CDR Documentation

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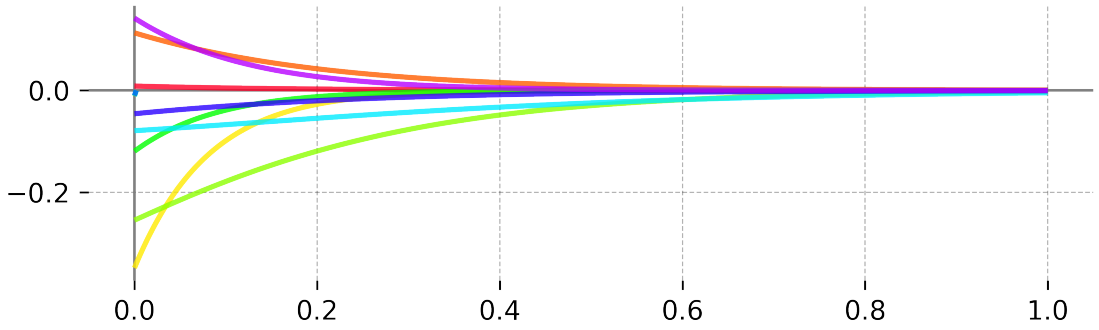
Documentation for the `cdr` Python package.

CHAPTER

ONE

INTRODUCTION



In many real world time series, events trigger "ripples" in a dependent variable that unfold slowly and overlap in time (temporal diffusion). Recovering the underlying dynamics of temporally diffuse effects is challenging when events and/or responses occur at irregular intervals. Continuous-time deconvolutional regression (CDR) is a regression technique for time series that directly models temporal diffusion of effects (Shain & Schuler, 2018, 2021). CDR uses machine learning to estimate continuous-time impulse response functions (IRFs) that mediate between predictors (event properties) and responses. Given data and a model template specifying the functional form(s) of the IRF kernel(s), CDR finds IRF parameters that optimize some objective function. This approach can be generalized to account for non-stationary, non-linear, non-additive, and context-dependent response functions by implementing the IRF as a deep neural network (Shain, 2021).

The `cdr` package documented here provides a Python implementation of a general-purpose CDR framework that allows users to flexibly select among neural network and kernel-based approaches to continuous-time deconvolution, and even to combine both approaches within a single model. This package provides (1) an API for programming with CDR(NN) and (2) executables that allow users to train and evaluate CDR(NN) models out of the box, without needing to write any code. Source code and bug reporting tools are available on Github.

1.1 Installation (PyPI)

Install python, then install CDR(NN) using `pip` as follows:

```
pip install cdrnn
```

Note that, despite the package name, both (kernel-based) CDR and (deep-neural) CDRNN are both implemented by the same codebase, so both kinds of models can be fitted using this package.

1.2 Installation (Anaconda)

Install anaconda and clone the CDR repository (https://github.com/coryshain/cdr) to the directory of your choice. From the CDR repository root, run the following commands to create a new conda environment:

```
conda env create -f conda_cdr.yml
conda activate cdr
```

(Optional) Run the following from the CDR repository root to install CDR system-wide (otherwise, simply run CDR from the repository root):

```
python setup.py install
```

The `cdr` environment must first be activated anytime you want to use the CDR codebase:

```
conda activate cdr
```

1.3 Basic Usage

Once the `cdr` package is installed system-wide as described above (and the `cdr` conda environment is activated via `conda activate cdr`), the `cdr` package can be imported into Python as shown:

```
import cdr
```

Most users will not need to program with CDR(NN), but will instead run command-line executables for model fitting and criticism. These can be run as:

```
python -m cdr.bin.<EXECUTABLE-NAME> ...
```

For documentation of available CDR(NN) executables, run:

```
python -m cdr.bin.help( <SCRIPT-NAME>)*
```

CDR(NN) models are defined using configuration (`*.ini`) files (fully described in *CDR Configuration Files*), which can be more convenient than shell arguments for specifying many settings at once, and which provide written documentation of the specific settings used to generate any given result. For convenience, we have provided a utility to initialize a new `*.ini` file, which can be run like this:

```
python -m cdr.bin.create_config > PATH.ini
```

This will initialize a CDR-oriented config file. To initialize a CDRNN-oriented config file, add the flag `-t cdrnn`. To initialize a plotting-oriented config file (which defines visualizations to run for an already fitted model), add the flag `-t plot`. To include annotation comments in the output file (which can help with customizing it), add the flag `-a`. The `PATH.ini` file can then be modified as needed to set up the analysis.

CDR model formula syntax resembles R-style model formulas (`DV ~ IV1 + IV2 + ...`) and is fully described in *CDR Model Formulas*. The core novelty is the `C(preds, IRF)` call (`C` for "convolve"), in which the first argument is a '+'-delimited list of predictors and the second argument is a call to an impulse response kernel (e.g. `Exp`, `Normal`, `ShiftedGammaShapeGT1`, see *CDR Model Formulas* for complete list). For example, a model with the following specification:

```
formula = DV ~ C(a + b + c, Normal())
```

will fit a CDR model that convolves predictors `a`, `b`, `c` using `Normal` IRFs with trainable location and scale parameters.

CDRNN models do not require user-specification of a kernel family, so their formula syntax is simpler:

```
formula = DV ~ a + b + c
```

The response shape to all variables (and all their interactions) will be fitted jointly.

Once a model file has been written (e.g. `model.ini`), the model(s) defined in it can be trained by running:

```
python -m cdr.bin.train model.ini
```

IRF estimates will be incrementally dumped into the output directory specified by `model.ini`, and learning curves can be inspected in Tensorboard:

```
python -m tensorboard.main --logdir=<PATH-TO-CDR-OUTPUT>
```

1.4 References

Shain, Cory and Schuler, William (2018). Deconvolutional time series regression: A technique for modeling temporally diffuse effects. *EMNLP18*.

Shain, Cory and Schuler, William (2021). Continuous-time deconvolutional regression for psycholinguistic modeling. *Cognition*.

Shain, Cory (2021). CDRNN: Discovering complex dynamics in human language processing. *ACL21*.

CHAPTER

TWO

GETTING STARTED

The `cdr` package provides utilities that support easy training and evaluation of CDR models. Most of these utilities depend on a config file `*.ini` containing metadata needed to construct the CDR model(s). At training time, a copy of the config file is placed in the output directory for the experiment, which can be useful for record keeping. The approach of using config files rather than command line arguments to define experiments has several advantages:

- Users only need to define the experiment once, and settings can be reused for arbitrarily many models
- The config file contains a permanent record of the settings used in the experiment, facilitating later reproduction
- The config file can be shared across many utilities (training, evaluation, statistical testing, plotting, etc.)

This guide describes how to write the config file and use it to train and evaluate CDR models.

2.1 Configuring CDR Experiments

A set of CDR experiments is definied in a config file `*.ini`, which can then be passed to CDR executables (). For example, once a config file `foo.ini` has been created, the models defined in it can be trained using the included `train` executable, like this:

```
python -m cdr.bin.train foo.ini
```

The config file must at minimum contain the sections `[data]` (with pointers to training/evaluation data) and `[global_settings]` (with the location of the output directory). A section `[cdr_settings]` can be (optionally) provided to override default settings. In addition, the config file should contain at least one model section, consisting of the prefix `model_` followed by a custom name for the model. For example, to define a model called `readingtimes`, use the section heading `[model_readingtimes]`. The identifier `readingtimes` will then be used by a number of utilities to designate this model. The data and settings configurations will be shared between all models defined a single config file. Each model section heading should contain at least the field `formula`. The value provided to `formula` must be a valid CDR model string. Additional fields may be provided to override inherited CDR settings on a model-specific basis. Experiments involving distinct datasets require distinct config files.

For more details on the available configuration parameters, see *CDR Configuration Files*. For more details on CDR model formulae, see *CDR Model Formulas*. To jump-start a new config file, run:

```
python -m cdr.bin.create_config > config.ini
```

Add the flag `-a` to include annotations that can help you fill in the fields correctly.

2.2 Running CDR executables

A number of executable utilities are contained in the module `cdr.bin` and can be executed using Python's `-m` flag. For example, the following call runs the `train` utility on all models specified in a config file `config.ini`:

```
python -m cdr.bin.train config.ini
```

Usage help for each utility can be viewed by running:

```
python -m cdr.bin.<UTIL-NAME> -h
```

for the utility in question. Or usage help for all utilities can be printed at once using:

```
python -m cdr.bin.help
```

The following sections go into more detail about training and evaluation utilities that will likely be useful to most users.

2.3 Training CDR Models

First, gather some data and write a config file defining your experiments. Data must be in a textual tabular format. CSV format is assumed; to specify the delimiter, use the **sep** field in your config file. Once the config file has been written, training a CDR model is simple using the `train` utility, which takes as its principle argument a path to the config file. For example, if the config file is names `experiment.ini`, all models defined in it can be trained with the call:

```
python -m dstr.bin.train experiment.ini
```

To restrict training to some subset of models, the `-m` flag is used. For example, the following call trains models `A` and `B` only:

```
python -m cdr.bin.train experiment.ini -m CDR_A CDR_B
```

CDR periodically saves training checkpoints to the model's output directory (every **save_freq** training epochs, where **save_freq** can be defined in the config file or left at its default of `1`). This allows training to be interrupted and resumed. To save space, checkpoints overwrite each other, so the output directory will contain only the most recent checkpoint. If the `train` utility discovers a checkpoint in the model's output directory, it loads it and resumes training from the saved state.

CDR learning curves can be visualized in Tensorboard. To run Tensorboard for a CDR model called `CDR_A` saved in experiment directory `EXP`, run:

```
python -m tensorboard.main --logdir=EXP/CDR_A
```

then open the returned address (usually `http://<USERNAME>:6006`) in a web browser.

2.4 Evaluating and Testing CDR Models

This package provides several utilities for inspecting and evaluating fitted CDR models. The principal evaluation utility is `predict`. The following generates predictions on test data from the model `CDR_A` defined in `experiment.ini`:

```
python -m cdr.bin.predict experiment.ini -m CDR_A -p test
```

This call will save files containing elementwise predictions, errors, and likelihoods, along with a performance summary. For more details on usage, run:

```
python -m cdr.bin.predict -h
```

Once `predict` has been run for multiple models, statistical model comparison (permutation test) can be performed using `test`, as shown:

```
python -m cdr.bin.test experiment.ini -p test
```

The above call will permutation test pairwise differences in mean squared error on test data for all unique pairs of models defined in `experiment.ini`. For more details on usage, run:

```
python -m cdr.bin.test -h
```

To compare a specific pair of models (e.g. `A` and `B`), use the `-m` flag:

```
python -m cdr.bin.test experiment.ini -p test -m A B
```

This kind of statistical model comparison is the foundation of hypothesis testing with CDR(NN)s. If model `A` above represents the null hypothesis (e.g. excludes predictor `P`) and model `B` represents the alternative (e.g. includes predictor `P`), then the test will give a *p* value for the effect of `P` (namely, does including `P` in the model improve fit to the test set?).

In addition to these core utilities, `convolve` convolves the input predictors using the fitted CDR data transform and saves the data table, and `plot` generates IRF plots with basic customization as permitted by the command line arguments.

CHAPTER

THREE

CDR CONFIGURATION FILES

The CDR utilities in this module read config files that follow the INI standard. Basic information about INI file syntax can be found e.g. here. This reference assumes familiarity with the INI protocol.

CDR configuration files contain the sections and fields described below.

3.1 Section: `[data]`

The `[data]` section supports the following fields:

REQUIRED

- **X_train**: `str`; Path to training data (predictor matrix)
- **y_train**: `str`; Path to training data (response matrix)
- **series_ids**: space-delimited list of `str`; Names of columns used to define unique time series

Note that, unlike e.g. linear models, CDR does not require synchronous predictors and responses, which is why separate data objects must be provided for each of these components. If the predictors and responses are synchronous, this is fine. The `X_train` and `y_train` fields can point to the same file. The system will treat each unique combination of values in the columns given in `series_ids` as constituting a unique time series.

OPTIONAL

- **X_dev**: `str`; Path to dev data (predictor matrix)
- **y_dev**: `str`; Path to dev data (response matrix)
- **X_test**: `str`; Path to test data (predictor matrix)
- **y_test**: `str`; Path to test data (response matrix)
- **history_length**: `int`; Length of history window in timesteps (default: `128`)
- **filters**: `str`; List of filters to apply to response data (`;`-delimited).

All variables used in a filter must be contained in the data files indicated by the `y_*` parameters in the `[data]` section of the config file. The variable name is specified as an INI field, and the condition is specified as its value. Supported logical operators are <, <=, >, >=, ==, and `!=`. For example, to keep only data points for which column `foo` is less or equal to 100, the following filter can be added:

```
filters = foo <= 100
```

To keep only data points for which the column `foo` does not equal `bar`, the following filter can be added:

```
filters = foo != bar
```

Filters can be conjunctively combined:

```
filters = foo > 5; foo <= 100
```

Count-based filters are also supported, using the designated `nunique` suffix. For example, if the column `subject` is being used to define a random effects level and we want to exclude all subjects with fewer than 100 data points, this can be accomplished using the following filter:

```
filters = subjectsnunique > 100
```

More complex filtration conditions are not supported automatically in CDR but can be applied to the data by the user as a preprocess.

