Data for Function–on–Function Regression

# Description

Generates synthetic datasets that mimic the structure analysed in *Beyaztas, Bakicierler Sezer, Inan* (2025): a functional response observed on a dense grid, multiple functional predictors, and multiple scalar predictors. Two regimes are available:

- "linear": response driven solely by linear integral effects.
- "nonlinear": adds strong, smooth nonlinear interactions (functional × functional, functional × scalar, scalar × scalar) scaled to dominate the linear part.

Every dataset also includes Ornstein-Uhlenbeck (OU) process noise to emulate realistic autocorrelated measurement error.

## Usage

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## **Arguments**

n	Number of subjects/curves.
j	Grid length $M$ ; all functional objects are evaluated on seq(0, 1, length.out = j).
model	Character string choosing the data-generating mechanism; partial matching is supported.
n_func	Number $P$ of functional predictors to simulate.
n_scl	Number $d_z$ of scalar predictors.
seed	Optional integer for reproducibility (set.seed(seed)).

## **Details**

Let  $X_i^{(p)}(s)$  denote functional predictor  $p=1,\ldots,P$  and  $\mathbf{Z}_i \in \mathbb{R}^{d_z}$  the scalar predictor vector for subject  $i \in \{1,\ldots,n\}$ . The latent *signal* generating the functional response on grid points  $t_1,\ldots,t_M$  is

$$\eta_i(t) = \underbrace{\sum_{p=1}^P \int_0^1 X_i^{(p)}(s) \, \beta_p(s,t) \, ds}_{\text{linear functional effects}} + \underbrace{\mathbf{Z}_i^\top \gamma(t)}_{\text{scalar effects}} + \mathcal{N}L_i(t),$$

where P=3 "strong" functional predictors drive the linear component,  $\beta_p$  are pre-specified wavy B-spline surfaces (see code), and  $\gamma(t)$  are smooth one-dimensional bases. If model == "linear" we set  $\mathcal{N}L_i(t)\equiv 0$ ; otherwise  $\mathcal{N}L_i(t)$  equals the *sum* of five carefully designed nonlinear terms (quadratic functional interactions, sinusoidal transforms, scalar–functional products, etc.) rescaled so that

$$SD\{NL\} \approx 2 SD\{\text{linear signal}\}.$$

The *observed* response is

$$Y_i(t_m) = \eta_i(t_m) + \varepsilon_i(t_m), \quad \varepsilon_i \sim OU(0, \alpha = 3, \sigma = 0.7),$$

i.e. an Ornstein–Uhlenbeck process discretised on the same grid. Noise is scaled so that its empirical standard deviation equals 10% of the signal standard deviation.

## Value

A named list:

У	$n \times j$ matrix of noisy responses $Y_i(t_m)$ .
yt	$n \times j$ matrix of true signals $\eta_i(t_m)$ .
х	list of length P; each element is an $n \times j$ matrix of functional predictors $X_i^{(p)}(s_m).$
x.scl	$n \times d_z$ numeric matrix of scalar predictors $\mathbf{Z}_i$ .
meta	List containing grids sx, sy, true beta surfaces (beta), and the model flag.

## Note

Requires the suggested package **goffda** for OU noise generation.

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#### Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

#### References

Kokoszka, P. and Reimherr, M.~(2017). *Introduction to Functional Data Analysis*. Chapman and Hall/CRC.

#### See Also

```
fonf_fit, r_ou
```

## **Examples**

```
## Not run:
# ------
# Simulate a nonlinear training set and inspect its structure
# -------
# n <- 100  # sample size
# simdata <- dgp_mixed(n, 101, model = "nonlinear")

# y <- simdata$y  # noisy response curves
# yt <- simdata$yt  # true (noise-free) curves
# x <- simdata$x  # list of functional predictors
# xscl <- simdata$x.scl  # scalar predictors
## End(Not run)</pre>
```

fonf\_fit

Fit a Hybrid Deep Tensor Network for Function-on-Function Regression with Mixed Predictors

## **Description**

Trains the hybrid deep tensor network (HDTN) of *Beyaztas, Bakicierler Sezer, Inan* (2025) to predict a *functional response* from multiple functional and scalar covariates. The model combines a first-layer tensor-product B-spline representation (capturing linear functional effects) with fully-connected dense layers (capturing higher-order nonlinear interactions) and supplies finite-sample, distribution-free prediction bands via conformal inference.