Several CDR utilities (e.g. for prediction and evaluation) are designed to handle train, dev, and test partitions of the input data, but these partitions must be constructed in advance. This package also provides a `partition` utility that can be used to partition input data by applying modular arithmetic to some subset of the variables in the data. For usage details run:

`python -m cdr.bin.partition -h`

IMPORTANT NOTES

- The files indicated in `X_*` must contain the following columns:
  - **time**: Timestamp associated with each observation
  - A column for each variable in `series_ids`
  - A column for each predictor variable indicated in the model formula
- The file in `y_*` must contain the following columns:
  - **time**: Timestamp associated with each observation
  - A column for the response variable in the model formula
  - A column for each variable in `series_ids`
  - A column for each random grouping factor in the in the model formula
  - A column for each variable used for data filtration (see below)
- Data in `y_*` may be filtered/partitioned, but data in `X_*` **must be uncensored** unless independent reason exists to assume that certain observations never have an impact on the response.

3.2 Section: `[global_settings]`

The `[global_settings]` section supports the following fields:

- **outdir**: `str`; Path to output directory where checkpoints, plots, and Tensorboard logs should be saved (default: `./cdr_model/`). If it does not exist, this directory will be created. At runtime, the `train` utility will copy the config file to this directory as `config.ini`, serving as a record of the settings used to generate the analysis.
- **use_gpu_if_available**: `bool`; If available, run on GPU. If `False`, always runs on CPU even when system has compatible GPU.

3.3 Section: [cdr_settings]

The [cdr_settings] section supports the following fields:

3.3.1 All Models

- **outdir**: str; Path to output directory, where logs and model parameters are saved. **Default**: ./cdr_model/
- **use_distributional_regression**: bool; Whether to model all parameters of the response distribution as dependent on IRFs of the impulses (distributional regression). If False, only the mean depends on the predictors (other parameters of the response distribution are treated as constant). **Default (CDR)**: False; **Default (CDRNN)**: True
- **response_distribution_map**: str or None; Definition of response distribution. Can be a single distribution name (shared across all response variables), a space-delimited list of distribution names (one per response variable), a space-delimited list of ';'-delimited tuples matching response variables to distribution names (e.g. response;Bernoulli), or None, in which case the response distribution will be inferred as JohnsonSU for continuous variables and Categorical for categorical variables. **Default**: None
- **center_inputs**: bool; DISCOURAGED UNLESS YOU HAVE A GOOD REASON, since this can distort rate estimates. Center inputs by subtracting training set means. Can improve convergence speed and reduce vulnerability to local optima. Only affects fitting – prediction, likelihood computation, and plotting are reported on the source values. **Default**: False
- **rescale_inputs**: bool; Rescale input features by dividing by training set standard deviation. Can improve convergence speed and reduce vulnerability to local optima. Only affects fitting – prediction, likelihood computation, and plotting are reported on the source values. **Default**: True
- **history_length**: int; Length of the history (backward) window (in timesteps). **Default**: 128
- **future_length**: int; Length of the future (forward) window (in timesteps). Note that causal IRF kernels cannot be used if **future_length** > 0. **Default**: 0
- **t_delta_cutoff**: float or None; Maximum distance in time to consider (can help improve training stability on data with large gaps in time). If 0 or None, no cutoff. **Default**: None
- **constraint**: str; Constraint function to use for bounded variables. One of ['abs', 'square', 'softplus']. **Default**: softplus
- **random_variables**: str; Space-delimited list of model components to instantiate as (variationally optimized) random variables, rather than point estimates. Can be any combination of: *['intercept', 'coefficient', 'interaction', 'irf_param', 'nn']*. Can also be *'all'*, *'none'*, or *'default'*, which defaults to all components except *'nn'*. **Default**: default
- **scale_loss_with_data**: bool; Whether to multiply the scale of the LL loss by N, where N is num batches. This turns the loss into an expectation over training set likelihood. **Default**: True
- **scale_regularizer_with_data**: bool; Whether to multiply the scale of all weight regularization by B * N, where B is batch size and N is num batches. If **scale_loss_with_data** is true, this approach ensures a stable regularization strength (relative to the loss) across datasets and batch sizes. **Default**: False
- **n_iter**: int; Number of training iterations. If using variational inference, this becomes the *expected* number of training iterations and is used only for Tensorboard logging, with no impact on training behavior. **Default**: 100000
- **minibatch_size**: int or None; Size of minibatches to use for fitting (full-batch if None). **Default**: 1024
- **eval_minibatch_size**: int; Size of minibatches to use for prediction/evaluation. **Default**: 1024
- **n_samples_eval**: int; Number of posterior predictive samples to draw for prediction/evaluation. Ignored for evaluating CDR MLE models. **Default**: 1000

- **optim_name**: `str` or `None`; Name of the optimizer to use. Must be one of:
  - `'SGD'`
  - `'Momentum'`
  - `'AdaGrad'`
  - `'AdaDelta'`
  - `'Adam'`
  - `'FTRL'`
  - `'RMSProp'`
  - `'Nadam'` **Default**: Adam
- **max_gradient**: `float` or `None`; Maximum allowable value for the gradient, which will be clipped as needed. If `None`, no max gradient. **Default**: None
- **max_global_gradient_norm**: `float` or `None`; Maximum allowable value for the global norm of the gradient, which will be clipped as needed. If `None`, no max global norm for the gradient. **Default**: 1.0
- **use_safe_optimizer**: `bool`; Stabilize training by preventing the optimizer from applying updates involving NaN gradients (affected weights will remain unchanged after the update). Incurs slight additional computational overhead and can lead to bias in the training process. **Default**: False
- **epsilon**: `float`; Epsilon parameter to use for numerical stability in bounded parameter estimation (imposes a positive lower bound on the parameter). **Default**: 1e-05
- **response_dist_epsilon**: `float`; Epsilon parameter to use for numerical stability in bounded parameters of the response distribution (imposes a positive lower bound on the parameter). **Default**: 1e-05
- **optim_epsilon**: `float`; Epsilon parameter to use if **optim_name** in `['Adam', 'Nadam']`, ignored otherwise. **Default**: 1e-08
- **learning_rate**: `float`; Initial value for the learning rate. **Default (CDR)**: 0.001; **Default (CDRNN)**: 0.01
- **learning_rate_min**: `float`; Minimum value for the learning rate. **Default**: 0.0
- **lr_decay_family**: `str` or `None`; Functional family for the learning rate decay schedule (no decay if `None`). **Default**: None
- **lr_decay_rate**: `float`; coefficient by which to decay the learning rate every `lr_decay_steps` (ignored if `lr_decay_family==None`). **Default**: 1.0
- **lr_decay_steps**: `int`; Span of iterations over which to decay the learning rate by `lr_decay_rate` (ignored if `lr_decay_family==None`). **Default**: 100
- **lr_decay_iteration_power**: `float`; Power to which the iteration number `t` should be raised when computing the learning rate decay. **Default**: 0.5
- **lr_decay_staircase**: `bool`; Keep learning rate flat between `lr_decay_steps` (ignored if `lr_decay_family==None`). **Default**: False
- **filter_outlier_losses**: `float`, `bool` or `None`; Whether outlier large losses are filtered out while training continues. If `False`, outlier losses trigger a restart from the most recent save point. Ignored unless *loss_cutoff_n_sds* is specified. Using this option avoids restarts, but can lead to bias if training instances are systematically dropped. If `None`, `False`, or `0`, no loss filtering. **Default**: False
- **loss_cutoff_n_sds**: `float` or `None`; How many moving standard deviations above the moving mean of the loss to use as a cut-off for stability (if outlier large losses are detected, training restarts from the preceding checkpoint). If `None`, or `0`, no loss cut-off. **Default**: 1000

- **ema_decay**: `float`; Decay factor to use for exponential moving average for parameters (used in prediction). **Default**: 0.999
- **convergence_n_iterates**: `int` or `None`; Number of timesteps over which to average parameter movements for convergence diagnostics. If `None` or `0`, convergence will not be programmatically checked (reduces memory overhead, but convergence must then be visually diagnosed). **Default (CDR)**: 500; **Default (CDRNN)**: 100
- **convergence_stride**: `int`; Stride (in iterations) over which to compute convergence. If larger than 1, iterations within a stride are averaged with the most recently saved value. Larger values increase the receptive field of the slope estimates, making convergence diagnosis less vulnerable to local perturbations but also increasing the number of post-convergence iterations necessary in order to identify convergence. If `early_stopping` is `True`, `convergence_stride` will implicitly be multiplied by `eval_freq`. **Default**: 1
- **convergence_alpha**: `float` or `None`; Significance threshold above which to fail to reject the null of no correlation between convergence basis and training time. Larger values are more stringent. **Default**: 0.5
- **early_stopping**: `bool`; Whether to diagnose convergence based on dev set performance (`True`) or training set performance (`False`). **Default**: True
- **regularizer_name**: `str` or `None`; Name of global regularizer; can be overridden by more regularizers for more specific parameters (e.g. `l1_regularizer`, `l2_regularizer`). If `None`, no regularization. **Default**: None
- **regularizer_scale**: `str` or `float`; Scale of global regularizer; can be overridden by more regularizers for more specific parameters (ignored if `regularizer_name==None`). **Default**: 0.0
- **intercept_regularizer_name**: `str`, `"inherit"` or `None`; Name of intercept regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: inherit
- **intercept_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of intercept regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: inherit
- **coefficient_regularizer_name**: `str`, `"inherit"` or `None`; Name of coefficient regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: inherit
- **coefficient_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of coefficient regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: inherit
- **irf_regularizer_name**: `str`, `"inherit"` or `None`; Name of IRF parameter regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: inherit
- **irf_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of IRF parameter regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: inherit
- **ranef_regularizer_name**: `str`, `"inherit"` or `None`; Name of random effects regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. Regularization only applies to random effects without variational priors. **Default (CDR)**: inherit; **Default (CDRNN)**: l2_regularizer
- **ranef_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of random effects regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. Regularization only applies to random effects without variational priors. **Default (CDR)**: inherit; **Default (CDRNN)**: 100.0
- **regularize_mean**: `bool`; Mean-aggregate regularized variables. If `False`, use sum aggregation. **Default**: False
- **save_freq**: `int`; Frequency (in iterations) with which to save model checkpoints. **Default**: 1
- **plot_freq**: `int`; Frequency (in iterations) with which to plot model estimates (or `0` to turn off incremental plotting). **Default**: 10

- **eval_freq**: `int`; Frequency (in iterations) with which to evaluate on dev data (or `0` to turn off incremental evaluation). **Default**: 10
- **log_freq**: `int`; Frequency (in iterations) with which to log model params to Tensorboard. **Default**: 1
- **log_fixed**: `bool`; Log random fixed to Tensorboard. Can slow training of models with many fixed effects. **Default**: True
- **log_random**: `bool`; Log random effects to Tensorboard. Can slow training of models with many random effects. **Default**: True
- **log_graph**: `bool`; Log the network graph to Tensorboard **Default**: False
- **indicator_names**: `str`; Space-delimited list of predictors that are indicators (0 or 1). Used for plotting and effect estimation (value 0 is always used as reference, rather than mean). **Default**:
- **default_reference_type**: `"mean"` or `0.0`; Reference stimulus to use by default for plotting and effect estimation. If *0*, zero vector. If *mean*, training set mean by predictor. **Default (CDR)**: 0.0; **Default (CDRNN)**: mean
- **reference_values**: `str`; Predictor values to use as a reference in plotting and effect estimation. Structured as space-delimited pairs `NAME=FLOAT`. Any predictor without a specified reference value will use either 0 or the training set mean, depending on **plot_mean_as_reference**. **Default**:
- **plot_step**: `str`; Size of step by predictor to take above reference in univariate IRF plots. Structured as space-delimited pairs `NAME=FLOAT`. Any predictor without a specified step size will inherit from **plot_step_default**. **Default**:
- **plot_step_default**: `str` or `float`; Default size of step to take above reference in univariate IRF plots, if not specified in **plot_step**. Either a float or the string `'sd'`, which indicates training sample standard deviation. **Default**: sd
- **reference_time**: `float`; Timepoint at which to plot interactions. **Default**: 0.0
- **plot_n_time_units**: `float`; Number of time units to use for plotting. **Default**: 1
- **plot_n_time_points**: `int`; Resolution of plot axis (for 3D plots, uses sqrt of this number for each axis). **Default**: 1024
- **plot_dirac**: `bool`; Whether to include any Dirac delta IRF's (stick functions at t=0) in plot. **Default**: False
- **plot_x_inches**: `float`; Width of plot in inches. **Default**: 6.0
- **plot_y_inches**: `float`; Height of plot in inches. **Default**: 4.0
- **plot_legend**: `bool`; Whether to include a legend in plots with multiple components. **Default**: True
- **generate_univariate_irf_plots**: `bool`; Whether to plot univariate IRFs over time. **Default**: True
- **generate_univariate_irf_heatmaps**: `bool`; Whether to plot univariate IRF heatmaps over time. **Default**: False
- **generate_curvature_plots**: `bool`; Whether to plot IRF curvature at time **reference_time**. **Default**: True
- **generate_irf_surface_plots**: `bool`; Whether to plot IRF surfaces. **Default**: False
- **generate_interaction_surface_plots**: `bool`; Whether to plot IRF interaction surfaces at time **reference_time**. **Default**: False
- **generate_err_dist_plots**: `bool`; Whether to plot the average error distribution for real-valued responses. **Default**: True
- **generate_nonstationarity_surface_plots**: `bool`; Whether to plot IRF surfaces showing non-stationarity in the response. **Default**: False
- **cmap**: `str`; Name of MatPlotLib cmap specification to use for plotting (determines the color of lines in the plot). **Default**: gist_rainbow

- **dpi**: `int`; Dots per inch of saved plot image file. **Default**: 300
- **keep_plot_history**: `bool`; Keep IRF plots from each checkpoint of a run, which can help visualize learning trajectories but can also consume a lot of disk space. If `False`, only the most recent plot of each type is kept. **Default**: False
- **declare_priors_fixef**: `bool`; Specify Gaussian priors for all fixed model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_ranef**: `bool`; Specify Gaussian priors for all random model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **intercept_prior_sd**: `str`, `float` or `None`; Standard deviation of prior on fixed intercept. Can be a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable), a `float` (applied to all responses), or `None`, in which case the prior is inferred from **prior_sd_scaling_coefficient** and the empirical variance of the response on the training set. **Default**: None
- **coef_prior_sd**: `str`, `float` or `None`; Standard deviation of prior on fixed coefficients. Can be a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable), a `float` (applied to all responses), or `None`, in which case the prior is inferred from **prior_sd_scaling_coefficient** and the empirical variance of the response on the training set. **Default**: None
- **irf_param_prior_sd**: `str` or `float`; Standard deviation of prior on convolutional IRF parameters. Can be either a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable) or a `float` (applied to all responses) **Default**: 1.0
- **y_sd_prior_sd**: `float` or `None`; Standard deviation of prior on standard deviation of output model. If `None`, inferred as **y_sd_prior_sd_scaling_coefficient** times the empirical variance of the response on the training set. **Default**: None
- **prior_sd_scaling_coefficient**: `float`; Factor by which to multiply priors on intercepts and coefficients if inferred from the empirical variance of the data (i.e. if **intercept_prior_sd** or **coef_prior_sd** is `None`). Ignored for any prior widths that are explicitly specified. **Default**: 1
- **y_sd_prior_sd_scaling_coefficient**: `float`; Factor by which to multiply prior on output model variance if inferred from the empirical variance of the data (i.e. if **y_sd_prior_sd** is `None`). Ignored if prior width is explicitly specified. **Default**: 1
- **ranef_to_fixef_prior_sd_ratio**: `float`; Ratio of widths of random to fixed effects priors. I.e. if less than 1, random effects have tighter priors. **Default**: 0.1
- **posterior_to_prior_sd_ratio**: `float`; Ratio of posterior initialization SD to prior SD. Low values are often beneficial to stability, convergence speed, and quality of final fit by avoiding erratic sampling and divergent behavior early in training. **Default**: 0.01
- **center_X_time**: `bool`; Whether to center time values as inputs under the hood. Times are automatically shifted back to the source location for plotting and model criticism. **Default**: False
- **center_t_delta**: `bool`; Whether to center time offset values under the hood. Offsets are automatically shifted back to the source location for plotting and model criticism. **Default**: False
- **rescale_X_time**: `bool`; Whether to rescale time values as inputs by their training SD under the hood. Times are automatically reconverted back to the source scale for plotting and model criticism. **Default**: True
- **rescale_t_delta**: `bool`; Whether to rescale time offset values by their training SD under the hood. Offsets are automatically reconverted back to the source scale for plotting and model criticism. **Default**: False
- **nn_use_input_scaler**: `bool`; Whether to apply a Hadamard scaling layer to the inputs to any NN components. **Default**: False

- **log_transform_t_delta**: `bool`; Whether to log-modulus transform time offset values for stability under the hood (log-modulus is used to handle negative values in non-causal models). Offsets are automatically reconverted back to the source scale for plotting and model criticism. **Default**: False
- **nonstationary**: `bool`; Whether to model non-stationarity in NN components by feeding impulse timestamps as input. **Default**: True
- **n_layers_ff**: `int` or `None`; Number of hidden layers in feedforward encoder. If `None`, inferred from length of **n_units_ff**. **Default**: 2
- **n_units_ff**: `int`, `str` or `None`; Number of units per feedforward encoder hidden layer. Can be an `int`, which will be used for all layers, or a `str` with **n_layers_rnn** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no feedforward encoder. **Default**: 128
- **n_layers_rnn**: `int` or `None`; Number of RNN layers. If `None`, inferred from length of **n_units_rnn**. **Default**: None
- **n_units_rnn**: `int`, `str` or `None`; Number of units per RNN layer. Can be an `int`, which will be used for all layers, or a `str` with **n_layers_rnn** space-delimited integers, one for each layer in order from bottom to top. Can also be `'infer'`, which infers the size from the number of predictors, or `'inherit'`, which uses size **n_units_hidden_state**. If `0` or `None`, no RNN encoding (i.e. use a context-independent convolution kernel). **Default**: None
- **n_layers_rnn_projection**: `int` or `None`; Number of hidden layers in projection of RNN state (or of timestamp + predictors if no RNN). If `None`, inferred automatically. **Default**: None
- **n_units_rnn_projection**: `int`, `str` or `None`; Number of units per hidden layer in projection of RNN state. Can be an `int`, which will be used for all layers, or a `str` with **n_units_rnn_projection** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no hidden layers in RNN projection. **Default**: None
- **n_layers_irf**: `int` or `None`; Number of IRF hidden layers. If `None`, inferred from length of **n_units_irf**. **Default**: 2
- **n_units_irf**: `int`, `str` or `None`; Number of units per hidden layer in IRF. Can be an `int`, which will be used for all layers, or a `str` with **n_units_irf** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no hidden layers. **Default**: 128
- **input_dependent_irf**: `bool`; Whether or not NN IRFs are input-dependent (can modify their shape at different values of the predictors). **Default**: True
- **ranef_l1_only**: `bool`; Whether to include random effects only on first layer of feedforward transforms (`True`) or on all neural components. **Default**: False
- **ranef_bias_only**: `bool`; Whether to include random effects only on bias terms of neural components (`True`) or also on weight matrices. **Default**: True
- **normalizer_use_ranef**: `bool`; Whether to include random effects in normalizer layers (`True`) or not. **Default**: False
- **ff_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in feedforward encoder. **Default**: gelu
- **ff_activation**: `str` or `None`; Name of activation function to use for output of feedforward encoder. **Default**: None
- **rnn_activation**: `str` or `None`; Name of activation to use in RNN layers. **Default**: tanh
- **recurrent_activation**: `str` or `None`; Name of recurrent activation to use in RNN layers. **Default**: sigmoid
- **rnn_projection_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in projection of RNN state. **Default**: gelu

- **rnn_projection_activation**: `str` or `None`; Name of activation function to use for final layer in projection of RNN state. **Default**: None
- **irf_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in IRF. **Default**: gelu
- **irf_activation**: `str` or `None`; Name of activation function to use for final layer in IRF. **Default**: None
- **kernel_initializer**: `str` or `None`; Name of initializer to use in encoder kernels. **Default**: glorot_uniform_initializer
- **recurrent_initializer**: `str` or `None`; Name of initializer to use in encoder recurrent kernels. **Default**: orthogonal_initializer
- **weight_sd_init**: `str`, `float` or `None`; Standard deviation of kernel initialization distribution (Normal, mean=0). Can also be `'glorot'`, which uses the SD of the Glorot normal initializer. If `None`, inferred from other hyperparams. **Default**: glorot
- **batch_normalization_decay**: `bool`, `float` or `None`; Decay rate to use for batch normalization in internal layers. If `True`, uses decay `0.999`. If `False` or `None`, no batch normalization. **Default**: None
- **layer_normalization_type**: `bool`, `str` or `None`; Type of layer normalization, one of `['z', 'length', None]`. If `'z'`, classical z-transform-based normalization. If `'length'`, normalize by the norm of the activation vector. If `True`, uses `'z'`. If `False` or `None`, no layer normalization. **Default**: z
- **normalize_ff**: `bool`; Whether to apply normalization (if applicable) to hidden layers of feedforward encoders. **Default**: True
- **normalize_irf**: `bool`; Whether to apply normalization (if applicable) to non-initial internal IRF layers. **Default**: True
- **normalize_after_activation**: `bool`; Whether to apply normalization (if applicable) after the non-linearity (otherwise, applied before). **Default**: False
- **shift_normalized_activations**: `bool`; Whether to use trainable shift in batch/layer normalization layers. **Default**: True
- **rescale_normalized_activations**: `bool`; Whether to use trainable scale in batch/layer normalization layers. **Default**: True
- **normalize_inputs**: `bool`; Whether to apply normalization (if applicable) to the inputs. **Default**: False
- **normalize_final_layer**: `bool`; Whether to apply normalization (if applicable) to the final layer. **Default**: False
- **nn_regularizer_name**: `str`, `"inherit"` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: None
- **nn_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of weight regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 1.0
- **activity_regularizer_name**: `str`, `"inherit"` or `None`; Name of activity regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no activity regularization. **Default**: None
- **activity_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of activity regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 5.0
- **ff_regularizer_name**: `str` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`) on output layer of feedforward encoders; overrides **regularizer_name**. If `None`, inherits from **nn_regularizer_name**. **Default**: None
- **ff_regularizer_scale**: `str` or `float`; Scale of weight regularizer (ignored if `regularizer_name==None`) on output layer of feedforward encoders. If `None`, inherits from **nn_regularizer_scale**. **Default**: 5.0

- **regularize_initial_layer**: `bool`; Whether to regulare the first layer of NN components. **Default**: True
- **regularize_final_layer**: `bool`; Whether to regulare the last layer of NN components. **Default**: False
- **rnn_projection_regularizer_name**: `str` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`) on output layer of RNN projection; overrides **regularizer_name**. If `None`, inherits from **nn_regularizer_name**. **Default**: None
- **rnn_projection_regularizer_scale**: `str` or `float`; Scale of weight regularizer (ignored if `regularizer_name==None`) on output layer of RNN projection. If `None`, inherits from **nn_regularizer_scale**. **Default**: 5.0
- **context_regularizer_name**: `str`, `"inherit"` or `None`; Name of regularizer on contribution of context (RNN) to hidden state (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: l1_l2_regularizer
- **context_regularizer_scale**: `float` or `"inherit"`; Scale of weight regularizer (ignored if `context_regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 10.0
- **maxnorm**: `float` or `None`; Bound on norm of dense kernel dimensions for max-norm regularization. If `None`, no max-norm regularization. **Default**: None
- **input_dropout_rate**: `float` or `None`; Rate at which to drop input_features. **Default**: None
- **ff_dropout_rate**: `float` or `None`; Rate at which to drop neurons of FF projection. **Default**: 0.5
- **rnn_h_dropout_rate**: `float` or `None`; Rate at which to drop neurons of RNN hidden state. **Default**: None
- **rnn_c_dropout_rate**: `float` or `None`; Rate at which to drop neurons of RNN cell state. **Default**: None
- **h_rnn_dropout_rate**: `float` or `None`; Rate at which to drop neurons of h_rnn. **Default**: 0.5
- **rnn_dropout_rate**: `float` or `None`; Rate at which to entirely drop the RNN. **Default**: 0.5
- **irf_dropout_rate**: `float` or `None`; Rate at which to drop neurons of IRF layers. **Default**: 0.5
- **ranef_dropout_rate**: `float` or `None`; Rate at which to drop random effects indicators. **Default**: None
- **dropout_final_layer**: `bool`; Whether to apply dropout to the last layer of NN components. **Default**: False
- **fixed_dropout**: `bool`; Whether to fix the dropout mask over the time dimension during training, ensuring that each training instance is processed by the same resampled model. **Default**: True
- **declare_priors_weights**: `bool`; Specify Gaussian priors for all fixed model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_biases**: `bool`; Specify Gaussian priors for model biases (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_gamma**: `bool`; Specify Gaussian priors for gamma parameters of any batch normalization layers (if `False`, use implicit improper uniform priors). **Default**: True
- **weight_prior_sd**: `str` or `float`; Standard deviation of prior on CDRNN hidden weights. A `float`, `'glorot'`, or `'he'`. **Default**: glorot
- **bias_prior_sd**: `str` or `float`; Standard deviation of prior on CDRNN hidden biases. A `float`, `'glorot'`, or `'he'`. **Default**: 1.0
- **gamma_prior_sd**: `str` or `float`; Standard deviation of prior on batch norm gammas. A `float`, `'glorot'`, or `'he'`. Ignored unless batch normalization is used **Default**: 1
- **bias_sd_init**: `str`, `float` or `None`; Initial standard deviation of variational posterior over biases. If `None`, inferred from other hyperparams. **Default**: None
- **gamma_sd_init**: `str`, `float` or `None`; Initial standard deviation of variational posterior over batch norm gammas. If `None`, inferred from other hyperparams. Ignored unless batch normalization is used. **Default**: None