# Usage

```
fonf_fit(resp,
         func_cov,
                            = NULL,
         scalar_cov
         nbasis_y
                             = NULL,
                              = NULL.
         nbasis_x
         hidden_layers = 2,
neurons_per_layer = c(32, 32),
         activations_in_layers = c("relu", "linear"),
                              = 100,
         epochs
         batch_size
                              = 32,
                              = 0.1,
         val_split
```

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learning_rate	= 1e-3,
patience_param	= 15,
dropout_rate	= 0.1,
12_lambda	= 1e-4,
cal_prop	= 0.2,
alpha	= 0.2,
verbose	= 1)

## **Arguments**

resp  $n \times M$  numeric matrix; row i stores the functional response  $Y_i(t_m)$  evaluated

on a common grid  $t_1, \ldots, t_M \subset \mathcal{I}_y$ .

func\_cov List of length P. Element p is an  $n \times G_p$  matrix that holds the functional pre-

dictor  $X_i^{(p)}(s_{pj})$  on its own grid  $s_{p1}, \ldots, s_{pG_p} \subset \mathcal{I}_{x_p}$ .

scalar\_cov Optional  $n \times d_z$  numeric matrix of scalar covariates  $\mathbf{Z}_i \in \mathbb{R}^{d_z}$ .

nbasis\_y Number of B-spline basis functions for the response domain  $(K_y)$ ; chosen auto-

matically when NULL.

nbasis\_x Integer vector of length P; element p gives the number of input-domain basis

functions  $K_x^{(p)}$ . Automatically selected when NULL.

 $hidden_{layers}$  Number R of fully-connected hidden layers.

neurons\_per\_layer

Vector of length hidden\_layers giving the width  $(D_r)$  of each dense layer.

activations\_in\_layers

Character vector of length hidden\_layers with Keras activation names ("relu",

"tanh", etc.).

epochs Maximum training epochs.

batch\_size Mini-batch size for stochastic optimisation.

val\_split Proportion of the training rows (not subjects) held out for on-line validation

during training.

learning\_rate Initial learning rate for the Adam optimiser (with cosine decay scheduler).

patience\_param Early-stopping patience; training stops when validation loss fails to improve for

this many epochs.

dropout\_rate Dropout probability applied after every dense hidden layer.

12\_lambda  $\ell_2$  (ridge) penalty applied to dense-layer weights.

cal\_prop Proportion of subjects set aside for the conformal *calibration* set.

alpha Mis-coverage level for conformal prediction bands (e.g. 0.2 yields 80% bands).

verbose Passed to keras; larger values give more console output.

## **Details**

Let  $Y_i(t) \in L^2(\mathcal{I}_y)$  be the response curve for subject  $i, X_i^{(p)}(s) \in L^2(\mathcal{I}_{x_p}), p \in \{1, \dots, P\}$ , the functional predictors, and  $\mathbf{Z}_i \in \mathbb{R}^{d_z}$  scalar predictors. The HDTN targets the nonlinear FoFR model

$$Y_i(t) = g \left\{ \beta_0(t) + \sum_{p=1}^P \langle X_i^{(p)}, \beta_p(\cdot, t) \rangle_{L^2} + \mathbf{Z}_i^\top \theta(t) \right\} + \varepsilon_i(t), \quad t \in \mathcal{I}_y,$$

with identity link g(u) = u in the present implementation.

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Tensor-product layer. Each bivariate coefficient surface is expanded

$$\beta_p(s,t) = \sum_{k=1}^{K_x^{(p)}} \sum_{\ell=1}^{K_y} w_{k\ell}^{(p)} \, \phi_k^{(p)}(s) \psi_\ell(t),$$

yielding first-layer weights  $w_{k\ell}^{(p)}$  to be learned. Subject-specific functional features are  $\tilde{\varphi}_{ik}^{(p)} = \langle X_i^{(p)}, \phi_k^{(p)} \rangle_{L^2}$  and  $u_{i\ell}^{(p)} = \sum_k \tilde{\varphi}_{ik}^{(p)} w_{k\ell}^{(p)}$ .