3.3.2 Variational Bayes

- **declare_priors_fixef**: `bool`; Specify Gaussian priors for all fixed model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_ranef**: `bool`; Specify Gaussian priors for all random model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **intercept_prior_sd**: `str`, `float` or `None`; Standard deviation of prior on fixed intercept. Can be a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable), a `float` (applied to all responses), or `None`, in which case the prior is inferred from **prior_sd_scaling_coefficient** and the empirical variance of the response on the training set. **Default**: None
- **coef_prior_sd**: `str`, `float` or `None`; Standard deviation of prior on fixed coefficients. Can be a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable), a `float` (applied to all responses), or `None`, in which case the prior is inferred from **prior_sd_scaling_coefficient** and the empirical variance of the response on the training set. **Default**: None
- **irf_param_prior_sd**: `str` or `float`; Standard deviation of prior on convolutional IRF parameters. Can be either a space-delimited list of `;`-delimited floats (one per distributional parameter per response variable) or a `float` (applied to all responses) **Default**: 1.0
- **y_sd_prior_sd**: `float` or `None`; Standard deviation of prior on standard deviation of output model. If `None`, inferred as **y_sd_prior_sd_scaling_coefficient** times the empirical variance of the response on the training set. **Default**: None
- **prior_sd_scaling_coefficient**: `float`; Factor by which to multiply priors on intercepts and coefficients if inferred from the empirical variance of the data (i.e. if **intercept_prior_sd** or **coef_prior_sd** is `None`). Ignored for any prior widths that are explicitly specified. **Default**: 1
- **y_sd_prior_sd_scaling_coefficient**: `float`; Factor by which to multiply prior on output model variance if inferred from the empirical variance of the data (i.e. if **y_sd_prior_sd** is `None`). Ignored if prior width is explicitly specified. **Default**: 1
- **ranef_to_fixef_prior_sd_ratio**: `float`; Ratio of widths of random to fixed effects priors. I.e. if less than 1, random effects have tighter priors. **Default**: 0.1
- **posterior_to_prior_sd_ratio**: `float`; Ratio of posterior initialization SD to prior SD. Low values are often beneficial to stability, convergence speed, and quality of final fit by avoiding erratic sampling and divergent behavior early in training. **Default**: 0.01

3.3.3 Neural Network Components

- **center_X_time**: `bool`; Whether to center time values as inputs under the hood. Times are automatically shifted back to the source location for plotting and model criticism. **Default**: False
- **center_t_delta**: `bool`; Whether to center time offset values under the hood. Offsets are automatically shifted back to the source location for plotting and model criticism. **Default**: False
- **rescale_X_time**: `bool`; Whether to rescale time values as inputs by their training SD under the hood. Times are automatically reconverted back to the source scale for plotting and model criticism. **Default**: True
- **rescale_t_delta**: `bool`; Whether to rescale time offset values by their training SD under the hood. Offsets are automatically reconverted back to the source scale for plotting and model criticism. **Default**: False
- **nn_use_input_scaler**: `bool`; Whether to apply a Hadamard scaling layer to the inputs to any NN components. **Default**: False

- **log_transform_t_delta**: `bool`; Whether to log-modulus transform time offset values for stability under the hood (log-modulus is used to handle negative values in non-causal models). Offsets are automatically reconverted back to the source scale for plotting and model criticism. **Default**: False
- **nonstationary**: `bool`; Whether to model non-stationarity in NN components by feeding impulse timestamps as input. **Default**: True
- **n_layers_ff**: `int` or `None`; Number of hidden layers in feedforward encoder. If `None`, inferred from length of **n_units_ff**. **Default**: 2
- **n_units_ff**: `int`, `str` or `None`; Number of units per feedforward encoder hidden layer. Can be an `int`, which will be used for all layers, or a `str` with **n_layers_rnn** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no feedforward encoder. **Default**: 128
- **n_layers_rnn**: `int` or `None`; Number of RNN layers. If `None`, inferred from length of **n_units_rnn**. **Default**: None
- **n_units_rnn**: `int`, `str` or `None`; Number of units per RNN layer. Can be an `int`, which will be used for all layers, or a `str` with **n_layers_rnn** space-delimited integers, one for each layer in order from bottom to top. Can also be `'infer'`, which infers the size from the number of predictors, or `'inherit'`, which uses size **n_units_hidden_state**. If `0` or `None`, no RNN encoding (i.e. use a context-independent convolution kernel). **Default**: None
- **n_layers_rnn_projection**: `int` or `None`; Number of hidden layers in projection of RNN state (or of timestamp + predictors if no RNN). If `None`, inferred automatically. **Default**: None
- **n_units_rnn_projection**: `int`, `str` or `None`; Number of units per hidden layer in projection of RNN state. Can be an `int`, which will be used for all layers, or a `str` with **n_units_rnn_projection** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no hidden layers in RNN projection. **Default**: None
- **n_layers_irf**: `int` or `None`; Number of IRF hidden layers. If `None`, inferred from length of **n_units_irf**. **Default**: 2
- **n_units_irf**: `int`, `str` or `None`; Number of units per hidden layer in IRF. Can be an `int`, which will be used for all layers, or a `str` with **n_units_irf** space-delimited integers, one for each layer in order from bottom to top. If `0` or `None`, no hidden layers. **Default**: 128
- **input_dependent_irf**: `bool`; Whether or not NN IRFs are input-dependent (can modify their shape at different values of the predictors). **Default**: True
- **ranef_l1_only**: `bool`; Whether to include random effects only on first layer of feedforward transforms (`True`) or on all neural components. **Default**: False
- **ranef_bias_only**: `bool`; Whether to include random effects only on bias terms of neural components (`True`) or also on weight matrices. **Default**: True
- **normalizer_use_ranef**: `bool`; Whether to include random effects in normalizer layers (`True`) or not. **Default**: False
- **ff_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in feedforward encoder. **Default**: gelu
- **ff_activation**: `str` or `None`; Name of activation function to use for output of feedforward encoder. **Default**: None
- **rnn_activation**: `str` or `None`; Name of activation to use in RNN layers. **Default**: tanh
- **recurrent_activation**: `str` or `None`; Name of recurrent activation to use in RNN layers. **Default**: sigmoid
- **rnn_projection_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in projection of RNN state. **Default**: gelu

- **rnn_projection_activation**: `str` or `None`; Name of activation function to use for final layer in projection of RNN state. **Default**: None
- **irf_inner_activation**: `str` or `None`; Name of activation function to use for hidden layers in IRF. **Default**: gelu
- **irf_activation**: `str` or `None`; Name of activation function to use for final layer in IRF. **Default**: None
- **kernel_initializer**: `str` or `None`; Name of initializer to use in encoder kernels. **Default**: glorot_uniform_initializer
- **recurrent_initializer**: `str` or `None`; Name of initializer to use in encoder recurrent kernels. **Default**: orthogonal_initializer
- **weight_sd_init**: `str`, `float` or `None`; Standard deviation of kernel initialization distribution (Normal, mean=0). Can also be `'glorot'`, which uses the SD of the Glorot normal initializer. If `None`, inferred from other hyperparams. **Default**: glorot
- **batch_normalization_decay**: `bool`, `float` or `None`; Decay rate to use for batch normalization in internal layers. If `True`, uses decay `0.999`. If `False` or `None`, no batch normalization. **Default**: None
- **layer_normalization_type**: `bool`, `str` or `None`; Type of layer normalization, one of `['z', 'length', None]`. If `'z'`, classical z-transform-based normalization. If `'length'`, normalize by the norm of the activation vector. If `True`, uses `'z'`. If `False` or `None`, no layer normalization. **Default**: z
- **normalize_ff**: `bool`; Whether to apply normalization (if applicable) to hidden layers of feedforward encoders. **Default**: True
- **normalize_irf**: `bool`; Whether to apply normalization (if applicable) to non-initial internal IRF layers. **Default**: True
- **normalize_after_activation**: `bool`; Whether to apply normalization (if applicable) after the non-linearity (otherwise, applied before). **Default**: False
- **shift_normalized_activations**: `bool`; Whether to use trainable shift in batch/layer normalization layers. **Default**: True
- **rescale_normalized_activations**: `bool`; Whether to use trainable scale in batch/layer normalization layers. **Default**: True
- **normalize_inputs**: `bool`; Whether to apply normalization (if applicable) to the inputs. **Default**: False
- **normalize_final_layer**: `bool`; Whether to apply normalization (if applicable) to the final layer. **Default**: False
- **nn_regularizer_name**: `str`, `"inherit"` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: None
- **nn_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of weight regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 1.0
- **activity_regularizer_name**: `str`, `"inherit"` or `None`; Name of activity regularizer (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no activity regularization. **Default**: None
- **activity_regularizer_scale**: `str`, `float` or `"inherit"`; Scale of activity regularizer (ignored if `regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 5.0
- **ff_regularizer_name**: `str` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`) on output layer of feedforward encoders; overrides **regularizer_name**. If `None`, inherits from **nn_regularizer_name**. **Default**: None
- **ff_regularizer_scale**: `str` or `float`; Scale of weight regularizer (ignored if `regularizer_name==None`) on output layer of feedforward encoders. If `None`, inherits from **nn_regularizer_scale**. **Default**: 5.0

- **regularize_initial_layer**: `bool`; Whether to regulare the first layer of NN components. **Default**: True
- **regularize_final_layer**: `bool`; Whether to regulare the last layer of NN components. **Default**: False
- **rnn_projection_regularizer_name**: `str` or `None`; Name of weight regularizer (e.g. `l1_regularizer`, `l2_regularizer`) on output layer of RNN projection; overrides **regularizer_name**. If `None`, inherits from **nn_regularizer_name**. **Default**: None
- **rnn_projection_regularizer_scale**: `str` or `float`; Scale of weight regularizer (ignored if `regularizer_name==None`) on output layer of RNN projection. If `None`, inherits from **nn_regularizer_scale**. **Default**: 5.0
- **context_regularizer_name**: `str`, `"inherit"` or `None`; Name of regularizer on contribution of context (RNN) to hidden state (e.g. `l1_regularizer`, `l2_regularizer`); overrides **regularizer_name**. If `'inherit'`, inherits **regularizer_name**. If `None`, no regularization. **Default**: l1_l2_regularizer
- **context_regularizer_scale**: `float` or `"inherit"`; Scale of weight regularizer (ignored if `context_regularizer_name==None`). If `'inherit'`, inherits **regularizer_scale**. **Default**: 10.0
- **maxnorm**: `float` or `None`; Bound on norm of dense kernel dimensions for max-norm regularization. If `None`, no max-norm regularization. **Default**: None
- **input_dropout_rate**: `float` or `None`; Rate at which to drop input_features. **Default**: None
- **ff_dropout_rate**: `float` or `None`; Rate at which to drop neurons of FF projection. **Default**: 0.5
- **rnn_h_dropout_rate**: `float` or `None`; Rate at which to drop neurons of RNN hidden state. **Default**: None
- **rnn_c_dropout_rate**: `float` or `None`; Rate at which to drop neurons of RNN cell state. **Default**: None
- **h_rnn_dropout_rate**: `float` or `None`; Rate at which to drop neurons of h_rnn. **Default**: 0.5
- **rnn_dropout_rate**: `float` or `None`; Rate at which to entirely drop the RNN. **Default**: 0.5
- **irf_dropout_rate**: `float` or `None`; Rate at which to drop neurons of IRF layers. **Default**: 0.5
- **ranef_dropout_rate**: `float` or `None`; Rate at which to drop random effects indicators. **Default**: None
- **dropout_final_layer**: `bool`; Whether to apply dropout to the last layer of NN components. **Default**: False
- **fixed_dropout**: `bool`; Whether to fix the dropout mask over the time dimension during training, ensuring that each training instance is processed by the same resampled model. **Default**: True

3.3.4 Variational Bayesian Neural Network Components

- **declare_priors_weights**: `bool`; Specify Gaussian priors for all fixed model parameters (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_biases**: `bool`; Specify Gaussian priors for model biases (if `False`, use implicit improper uniform priors). **Default**: True
- **declare_priors_gamma**: `bool`; Specify Gaussian priors for gamma parameters of any batch normalization layers (if `False`, use implicit improper uniform priors). **Default**: True
- **weight_prior_sd**: `str` or `float`; Standard deviation of prior on CDRNN hidden weights. A `float`, `'glorot'`, or `'he'`. **Default**: glorot
- **bias_prior_sd**: `str` or `float`; Standard deviation of prior on CDRNN hidden biases. A `float`, `'glorot'`, or `'he'`. **Default**: 1.0
- **gamma_prior_sd**: `str` or `float`; Standard deviation of prior on batch norm gammas. A `float`, `'glorot'`, or `'he'`. Ignored unless batch normalization is used **Default**: 1

- **bias_sd_init**: `str`, `float` or `None`; Initial standard deviation of variational posterior over biases. If `None`, inferred from other hyperparams. **Default**: None
- **gamma_sd_init**: `str`, `float` or `None`; Initial standard deviation of variational posterior over batch norm gammas. If `None`, inferred from other hyperparams. Ignored unless batch normalization is used. **Default**: None

3.4 Section: `[irf_name_map]`

The optional `[irf_name_map]` section simply permits prettier variable naming in plots. For example, the internal name for a convolution applied to predictor `A` may be `ShiftedGammaKgt1.s(A)-Terminal.s(A)`, which is not very readable. To address this, the string above can be mapped to a more readable name using an INI key-value pair, as shown:

```
ShiftedGammaKgt1.s(A)-Terminal.s(A) = A
```

The model will then print `A` in plots rather than `ShiftedGammaKgt1.s(A)-Terminal.s(A)`. Unused entries in the name map are ignored, and model variables that do not have an entry in the name map print with their default internal identifier.

3.5 Sections: `[model_CDR_*]`

Arbitrarily many sections named `[model_CDR_*]` can be provided in the config file, where * stands in for a unique identifier. Each such section defines a different CDR model and must contain at least one field — `formula` — whose value is a CDR model formula (see *CDR Model Formulas* for more on CDR formula syntax) The identifier `CDR_*` will be used by the CDR utilities to reference the fitted model and its output files.

For example, to define a CDR model called `readingtimes`, the section header `[model_CDR_readingtimes]` is included in the config file along with an appropriate `formula` specification. To use this specific model once fitted, it can be referenced using the identifier `CDR_readingtimes`. For example, the following call will extract predictions on dev data from a fitted `CDR_readingtimes` defined in config file **config.ini**:

```
python -m cdr.bin.predict config.ini -m CDR_readingtimes -p dev
```

Additional fields from `[cdr_settings]` may be specified for a given model, in which case the locally-specified setting (rather than the globally specified setting or the default value) will be used to train the model. For example, imagine that `[cdr_settings]` contains the field `n_iter = 1000`. All CDR models subsequently specified in the config file will train for 1000 iterations. However, imagine that model `[model_CDR_longertrain]` should train for 5000 iterations instead. This can be specified within the same config file as:

```
[model_CDR_longertrain]
n_iter = 5000
formula = ...
```

This setup allows a single config file to define a variety of CDR models, as long as they all share the same data. Distinct datasets require distinct config files.

For hypothesis testing, fixed effect ablation can be conveniently automated using the `ablate` model field. For example, the following specification implicitly defines 7 unique models, one for each of the `|powerset(a, b, c)| - 1 = 7` non-null ablations of `a`, `b`, and `c`:

```
[model_CDR_example]
n_iter = 5000
```

(continues on next page)

(continued from previous page)

```
ablate = a b c
formula = C(a + b + c, Normal()) + (C(a + b + c, Normal()) | subject)
```

The ablated models are named using `'!'` followed by the name for each ablated predictor. Therefore, the above specification is equivalent to (and much easier to write than) the following:

```
[model_CDR_example]
n_iter = 5000
formula = C(a + b + c, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!a]
n_iter = 5000
formula = C(b + c, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!b]
n_iter = 5000
formula = C(a + c, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!c]
n_iter = 5000
formula = C(a + b, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!a!b]
n_iter = 5000
formula = C(c, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!a!c]
n_iter = 5000
formula = C(b, Normal()) + (C(a + b + c, Normal()) | subject)

[model_CDR_example!b!c]
n_iter = 5000
formula = C(a, Normal()) + (C(a + b + c, Normal()) | subject)
```

CHAPTER

FOUR

CDR MODEL FORMULAS

4.1 Basic Overview

This package constructs CDR models from **R**-style formula strings defining the model structure. A CDR formula has the following template:

```
RESPONSE ~ FIXED_EFFECTS + RANDOM_EFFECTS
```

The left-hand side (LHS) of the formula contains the name a single (possibly transformed) variable from the input data table, and the right-hand side (RHS) contains fixed and random effects, each of which must consist exclusively of intercept terms and/or convolutional terms. Intercept terms can be added by including `1` in the RHS and removed by including `0` in the RHS. If neither of these appears in the RHS, an intercept is added by default.

WARNING: The compiler for CDR formulas is still in development and may fail to correctly process certain formula strings, especially ones that contain hierarchical term expansions, categorical variable expansions, and/or interactions. Please double-check the correctness of the model formula reported at the start of training and report problems in the issue tracker on Github.

WARNING: If you are using interaction terms, it is easy to accidentally mis-specify your formula because interactions are trickier in CDR than in linear models. Make sure to read *Interactions in CDR* before fitting models with interactions.

WARNING: Column names in your data must be valid Python identifiers in order to be parsed correctly in model formulas. Numeric names, names containing punctuation other than underscore, and other violations of Python's variable naming rules can result in an incorrect formula parse, which will at best crash and at worse quietly build a different model than the one you wanted.

4.2 CDR Model Formulas

4.2.1 Linear (DiracDelta) Predictors

A trivial way of "deconvolving" a predictor `A` is to assume a Dirac delta response to `A`: A at $t = 0$, 0 otherwise. DiracDelta IRF are thus equivalent to predictors in linear models; only the value of the predictor that coincides with the response measurement is used for prediction. Linear (mixed) models of time series are therefore a special subtype of CDR, namely CDR models that exclusively use Dirac delta response kernels. While you therefore *can* use this package to fit LME models, that doesn't mean you should! The stochastic optimization used here is likely much less efficient in this simple case than that of specialized LME regression tools.

However, the availability of Dirac delta responses in this package means that CDR can combine linear and convolved substructures into a single model, which is important for many use cases. For example, imagine a bi-variate model with predictors `stimulus` and `condition`, where `stimulus` varies within each time series can might engender a temporally diffise response while `condition` is held fixed within each time series. In this case, a convolution of `condition` would

be meaningless (or at least perfectly confounded with `rate`, the deconvolutional intercept); instead, we're interested in a *linear* effect of `condition` and a *convolved* effect of `stimulus` on the response. Dirac delta responses can specified manually using the syntax described in the following sections. However, for convenience, bare predictor names in model formulas (outside of convolution calls `C()`) are automatically interpreted as Dirac delta. This allows you to retain stock formula syntax that might already be familiar from linear (mixed) models in **R** in order to define linear substructures of your CDR model. For example, the following is interpreted as specifying linear effects for each of `A`, `B`, and the interaction `A:B`:

```
y ~ A + B + C:B
```

An important caveat in using Dirac delta responses is that the predictors they apply to should be *response-aligned*, that is, measured at the same moments in time that the responses themselves are. If the stimuli and responses are measured at different points in time, you cannot fit a Dirac delta response to a stimulus-aligned variable unless that variable happens at least sometimes to accidentally be measured concurrently with the response. CDR does not internally distinguish stimulus-aligned and response-aligned predictors, so it's up to users to make sure that models are sensible in this regard. However, the model does internally mask all elements in a Dirac delta predictor that are not simultaneous with the response. Therefore, fitting a Dirac delta response to a stimulus-aligned predictor will not produce an erroneous model; in the worst case, the entire predictor will be masked and therefore ignored by the model.

4.2.2 Defining an Impulse Response Function (IRF)

A convolutional term is defined using the syntax `C(..., IRF_FAMILY())`, where `...` is replaced by names of predictors contained in the input data. For example, to define a Gamma convolution of predictor `A`, the expression `C(A, Gamma())` is added to the RHS. Separate terms are delimited by +. For example, to add a Gaussian convolution of predictor `B`, the RHS above becomes `C(A, Gamma()) + C(B, Normal())`.

4.2.3 Supported Parametric IRFs

The currently supported parametric IRF families are the following. All IRFs are normalized to integrate to 1 over the positive real line. For simplicity, normalization constants are omitted from the equations below. For details, see Shain & Schuler (2021).

- `DiracDelta`: Stick function (equivalent to a predictor in linear regression, see *Linear (DiracDelta) Predictors*)
  - Parameters:
    - None
  - Definition: 1 at $x = 0$, 0 otherwise
- `Exp`: PDF of exponential distribution
  - Parameters:
    - $\beta > 0$: `beta` (rate)
  - Definition: $\beta e^{-\beta x}$
  - Note: Dropping the normalization constant from the PDF helps deconfound IRF shape and magnitude. Normalization is unnecessary since this kernel defines an IRF, not a probability distribution.
- `Gamma`: PDF of gamma distribution
  - Parameters:
    - $\alpha > 0$: `alpha` (shape)
    - $\beta > 0$: `beta` (rate)

  - Definition: $\frac{\beta^\alpha x^{\alpha-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha)}$

- `ShiftedGamma`: PDF of gamma distribution with support starting at $0 + \delta$
  - Parameters:
    - $\alpha > 0$: `alpha` (shape)
    - $\beta > 0$: `beta` (rate)
    - $\delta < 0$: `delta` (shift)
  - Definition: $\frac{\beta^\alpha (x-\delta)^{\alpha-1} e^{-\frac{x-\delta}{\beta}}}{\Gamma(\alpha)}$
- `GammaShapeGT1`: PDF of gamma distribution, $\alpha > 1$ (enforces rising-then-falling shape)
  - Parameters:
    - $\alpha > 1$: `alpha` (shape)
    - $\beta > 1$: `beta` (rate)
  - Definition: $\frac{\beta^\alpha x^{\alpha-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha)}$
- `ShiftedGammaShapeGT1`: PDF of gamma distribution with support starting at $0 + \delta$, $\alpha > 1$ (enforces rising-then-falling shape)
  - Parameters:
    - $\alpha > 1$: `alpha` (shape)
    - $\beta > 0$: `beta` (rate)
    - $\delta < 0$: `delta` (shift)
  - Definition: $\frac{\beta^\alpha (x-\delta)^{\alpha-1} e^{-\frac{x-\delta}{\beta}}}{\Gamma(\alpha)}$
- `Normal`: PDF of Gaussian (normal) distribution
  - Parameters:
    - μ: `mu` (mean)
    - $\sigma^2 > 0$: `sigma2` (variance)
  - Definition: $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
  - Note: Dropping the normalization constant from the PDF helps deconfound IRF shape and magnitude. Normalization is unnecessary since this kernel defines an IRF, not a probability distribution.
- `SkewNormal`: PDF of SkewNormal distribution (normal distribution augmented with left/right skew parameter)
  - Parameters:
    - μ (mean)
    - $\sigma > 0$ (standard deviation)
    - α (skew)
  - Definition: Let ϕ and Φ denote the PDF and CDF (respectively) of the standard normal distribution. Then the SkewNormal distribution is: $\frac{2}{\sigma}\phi\left(\frac{x-\mu}{\sigma}\right)\Phi(\alpha\frac{x-\mu}{\sigma})$
- `EMG`: PDF of exponentially modified gaussian distribution (convolution of a normal with an exponential distribution, can be right-skewed)
  - Parameters:

        * μ: `mu` (mean)
        * $\sigma > 0$: `sigma` (standard deviation)
        * $\beta > 0$: `beta` (rate)
    - Definition: $\frac{\beta}{2} e^{\frac{\beta}{2}\left(2\mu + \beta\sigma^2 - 2x\right)} \operatorname{erfc}\left(\frac{m + \beta\sigma^2 - x}{\sqrt{2}\sigma}\right)$, where $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$.
- `BetaPrime`: PDF of BetaPrime (inverted beta) distribution
    - Parameters:
        * $\alpha > 0$: `alpha` (shape)
        * $\beta > 0$: `beta` (shape)
    - Definition: $\frac{x^{\alpha-1}(1+x)^{-\alpha-\beta}}{B(\alpha,\beta)}$
- `ShiftedBetaPrime`: PDF of BetaPrime (inverted beta) distribution with support starting at $0 + \delta$
    - Parameters:
        * $\alpha > 0$: `alpha` (shape)
        * $\beta > 0$: `beta` (shape)
        * $\delta < 0$: `delta` (shift)
    - Definition: $\frac{(x-\delta)^{\alpha-1}(1+(x-\delta))^{-\alpha-\beta}}{B(\alpha,\beta)}$
- `HRFSingleGamma`: Single-gamma hemodynamic response function (fMRI). Identical to `GammaShapeGT1` except in its initial parameter values, which are inherited from the peak response model of the canonical HRF in SPM ($\alpha = 6$ and $\beta = 1$)
    - Parameters:
        * $\alpha > 0$: `alpha` (shape)
        * $\beta > 0$: `beta` (rate)
    - Definition: $\frac{\beta^\alpha x^{\alpha-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha)}$
- `HRFDoubleGamma1`: 1-parameter double-gamma hemodynamic response function (fMRI). Shape parameters are fixed at SPM's defaults for both the first and second gammas (6 and 16, respectively). Parameter β is tied between both gammas. The coefficient on the second gamma is fixed at SPM's default ($\frac{1}{6}$). This is a "stretchable" canonical HRF.
    - Parameters:
        * $\beta > 0$: `beta` (peak and undershoot rate)
    - Definition: $\frac{\beta^6 x^{6-1} e^{-\frac{x}{\beta}}}{\Gamma(6)} - \frac{1}{6}\frac{\beta^{16} x^{15} e^{-\frac{x}{\beta}}}{\Gamma(16)}$
- `HRFDoubleGamma2`: 2-parameter double-gamma hemodynamic response function (fMRI). Parameter α of the second gamma is fixed to the $alpha$ of the first gamma using SPM

s default offset (10). Parameter β is tied between both gammas. The coefficient on the second gamma is fixed at SPM's default ($\frac{1}{6}$).