**Dense layers**. The concatenated feature vector  $\mathbf{h}_i^{(0)} = \left(u_{i\cdot}^{(1)\top}, \dots, u_{i\cdot}^{(P)\top}, \mathbf{Z}_i^{\top}\right)^{\top}$  is propagated through R fully-connected layers  $\mathbf{h}_i^{(r)} = \sigma_r (W^{(r)} \mathbf{h}_i^{(r-1)} + b^{(r)})$  with dropout and ridge penalty  $\lambda \|W^{(r)}\|_F^2/2$ . The final linear layer outputs  $\hat{\eta}_i(t_m)$ , giving  $\hat{Y}_i(t_m) = \hat{\eta}_i(t_m)$  for identity link.

**Loss and optimisation**. Training minimises mean integrated squared error plus the ridge penalty,  $\mathcal{L} = \frac{1}{nM} \sum_{i=1}^n \sum_{m=1}^M \left\{ Y_i(t_m) - \hat{Y}_i(t_m) \right\}^2 + \frac{\lambda}{2} \sum_{r=1}^R \|W^{(r)}\|_F^2, \text{ via Adam with cosine-decay learning rate.}$ 

Conformal prediction. A calibration subset C (size cal\_prop \* n subjects) yields residuals  $e_{jm} = |Y_j(t_m) - \hat{Y}_j(t_m)|$ . The empirical  $1 - \alpha$  quantile  $q_{1-\alpha}$  of length(C)\*M pooled residuals provides a constant-width  $(1 - \alpha)$  band  $\left[\hat{Y}_i(t_m) - q_{1-\alpha}, \ \hat{Y}_i(t_m) + q_{1-\alpha}\right]$  for every new subject i and grid point  $t_m$ . Finite-sample marginal coverage is guaranteed (Lei, G'Sell, et al., 2018).

#### Value

An object of class "fonf\_dl" to be consumed by fonf\_predict:

model Trained Keras model.

center, scale Vectors used to standardise the design matrix.

py Number of response grid points (M).

nbasis\_y, nbasis\_x

Basis dimensions actually used.

q\_hat Half-width  $q_{1-\alpha}$  of the conformal prediction band.

alpha User-supplied mis-coverage level.

history keras\_training\_history object returned by fit().

## Note

Requires TensorFlow/Keras (tested with TensorFlow >= 2.16).

## Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

## References

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. and Wasserman, L. (2018). *Distribution-Free Predictive Inference for Regression. Journal of the American Statistical Association*, 113(523), 1094-1111.

## See Also

fonf\_predict, keras\_model\_sequential

fonf\_fnc

#### **Examples**

```
## Not run:
# 1. Simulate training data
# n <- 100
# simdata <- dgp_mixed(n, 101, model = "nonlinear")</pre>
     <- simdata$y
# yt <- simdata$yt</pre>
                       # (true curves, if needed)
     <- simdata$x
                       # list of functional predictors
# x
                      # scalar predictors
# xscl <- simdata$x.scl</pre>
# ------
# 2. Fit the hybrid deep tensor network
# ------
# nfof_model <- fonf_fit(resp</pre>
                           = y,
                  func\_cov = x,
                   scalar_cov = xscl)
## End(Not run)
```

fonf\_fnc

Extract and Visualise Estimated Coefficient Surfaces

## **Description**

Given a fitted fonf\_fit model, this helper recovers the bivariate coefficient surfaces  $\widehat{\beta}_p(t,s)$  that link functional predictor  $X^{(p)}(s)$  to the functional response Y(t), evaluates them on user-supplied grids, and—optionally—renders compact, printer-friendly 3-D perspective plots via **plot3D**.