- Parameters:
    - $\alpha > 1$: `alpha` (peak shape)
    - $\beta > 0$: `beta` (peak and undershoot rate)
- Definition: $\frac{\beta^\alpha x^{\alpha-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha)} - \frac{1}{6}\frac{\beta^{\alpha+10} x^{\alpha+9} e^{-\frac{x}{\beta}}}{\Gamma(\alpha+10)}$

- `HRFDoubleGamma3`: 3-parameter double-gamma hemodynamic response function (fMRI). Parameter α of the second gamma is fixed to the $alpha$ of the first gamma using SPM

s default offset (10). Parameter β is tied between both gammas.

- Parameters:
  - $\alpha > 1$: `alpha` (peak shape)
  - $\beta > 0$: `beta` (peak and undershoot rate)
  - c: `c` (undershoot coefficient)
- Definition: $\frac{\beta^{\alpha} x^{\alpha-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha)} - c\frac{\beta^{\alpha+10} x^{\alpha+9} e^{-\frac{x}{\beta}}}{\Gamma(\alpha+10)}$
- `HRFDoubleGamma4`: 4-parameter double-gamma hemodynamic response function (fMRI). Parameter β is tied between both gammas.
  - Parameters:
    - $\alpha_1 > 1$: `alpha_main` (peak shape)
    - $\alpha_2 > 1$: `alpha_undershoot` (undershoot shape)
    - $\beta > 0$: `beta` (peak and undershoot rate)
    - c: `c` (undershoot coefficient)
  - Definition: $\frac{\beta^{\alpha_1} x^{\alpha_1-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha_1)} - c\frac{\beta^{\alpha_2} x^{\alpha_2-1} e^{-\frac{x}{\beta}}}{\Gamma(\alpha_2)}$
- `HRFDoubleGamma5`: 5-parameter double-gamma hemodynamic response function (fMRI). All parameters are free.
  - Parameters:
    - $\alpha_1 > 1$: `alpha_main` (peak shape)
    - $\alpha_2 > 1$: `alpha_undershoot` (undershoot shape)
    - $\beta_1 > 0$: `beta_main` (peak rate)
    - $\beta_2 > 0$: `beta_undershoot` (undershoot rate)
    - c: `c` (undershoot coefficient)
  - Definition: $\frac{\beta^{\alpha_1} x^{\alpha_1-1} e^{-\frac{x}{\beta_1}}}{\Gamma(\alpha_1)} - c\frac{\beta^{\alpha_2} x^{\alpha_2-1} e^{-\frac{x}{\beta_2}}}{\Gamma(\alpha_2)}$

4.2.4 Interactions in CDR

In comparison to interactions in linear models, deconvolution introduces the additional complexity of needing to decide and specify whether interactions precede (impulse-level interactions) or follow (response-level interactions) the convolution step. Impulse-level interactions consider interactions as *events* which may trigger a temporally diffuse response (i.e. a response to both A and B happening together at a particular point in time). Response-level interactions capture non-additive effects of multiple (possibly convolved) variables; they do not get their own impulse responses. Response-level interactions correspond to interactions in linear models and are almost always what you want except in the special case of linear (DiracDelta IRF) predictors, where impulse-level interactions should be used (just like in linear models).

CDR formulas use a simple syntax to distinguish these two types of interactions: impulse-level interactions are specified *inside* the first argument of convolution calls *C()*, while response-level interactions are specified outside them. As in **R**, interaction terms are designated with `:`, as in `A:B`. And as in **R**, for convenience, two-way cross-product interactions can be designated with `*` (e.g. `A*B` is shorthand for `A + B + A:B`) and multi-way cross-product interactions can be

designated with power notation `^<INT>` or `**<INT>` (e.g. `(A+B+C)^3` equals `A + B + C + A:B + B:C + A:C + A:B:C`). The following defines an impulse-level interaction between `A` and `B` underneath a `Normal` IRF kernel:

```
C(A:B, Normal())
```

The following defines a response-level interaction between Normal convolutions of `A` and `B`:

```
C(A, Normal()):C(B, Normal())
```

In order to fit interactions between convolved variables, the convolutions themselves must exist. Therefore, unlike linear interactions, which can be fit even if their subcomponents are not included in the model, `C(A, Normal()):C(B, Normal())` requires the existence of model estimates for both `C(A, Normal())` and `C(B, Normal())`, and these terms are therefore automatically inserted when used by any response-level interactions.

Response-level interactions do not need to be convolved variables. They can also be predictors supplied by the data *as long as the predictors are response-aligned* (i.e. measured concurrently with the responses, rather than the impulses). For example, suppose we have a response-aligned variable `C` provided by our data. We can interact responses with it, like so:

```
C(A, Normal()):C
```

This will fit a normal response to A, along with an estimate for the modulation of that response by C. Unlike convolved inputs to response-level interactions, estimates for regular variables are not automatically added to the model. In order to fit a separate (linear) effect for C, we could use the multiplication operator instead:

```
C(A, Normal())*C = C(A, Normal() + C + C(A, Normal()):C
```

For convenience, response-level interactions distribute across the inputs to a convolution call `C()`. Thus, interacting a variable with a convolution of multiple inputs is equivalent to interacting the variable with a convolution of each of the inputs:

```
C(A + B, Gamma()):C = C(A + B, Gamma()) + C(A, Gamma()):C + C(B, Gamma()):C
```

Similarly, interacting multiple convolution calls each containing multiple inputs is equivalent to defining interactions over the Cartesian-product of the responses to the two sets of inputs:

```
C(A + B, Gamma()):C(C + D, EMG()) = C(A + B, Gamma()) + C(C + D, EMG()) + \
                                    C(A, Gamma()):C(C, EMG()) + C(B, Gamma()):C(C,␣
↪EMG()) + \
                                    C(A, Gamma()):C(D, EMG()) + C(B, Gamma()):C(D, EMG())
```

Order of operations between term expansions can be enforced through parentheses:

```
(A*B):E = A:E + B:E + A:B:E
A*(B:E) = A + B:E + A:B:E
```

4.2.5 Automatic Term Expansion

For convenience, the `C()` function distributes the impulse response family over multiple +-delimited terms in its first argument. Therefore, the following two expressions are equivalent:

```
C(A + B, Gamma())
C(A, Gamma()) + C(B, Gamma())
```

R-style expansions for interactions are also available, as discussed above. IRF distribute across the expansion of interaction terms, such that the following expressions are equivalent:

```
C((A + B + C)**3, Gamma())
C(A, Gamma()) + C(B, Gamma()) + C(C, Gamma()) + C(A:B, Gamma()) + C(B:C, Gamma()) +␣
↪C(A:C, Gamma()) + C(A:B:C, Gamma())
```

Categorical variables are automatically discovered and expanded in CDR models. This process imposes a transformation on the model. For example, imagine that predictor `B` in the following model turns out to be categorical in the data set with categories `B1`, `B2`, and `B3`:

```
C(A + B, EMG())
```

When the CDR model is initialized, the categorical nature of `B` is detected and the model is expanded out as:

```
C(A + B2 + B3, EMG())
```

However, they can be included simply by adding binary indicator vectors for each of $n-1$ of the levels of the variable to the input data as a preprocessing step, then defining the model in terms of the binary indicators.

Note that the term expansions described above add *separate* IRF for each term in the expansion. For example, `C(A + B, Gamma())` adds two distinct Gamma IRF parameterizations to the model, one for each predictor. It is also possible to tie IRF between predictor variables (details below).

Note also that (unlike **R**) redundant terms are **not** automatically collapsed, so care must be taken to ensure that no duplicate terms are produced via term expansion.

4.2.6 Random Effects

Random effects in CDR are specified using the following syntax:

```
(RANDOM_TERMS | GROUPING_FACTOR)
```

where `RANDOM_TERMS` are terms as they would appear in the RHS of the model described above and `GROUPING_FACTOR` is the name of a categorical variable in the input that is used to define the random effect (e.g. a vector of ID's of human subjects). As in the case of fixed effects, a random intercept is automatically added unless `0` appears among the random terms. Mixed models are constructed simply by adding random effects to fixed effects in the RHS of the formula. For example, to construct a mixed model with a fixed and by-subject random coefficient for a Gaussian IRF for predictor `A` along with a random intercept by subject, the following RHS would be used:

```
C(A, Normal()) + (C(A, Normal()) | subject)
```

IRF in random effects statements are treated as tied to any corresponding fixed effects unless explicitly distinguished by distinct IRF ID's (see section below on parameter tying).

The above formula uses a single parameterization for the Gaussian IRF and fits by-subject coefficients for it. However it is also possible to fit by-subject IRF parameterizations. This can be accomplished by adding `ran=T` to the IRF call, as shown below:

```
C(A, Normal()) + (C(A, Normal(ran=T)) | subject)
```

This formula will fit separate coefficients *and* IRF shapes for this predictor for each subject.

An important complication in fitting mixed models with CDR is that the relevant grouping factor is determined by the current *regression target*, not the properties of the independent variable observations in the series history. This means that random effects are only guaranteed to be meaningful when fit using grouping factors that are constant for the entire series (e.g. the ID of the human subject completing the experiment). Random effects fit for grouping factors that vary during the experiment should therefore be avoided unless they are intercept terms only, which are not affected by the temporal convolution.

4.2.7 Parameter Initialization

IRF parameters can be initialized for a given convolutional term by specifying their initial values in the IRF call, using the parameter name as the keyword (see supported IRF and their associated parameters above). For example, to initialize a Gamma IRF with $\alpha = 2$ and $\beta = 2$ for predictor `A`, use the following call:

```
C(A, Gamma(alpha=2, beta=2))
```

These values will serve as initializations in both CDRMLE and CDRBayes, and in CDRBayes they will additionally serve as the mean of the prior distribution for that parameter. If no initialization is specified, defaults will be used. These defaults are not guaranteed to be plausible for your particular application and may have a detrimental impact on training. Therefore, it is generally a good idea to think carefully in advance about what kinds of IRF shapes are *a priori* reasonable and choose initializations in that range.

Note that the initialization values are on the constrained space, so make sure to respect the constraints when choosing them. For example, α of the Gamma distribution is constrained to be > 0, so an initial α of <=0 will result in incorrect behavior. However, keep in mind that for CDRBayes, prior variances are necessarily on the unconstrained space and get squashed by the constraint function, so choosing initializations that are very close to constraint boundaries can indirectly tighten the prior. For example, choosing an initialization $\alpha = 0.001$ for the Gamma distribution will result in a much tighter prior around small values of α.

Initializations for irrelevant parameters in ill-specified formulas will be ignored and the defaults for the parameters will be used instead. For example, if the model receives the IRF specification `Normal(alpha=1, beta=1)`, it will initialize a Normal IRF at $\mu = 0$, $\sigma = 1$ (the defaults for this kernel), since α and β are not recognized parameter names for the Normal distribution. Therefore, make sure to match the parameter names above when specifying parameter defaults. The correctness of initializations can be checked in the Tensorboard logs.

4.2.8 Using Constant (Non-trainable) Parameters

By default, CDR trains all the variables that parameterize an IRF kernel (e.g. both μ and σ for a Gaussian IRF kernel). But in some cases it's useful to treat certain IRF parameters as constants and leave them untrained. To do this, specify a list of trainable parameters with the keyword argument `trainable`, using Python list syntax. For example, to specify a ShiftedGamma IRF in which the shift parameter δ is held constant at -1, use the following IRF specification:

```
ShiftedGamma(delta=-1, trainable=[alpha, beta])
```

The model will then only train the α and β parameters of the response. As with parameter initialization, unrecognized parameter names in the `trainable` argument will be ignored, and parameter name mismatches can result in more parameters being held constant than intended. For example, the IRF specification `Normal(trainable=[alpha, beta])`, will result in an (untrainable) Normal IRF with all parameters held fixed at their defaults. It is therefore important to make sure that parameter names match those given above. The correctness of the `trainable` specification can be checked in the Tensorboard logs, as well as by the number of trainable parameters reported to standard error at the start of CDR training. Constant parameters will show 0 trainable parameters.

4.2.9 Parameter Tying

A convolutional term in a CDR model is factored into two components, an IRF component with appropriate parameters and a coefficient governing the overall amplitude of the estimate. Unless otherwise specified, both of these terms are fit separately for every predictor in the model. However, parameter tying is possible by passing keyword arguments to the IRF calls in the model formula. Coefficients can be tied using the `coef_id` argument, and IRF parameters can be tied using the `irf_id` argument. For example, the following RHS fits separate IRF and coefficients for each of `A` and `B`:

```
C(A, Normal()) + C(B, Normal())
```

The following fits a single IRF (called "IRF_NAME") but separate coefficients for `A` and `B`:

```
C(A, Normal(irf_id=IRF_NAME)) + C(B, Normal(irf_id=IRF_NAME))
```

The following fits separate IRF but a single coefficient (called "COEF_NAME") for both `A` and `B`:

```
C(A, Normal(coef_id=COEF_NAME)) + C(B, Normal(coef_id=COEF_NAME))
```

And the following fits a single IRF (called "IRF_NAME") and a single coefficient (called "COEF_NAME"), both of which are shared between `A` and `B`:

```
C(A, Normal(irf_id=IRF_NAME, coef_id=COEF_NAME)) + C(B, Normal(irf_id=IRF_NAME, coef_
↪id=COEF_NAME))
```

4.2.10 Transforming Variables

CDR provides limited support for automatic variable transformations based on model formulas. As in **R** formulas, a transformation is applied by wrapping the predictor name in the transformation function. For example, to fit a Gamma IRF to a log transform of predictor `A`, the following is added to the RHS:

```
C(log(A), Gamma())
```

Transformations may be applied to the predictors and/or the response.

The following are the currently supported transformations:

- `log()`: Applies a natural logarithm transformation to the variable
- `log1p()`: Adds 1 to the variable an applies a natural logarithm transformation (useful if predictor can include 0)
- `exp()`: Exponentiates the variable
- `z()`: Z-transforms the variable (subtracts its mean and divides by its standard deviation)
- `c()`: 0-centers the variable (subtracts its mean)
- `s()`: Scales the variable (divides by its standard deviation)

Other transformations must be applied via data preprocessing.

4.2.11 Pseudo Non-Parametric IRFs

CDR also supports pseudo non-parametric IRFs in the form of Gaussian kernel functions (linear combination of Gaussians or LCG). Instead of a parametric IRF kernel, the model implements the IRF as a sum of Gaussian kernel functions whose location, spread, and height can be optimized by the model. The advantage of LCG IRFs is that they do not require precommitment to a particular functional form for the IRF. The disadvantage is that fitting them is slower because they involve more parameters and computation.

The kernels themselves have a number of free parameters which are specified by the name of the kernel in the IRF call of the model formula. The syntax for an LCG IRF kernel is as follows:

```
LCG(b([0-9]+))?
```

This is a string representation of a function call `LCG` with optional keyword argument `b`.

The keyword argument is defined as follows:

- **b** (bases): `int`, number of bases (control points). **Default**: 10.

4.2.12 IRF Composition

In some cases it may be desirable to decompose the response into multiple convolutions of an impulse. For example, it is possible that the BOLD response in fMRI consists underlyingly of 2 convolutional responses: a **neural response** that convolves the impulse into a timecourse of neural activation, which is then convolved with a **hemodynamic response** into a BOLD signal. In this case, it would be desirable to be able to model the BOLD response as a composition of neural and hemodynamic responses.

Exact parametric composition of IRF is not possible in the general case because many pairs of IRF do not have a tractable analytical convolution. Instead, the CDR package uses a discrete approximation to the continuous integral of composed IRF by (1) computing the value of each IRF for some number of interpolation points, (2) computing their convolution via FFT, and (3) rescaling by the temporal distance between interpolation points. The number of interpolation points is defined by the model's **n_interp** initialization parameter.

To compose IRF in a model, simply insert one IRF call into the first argument position of another IRF call. For example, the following first convolves impulse `A` with a normal IRF and then convolves this convolved response with an exponential IRF:

```
C(A, Exp(Normal()))
```

Because convolution has the associative property, the order of composition does not matter, and the above is equivalent to:

```
C(A, Normal(Exp()))
```

The advantage of IRF composition is that it affords the possibility of discovering the structure of latent responses that are not directly observable in the measured response, as in the example described above. The disadvantage is that it is much more computationally expensive due to the interpolation and FFT steps required.

Care must also be taken when using IRF composition to avoid constructing unidentifiable models. For example, the convolution of two Gaussians $N(\mu_1, \sigma_1^2)$ and $N(\mu_2, \sigma_2^2)$ is known to be $N(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$. As a result, the following composed IRF has infinitely many solutions, and the resulting model is unidentifiable:

```
C(A, Normal(Normal()))
```

CDR is not able to recognize and flag identifiability problems and it will happily find a solution to such a model, disguising the fact that there are infinitely many other optimal solutions. It is up to the user to think carefully about whether the model structure could introduce such problems. For example, in the BOLD example discussed above,

the neural response is predictor-specific while the hemodynamic response is predictor-independent given the neural response. The two responses can thus be separated via parameter tying of the hemodynamic response portion (see below), requiring all predictors to share a single hemodynamic response and forcing predictor-level variation into the neural response alone. **NOTE:**: Only parametric (not neural network) IRFs can be composed in this way. Numerical integration of neural network IRFs is computationally prohibitive.

4.3 Neural Network Components

CDR allows two kinds of neural network components in the model architecture. First, rather than using a parametric IRF kernel, you can use a deep neural network IRF, simply by using the term `NN()` as the second argument of a `C()` call:

```
y ~ C(A + B, NN())
```

NN hyperparameters can either be globally defined through keywords in `[cdr_settings]` or locally defined in the formula via keyword arguments to `NN()` (for available options, see *CDR Configuration Files*). The main reason to define a hyperparameter locally within the formula is if you want to override a global setting for a particular neural network component. For example, imagine we have two predictors `A` and `B` and we want to constrain the response to be linear on `A` (but not `B`). We can achieve this by varying the value of the `input_dependent_irf` setting (which determines whether the IRF is allowed to differ at different input values, opening the possibility of non-linear responses), as follows:

```
[model_CDR_example]
input_dependent_irf = True
formula = y ~ C(A, NN(input_dependent_irf=False)) + C(B, NN())
```

In the above, the default setting for `input_dependent_irf` is set to `True` in the model settings (thus, non-linear by default), but this default is overridden in the NN response to `A` by using the keyword argument `input_dependent_irf=False` in the relevant `NN()` call of the model formula. Using this definition, the IRF to `B` depends on the value of `B`, but the IRF to `A` is independent of the value of `A`, and thus linear.

Just like other IRFs, neural network IRFs can participate in both fixed and random effects. For example, the following defines a single population-level neural network IRF but allows the coefficients to vary by subject:

```
y ~ C(A + B, NN()) + (C(A + B, NN()) | subject)
```

By contrast, the following allows by-subject variation in both in the coefficients and in the neural network parameters themselves:

```
y ~ C(A + B, NN()) + (C(A + B, NN(ran=T)) | subject)
```

In addition, formulas can include trainable neural network transformations of predictors, simply by placing `NN()` in the first argument of a `C()` call and entering the sum of predictors to transform as its argument:

```
y ~ C(NN(A + B + C), Normal())
```

The above formula will first apply a feedforward neural network to transform the vector `[A, B, C]` into a scalar, which is then treated as a predictor with a `Normal` IRF kernel. Neural net predictor transforms can also take neural network IRFs:

```
y ~ C(NN(A + B + C), NN())
```

In this case, one NN defines a transform on `A`, `B`, and `C`, and another defines an IRF that describes the diffusion of the effect of that transformed value over time. Note that in the above formula, the two NNs operate independently, one transforming data, the other convolving it. But this implementation also supports input-dependent NN IRFs that

take the input values into account in determining the IRF shape. Input-dependent IRFs can be used by setting the `input_dependent_irf` field to `True` in the `[cdr_settings]` section of the config. Input-dependent IRFs make predictor transformations unnecessary (since the IRF implicitly represents a transformation of the predictors), so the above formula would only make sense if input-dependence were turned off.

Parametric IRFs distribute over their inputs. Thus, the following two formulas are equivalent, and both express distinct IRF transforms for the variables A and B:

```
y ~ C(A + B, Normal())
y ~ C(A, Normal()) + C(B, Normal())
```

However, this is not the case for deep neural IRFs, where the elements in the first argument of `C()` determine the number of convolution weights that the neural IRF will generate. Thus, the following two formulas are not equivalent:

```
y ~ C(A + B, NN())
y ~ C(A, NN()) + C(B, NN())
```

The first defines a single NN IRF with two outputs that jointly convolves `A` and `B`. The second defines two distinct NN IRFs, each with one output, that separately convolve `A` and `B`.

Neural components can be flexibly combined with non-neural components. For example, the following treats `A` as a linear (`DiracDelta`) predictor, convolves `B` with a neural IRF, and convolves `C` with a `Normal` IRF:

```
y ~ A + C(B, NN()) + C(C, Normal())
```

4.4 Multivariate Responses

CDR can jointly model multiple response variables. Unless the model contains neural components, this is equivalent to fitting a distinct CDR model to each response vector, but it can be more computationally efficient. When neural components are used, distributed representations entail that multivariate models can substantively differ from separate univariate models. Information about one response variable can inform inferences made about other response variables.

To model multiple response variables, simply enter them all on the left-hand side of the model formula, delimited by +. For example, the following jointly models `y1` and `y2` as a function of `A` and `B`:

```
y1 + y2 ~ C(A + B, Gamma())
```

CHAPTER

FIVE

IRF TREES IN CDR

The network of IRFs for each CDR model are represented by the implementations in this package as *trees* from which properties can be read off for the purposes of model construction. This is an implementation detail that will not be pertinent to most users, especially those primarily training and using CDR models through the bundled executables. However, for users who want to program with CDR classes or directly interface with the associated `Formula` class, which is used to store and manipulate information about the model structure, this reference provides a conceptual overview of tree representations of CDR impulse response structures.

There are several reasons for representing IRFs as nodes on a tree. In particular, tree representations facilitate:

- **Factorization** of separable model components, especially *impulses*, *coefficients*, and *IRFs* (see discussion below)
- **IRF composition**: convolving multiple IRF with each other in a hierarchical fashion
- **Parameter tying**: sharing a single IRF or coefficient across multiple portions of the model

Note that these components cannot be cleanly factorized in CDRNN, so CDRNN "trees" are flat. The remainder of this page applies only to CDR.

5.1 Factorization

CDR models contain *impulses*, *coefficients*, and *IRFs*, each of whose structure can be separately manipulated. Impulses are timestamped data streams that constitute the predictors of the model. Impulses are computed from the input data prior to entering the CDR computation graph.

Coefficients govern the amplitude of the response to a predictor. Specifically, the IRF for a given predictor is multiplied by a coefficient governing the magnitude and sign of the overall response. Because multiplication distributes over convolution, coefficients are only needed at the point at which an IRF is convolved with an impulse. In hierarchical models involving convolution of multiple IRFs together, the coefficient can be seen as the product of all coefficients on all composed IRFs. It is therefore desirable to restrict coefficients only to those IRF that "make contact" with the impulse data.

IRFs govern the shape of the response to a predictor. The response is subsequently scaled using a coefficient. Arbitrary IRF can be convolved together in a hierarchical fashion using a fast Fourier transform-based discrete approximation to the continuous convolution.

Tree structures permit natural separation of these three components. Specifically, the CDR IRF tree consists of *nodes*, each of which represents the application of an IRF. IRF composition is represented in the tree as *dominance*: parent IRF are convolved with their children, which are they convolved with their children, etc. Coefficients are disallowed except at *terminal* IRF nodes, i.e. "leaves" of the tree that have no children. In this implementation, `Terminal` is distinguished as special type of IRF kernel. The leaves of the IRF tree must always and only be `Terminal`. Only `Terminal` IRF nodes are permitted to have coefficients. Attempts to specify coefficients at other portions of the tree are ignored. Terminals always have a 1-to-1 link to an impulse contained in the data.

Thus, impulses, coefficients, and IRFs are kept separate by representing the IRF as nodes in a tree and the impulses and coefficients as decorations on a distinguished `Terminal` node type.

5.2 IRF composition

All IRF trees are rooted at a special `ROOT` node, and subsequent application and composition of IRF is represented by tree structures dominated by `ROOT`. A simple model with no IRF composition will have a tree depth of 3:

```
ROOT --> IRF --> Terminals.
```

Models involving composition of IRF will have greater depth, as composition of IRF is represented as dominance relations between them. For example, imagine that the IRF for a given predictor is expected to be a Gamma convolved with another Gamma, which is then convolved with a Normal. The path through the tree describing this structure will be:

```
ROOT --> Gamma1 --> Gamma2 --> Terminal
```

At the terminal, the composed IRF is multiplied by its coefficient and then convolved with its associated impulse. Although IRF composition in CDR respects the hierarchical order in which the IRF are specified, in most cases order of composition does not matter because of associativity of convolution.

5.3 Parameter tying

IRF can be tied in CDR, a property which can be conveniently represented via branching structures in the tree. Specifically, if a single IRF is convolved with (1) multiple downstream IRF in a composition hierarchy or (2) multiple impulses, this fact can be represented by attaching multiple child nodes to a node representing the IRF. For example, consider the following two IRF trees involving impulses A, B, and C:

```
1)
            ROOT
         /     |     \
  NormalA  NormalB  NormalC
     |        |        |
   TermA    TermB    TermC

2)
         ROOT
           |
         Normal
       /   |    \
  TermA TermB TermC
```

In Tree (1), each terminal has its own IRF, so the branching occurs below `ROOT`, while in Tree (2), a single IRF is shared by all three impulses, so the branch occurs below `IRF`. More complex models could be formed e.g. by replacing one of the terminals in these examples with other IRF treelets, and so on.

Tying of coefficients is also supported but this is not represented in the tree structure. It is enforced simply by requiring multiple terminals to share the same value for the coefficient ID property.