### Usage

```
fonf_fnc(model,
        y_grid
                = NULL,
= NULL,
        x_grid
        agg_fun
                   = mean,
                    = TRUE,
        plot
                  = 101,
        grid_len
        view_theta = 40,
        view_phi
                  = 2,
        surface_col = "royalblue",
        border_col = "black",
        shade_fac = 0.5,
        title_mgp = c(2.8, 0.8, 0),
         ...)
```

## **Arguments**

```
model Object of class "fonf_dl" returned by fonf_fit.   y\_grid \qquad \qquad \text{Numeric vector of evaluation points } t_1, \ldots, t_M \text{ in the interval } [0,1]. \text{ Defaults to } \\  seq(0, 1, length.out = grid_len).
```

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x\_grid List of length P; element p is the grid  $s_{k1}, \ldots, s_{kL_k}$  for predictor p. Defaults to a length-grid\_len equi-spaced grid for every predictor. Function used to collapse the first-layer tensor weights into a single set of Bagg\_fun spline coefficients. With the default mean:  $\widehat{\beta}_p(t,s) = \frac{1}{D_1} \sum_{d=1}^{D_1} w_d^{(p)} B_y(t) B_x^{(p)}(s).$ Logical; if TRUE (default) one 3-D plot is produced for each predictor. plot grid\_len Length of the default equi-spaced grids when y\_grid or an element of x\_grid is NULL. view\_theta, view\_phi Viewing angles (in degrees) passed to persp3D. surface\_col, border\_col, shade\_fac Graphical parameters for the surfaces. Margin settings for titles (argument passed to par (mgp = ...) inside each plot). title\_mgp Currently ignored, reserved for future extensions.

#### **Details**

Let  $B_y(t)$  be the vector of  $K_y$  B-spline basis functions for t and let  $B_x^{(p)}(s)$  be the vector of  $K_x^{(p)}$  basis functions for s in predictor p. The first layer of the network stores a weight matrix  $W^{(1)}$  whose rows correspond to the spline products  $B_y(t)$   $B_x^{(p)}(s)$ . For each predictor p we:

- 1. Extract the contiguous block of  $K_y K_x^{(p)}$  weights.
- 2. Fold it into a  $K_y \times K_x^{(p)}$  matrix  $C_k$ .
- 3. Evaluate  $\widehat{\beta}_p(t,s) = B_y(t)^{\top} C_k B_x^{(p)}(s)$  on the requested grids.

If plot = TRUE every surface is drawn with persp3D; otherwise the numeric matrices are returned silently.

## Value

Invisibly returns a list with components:

beta\_hat List of length P; element p is a length(y\_grid) by length(x\_grid[[p]]) matrix containing  $\widehat{\beta}_p(t,s)$ .

y\_grid Evaluation grid for t.

x\_grid Evaluation grids for s.

List of closure functions; calling plots[[p]]() re-draws the p-th surface.

#### Note

Requires the suggested packages fda, keras, and plot3D. An error is thrown if any are missing.

# Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

## See Also

```
fonf_fit, persp3D, eval.basis
```

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#### **Examples**

fonf\_param\_grid

Create a Parameter Grid Without Factors

## **Description**

Generates a data frame from all combinations of input vectors, ensuring that character variables are not converted to factors. This is a convenient wrapper around expand.grid(..., stringsAsFactors = FALSE).

#### Usage

```
fonf_param_grid(...)
```

## Arguments

One or more vectors, factors, or lists to be combined into a data frame of parameter combinations.

# **Details**

This function simplifies the creation of parameter grids for tuning models. Unlike the base R expand.grid, it ensures that character vectors remain as characters, which is often desirable when building machine learning or neural network models where hyperparameter names or tags are string-based.

## Value

A data frame containing one row for each combination of the supplied vectors.

#### Note

This function is mainly used to build cross-product grids of model parameters when performing grid search for tuning.

# Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

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fonf_predict	Predict With a Trained Hybrid Deep Tensor Network

## **Description**

Generates point predictions and, optionally, distribution-free conformal prediction bands for a fonf\_fit model given new functional and scalar covariates.

# Usage

## **Arguments**

## **Details**

Let  $f_{\text{hat}}$  denote the trained network and let  $(x_i, z_i)$  be the design-matrix rows for a new subject, built with the same tensor-product bases used in training. fonf\_predict:

- 1. Builds the design matrix with design\_matrix\_build.
- 2. Standardises it with the training means and scales stored in the fitted object.
- 3. Computes the predictions, then reshapes the vector into an  $n_{\text{new}} \times M$  matrix, where M = object\$py.

**Conformal bands:** If interval == "conformal" the returned bands are  $\hat{Y}_i(t_m) \pm q_{1-\alpha}$ , where  $q_{1-\alpha}$  is the  $(1-\alpha)$ -quantile of the absolute residuals on the calibration set chosen during training. Split-conformal theory (Lei *et al.*, 2018) guarantees marginal coverage  $1-\alpha$  at each grid point, without distributional assumptions beyond independent rows.

#### Value

```
interval = "none" A numeric matrix with nrow = n_{new} and ncol = py containing point predictions.
```

interval = "conformal" A list with components mean, lower, and upper, each a matrix whose columns are named "t1", "t2", ..., "tM".

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#### Note

The feature grids supplied here must match those used at training time, and the length of the prediction vector must be divisible by object\$py; otherwise an error is raised.

#### Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

#### References

Lei, J., G'Sell, M., Rinaldo, A., Tibshirani, R. & Wasserman, L. (2018). Distribution-Free Predictive Inference for Regression. *Journal of the American Statistical Association*, 113(523), 1094–1111.

#### See Also

```
fonf_fit, dgp_mixed
```

# **Examples**

fonf\_tune

Simple Grid-Search Hyper-parameter Tuner for fonf\_fit

# **Description**

Evaluates every row of a user-supplied hyper-parameter grid via *K*-fold cross-validation (fonf\_cv), reports the cross-validated mean-squared error (CV-MSE), and then refits the best combination on the *full* data set. The implementation is deliberately lightweight—single-core, base R only—so it runs on any system where **fonf** installs.

## Usage

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## **Arguments**

grid	A data frame created by fonf_param_grid describing the hyper-parameter combinations to be tested. Each column corresponds to an argument of fonf_fit.
resp	Numeric matrix of size $n \times p_y$ ; functional response curves sampled on a common grid.
func_cov	List of length $P$ ; element $p$ is an $n \times G_p$ matrix containing the $p$ -th functional predictor.
scalar_cov	Optional $n \times q$ numeric matrix of scalar predictors. Omit or set to NULL if none.
nfolds	Number of folds used by fonf_cv (default 5).

#### **Details**

**How it works:** For each row g = 1, ..., G of grid:

- 1. The row is coerced to a named list of arguments compatible with fonf\_fit (vectors such as neurons\_per\_layer are replicated to the correct length).
- 2. fonf\_cv performs K-fold CV and stores the average test MSE in cv\_vec[g].

After all rows are processed the index of the minimum CV-MSE is selected, the corresponding parameter list is re-sanitised by sanitize\_basis(), and a final model is fitted on the whole data via fonf\_fit with verbose = TRUE.

## Value

results Data frame combining the original grid and a new column CV\_MSE (lower is better).

**best\_params** Named list containing the best-performing hyper-parameters in a format ready for fonf\_fit.

best\_model Object of class "fonf\_dl" fitted on the full data with best\_params.

## Note

- This function is single-threaded. For large grids consider a parallel wrapper (e.g. **future.apply**).
- Internal helpers flatten1() and sanitize\_basis() are not exported but are documented in the source code.

# Author(s)

Ufuk Beyaztas, Gizel Bakicierler Sezer, Deniz Inan

# **Examples**

fonf\_tune

```
# 2. Construct a small hyper-parameter grid
# -----
# grid <- fonf_param_grid(</pre>
# hidden_layers = c(1, 2),
# neurons_per_layer = list(32, c(64, 32)),
# activations_in_layers = list("relu", c("relu", "linear")),
# learning_rate = c(1e-3, 5e-4),
# epochs = 25
# epochs
#)
# -----
# 3. Tune and refit
# -----
# tune_out <- fonf_tune(grid,</pre>
                  resp = y,
func_cov = x,
#
#
                  scalar_cov = xscl,
#
                  nfolds = 5)
# tune_out$results
                     # CV table
# best_mod <- tune_out$best_model</pre>
## End(Not run)
```

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