5.4 CDR tree summaries

In the CDR model summary, the IRF tree is printed in string format with indentation representing dominance. The ID of each IRF on the tree is printed on its own line, along with other metadata when relevant (such as trainable params and associated random grouping factors). For example, Tree (1) above would be represented as follows:

```
ROOT
  Normal.A; trainable params: mu, sigma
    Normal.A-Terminal.A
  Normal.B; trainable params: mu, sigma
    Normal.B-Terminal.B
  Normal.C; trainable params: mu, sigma
    Normal.C-Terminal.C
```

while Tree (2) would be represented as follows:

```
ROOT
  Normal; trainable params: mu, sigma
    Normal-Terminal.A
    Normal-Terminal.B
    Normal-Terminal.C
```

CHAPTER

SIX

CDR PACKAGE API

Complete API for all public classes and methods in this package.

6.1 cdr.backend module

6.2 cdr.config module

class cdr.config.**Config**(*path*)

Bases: `object`

Parses an *.ini file and stores settings needed to define a set of CDR experiments.

Parameters
path – Path to *.ini file

build_cdr_settings(*settings*, *add_defaults=True*, *global_settings=None*, *is_cdr=True*, *is_cdrnn=False*)

Given a settings object parsed from a config file, compute CDR parameter dictionary.

Parameters

- **settings** – settings from a `ConfigParser` object.
- **add_defaults** – `bool`; whether to add default settings not explicitly specified in the config.
- **global_settings** – `dict` or `None`; dictionary of global defaults for parameters missing from **settings**.
- **is_cdr** – `bool`; whether this is a CDR(NN) model.
- **is_cdrnn** – `bool`; whether this is a CDRNN model.

Returns
`dict`; dictionary of settings key-value pairs.

expand_submodels()

Expand models into cross-validation folds and/or ensembles.

return: `None`

set_model(*model_name=None*)

Change internal state to that of model named **model_name**. `Config` instances can store settings for multiple models. `set_model()` determines which model's settings are returned by `Config` getter methods.

Parameters
model_name – `str`; name of target model

Returns
None

class cdr.config.**PlotConfig**(*path=None*)

Bases: object

Parses an *.ini file and stores settings needed to define CDR plots

Parameters
path – Path to *.ini file

build_plot_settings(*settings*)

Given a settings object parsed from a config file, compute plot parameters.

Parameters
settings – settings from a ConfigParser object.

Returns
dict; dictionary of settings key-value pairs.

6.3 cdr.data module

cdr.data.**add_responses**(*names*, *y*)

Add response variable(s) to a dataframe, applying any preprocessing required by the formula string.

Parameters

- **names** – str or list of str; name(s) of dependent variable(s)
- **y** – pandas DataFrame; response data.

Returns
pandas DataFrame; response data with any missing ops applied.

cdr.data.**build_CDR_impulse_data**(*X*, *first_obs*, *last_obs*, *X_in_Y_names=None*, *X_in_Y=None*, *impulse_names=None*, *history_length=128*, *future_length=0*, *int_type='int32'*, *float_type='float32'*)

Construct impulse data arrays in the required format for CDR fitting/evaluation for a single response array.

Parameters

- **X** – list of pandas tables; impulse (predictor) data.
- **first_obs** – list of index vectors (list, pandas series, or numpy vector) of first observations; the list contains vectors of row indices, one for each element of **X**, of the first impulse in the time series associated with the response. If None, inferred from **Y**.
- **last_obs** – list of index vectors (list, pandas series, or numpy vector) of last observations; the list contains vectors of row indices, one for each element of **X**, of the last impulse in the time series associated with the response. If None, inferred from **Y**.
- **X_in_Y_names** – list of str; names of predictors contained in **Y** rather than **X**. If None, no such predictors.
- **X_in_Y** – pandas DataFrame or None; table of predictors contained in **Y** rather than **X**. If None, no such predictors.
- **impulse_names** – list of str; names of columns in **X** to be used as impulses by the model. If None, all columns returned.
- **history_length** – int; maximum number of history (backward) observations.

- **future_length** – int; maximum number of future (forward) observations.
- **int_type** – str; name of int type.
- **float_type** – str; name of float type.

Returns

triple of numpy arrays; let N, T, I, R respectively be the number of rows in **Y**, history length, number of impulse dimensions, and number of response dimensions. Outputs are (1) impulses with shape (N, T, I), (2) impulse timestamps with shape (N, T, I), and impulse mask with shape (N, T, I).

cdr.data.**build_CDR_response_data**(*responses*, *Y=None*, *first_obs=None*, *last_obs=None*, *Y_time=None*, *Y_gf=None*, *X_in_Y_names=None*, *X_in_Y=None*, *Y_category_map=None*, *response_to_df_ix=None*, *gf_names=None*, *gf_map=None*)

Construct response data arrays in the required format for CDR fitting/evaluation for one or more response arrays.

Parameters

- **responses** – list of str; names of columns in **Y** to be used as responses (dependent variables) by the model.
- **Y** – list of pandas tables, or None; response data. If None, does not return a response array.
- **first_obs** – list of list of index vectors (list, pandas series, or numpy vector) of first observations, or None; the list contains one element for each response array. Inner lists contain vectors of row indices, one for each element of **X**, of the first impulse in the time series associated with each response. If None, inferred from **Y**.
- **last_obs** – list of list of index vectors (list, pandas series, or numpy vector) of last observations, or None; the list contains one element for each response array. Inner lists contain vectors of row indices, one for each element of **X**, of the last impulse in the time series associated with each response. If None, inferred from **Y**.
- **Y_time** – list of response timestamp vectors (list, pandas series, or numpy vector), or None; vector(s) of response timestamps, one for each response array. Needed to timestamp any response-aligned predictors (ignored if none in model).
- **Y_gf** – list of pandas DataFrame, or None; vector(s) of response timestamps, one for each response array. Data frames containing random grouping factor levels, if applicable.
- **X_in_Y_names** – list of str; names of predictors contained in **Y** rather than **X** (must be present in all elements of **Y**). If None, no such predictors.
- **X_in_Y** – list of pandas DataFrame or None; tables (one per response array) of predictors contained in **Y** rather than **X** (must be present in all elements of **Y**). If None, no such predictors.
- **Y_category_map** – dict or None; map from category labels to integers for each categorical response.
- **response_to_df_ix** – dict or None; map from response names to lists of indices of the response files that contain them.
- **gf_names** – list or None; list of names of random grouping factor variables. If None and **Y_gf** provided, will use all columns of **Y_gf**.
- **gf_map** – list of dict or None; list maps from random grouping factor levels to their indices, one map per grouping factor variable in **gf_names**.

Returns

7-tuple of `numpy` arrays; let N, R, XF, YF, Z, and K respectively be the number of rows (sum total number of rows in **Y**), number of response dimensions, number of distinct predictor files (X), number of distinct response files (Y), number of random grouping factor variables, and number of response_aligned predictors. Outputs are (1) responses with shape (N, R) or `None` if **Y** is `None`, (2) an XF-tuple of first observation vectors indexing start indices for each entry in X, (3) a YF-tuple of first observation vectors indexing end indices for each entry in X, (4) response timestamps with shape (N,), (5) response masks (masking out any missing response variables per row) with shape (N, R), (6) random grouping factor matrix with shape (N, Z), or `None` if no random grouping factors provided, and (7) response-aligned predictors with shape (N, K).

`cdr.data.c(`*df*`)`

Zero-center pandas series or data frame

Parameters

df – `pandas Series` or `DataFrame`; input date

Returns

`pandas Series` or `DataFrame`; centered data

`cdr.data.compare_elementwise_perf(`*a*, *b*, *y=None*, *mode='err'*`)`

Compare model performance elementwise.

Parameters

- **a** – `numpy` vector; vector of elementwise scores (or predictions if **mode** is `corr`) for model a.
- **b** – `numpy` vector; vector of elementwise scores (or predictions if **mode** is `corr`) for model b.
- **y** – `numpy` vector or `None`; vector of observations. Used only if **mode** is `corr`.
- **mode** – `str`; Type of performance metric. One of `err`, `loglik`, or `corr`.

Returns

`numpy` vector; vector of elementwise performance differences

`cdr.data.compute_filter(`*y*, *field*, *cond*`)`

Compute filter given a field and condition

Parameters

- **y** – `pandas DataFrame`; response data.
- **field** – `str`; name of column on whose values to filter.
- **cond** – `str`; string representation of condition to use for filtering.

Returns

`numpy` vector; boolean mask to use for `pandas` subsetting operations.

`cdr.data.compute_filters(`*Y*, *filters=None*`)`

Compute filters given a filter map.

Parameters

- **Y** – `pandas DataFrame`; response data.
- **filters** – `list`; list of key-value pairs mapping column names to filtering criteria for their values.

Returns

`numpy` vector; boolean mask to use for `pandas` subsetting operations.

cdr.data.**compute_partition**(*y*, *modulus*, *n*)

Given a `splitID` column, use modular arithmetic to partition data into **n** subparts.

Parameters

- **y** – `pandas DataFrame`; response data.
- **modulus** – `int`; modulus to use for splitting, must be at least as large as **n**.
- **n** – `int`; number of subparts in the partition.

Returns

`list` of `numpy` vectors; one boolean vector per subpart of the partition, selecting only those elements of **y** that belong.

cdr.data.**compute_splitID**(*y*, *split_fields*)

Map tuples in columns designated by **split_fields** into integer ID to use for data partitioning.

Parameters

- **y** – `pandas DataFrame`; response data.
- **split_fields** – `list` of `str`; column names to use for computing split ID.

Returns

`numpy` vector; integer vector of split ID's.

cdr.data.**compute_time_mask**(*X_time*, *first_obs*, *last_obs*, *history_length=128*, *future_length=0*, *int_type='int32'*, *float_type='float32'*)

Compute mask for expanded impulse data zeroing out non-existent impulses.

Parameters

- **X_time** – `pandas Series`; timestamps associated with each impulse in **X**.
- **first_obs** – `pandas Series`; vector of row indices in **X** of the first impulse in the time series associated with each response.
- **last_obs** – `pandas Series`; vector of row indices in **X** of the last preceding impulse in the time series associated with each response.
- **history_length** – `int`; maximum number of history (backward) observations.
- **future_length** – `int`; maximum number of future (forward) observations.
- **int_type** – `str`; name of int type.
- **float_type** – `str`; name of float type.

Returns

`numpy` array; boolean impulse mask.

cdr.data.**corr_cdr**(*X_2d*, *impulse_names*, *impulse_names_2d*, *time*, *time_mask*)

Compute correlation matrix, including correlations across time where necessitated by 2D predictors.

Parameters

- **X_2d** – `numpy` array; the impulse data. Must be of shape `(batch_len, history_length+future_length, n_impulses)`, can be computed from sources by `build_CDR_impulse_data()`.
- **impulse_names** – `list` of `str`; names of columns in **X_2d** to be used as impulses by the model.

- **impulse_names_2d** – list of str; names of columns in **X_2d** that designate to 2D predictors.
- **time** – 3D numpy array; array of timestamps for each event in **X_2d**.
- **time_mask** – 3D numpy array; array of masks over padding events in **X_2d**.

Returns
pandas DataFrame; the correlation matrix.

cdr.data.**expand_impulse_sequence**(*X*, *X_time*, *first_obs*, *last_obs*, *window_length*, *int_type='int32'*, *float_type='float32'*, *fill=0.0*)

Expand out impulse stream in **X** for each response in the target data.

Parameters

- **X** – pandas DataFrame; impulse (predictor) data.
- **X_time** – pandas Series; timestamps associated with each impulse in **X**.
- **first_obs** – pandas Series; vector of row indices in **X** of the first impulse in the time series associated with each response.
- **last_obs** – pandas Series; vector of row indices in **X** of the last preceding impulse in the time series associated with each response.
- **window_length** – int; number of steps in time dimension of output
- **int_type** – str; name of int type.
- **float_type** – str; name of float type.
- **fill** – float; fill value for padding cells.

Returns
3-tuple of numpy arrays; the expanded impulse array, the expanded timestamp array, and a boolean mask zeroing out locations of non-existent impulses.

cdr.data.**filter_invalid_responses**(*Y*, *dv*, *crossval_factor=None*, *crossval_fold=None*)

Filter out rows with non-finite responses.

Parameters

- **Y** – pandas table or list of pandas tables; response data.
- **dv** – str or list of str; name(s) of column(s) containing the dependent variable(s)
- **crossval_factor** – str or None; name of column containing the selection variable for cross validation. If None, no cross validation filtering.
- **crossval_fold** – list or None; list of valid values for cross-validation selection. Used only if crossval_factor is not None.

Returns
2-tuple of pandas DataFrame and pandas Series; valid data and indicator vector used to filter out invalid data.

cdr.data.**get_first_last_obs_lists**(*y*)

Convenience utility to extract out all first_obs and last_obs columns in **Y** sorted by file index

Parameters
y – pandas DataFrame; response data.

Returns
pair of list of str; first_obs column names and last_obs column names

cdr.data.**get_rangf_array**(*Y*, *rangf_names*, *rangf_map*)

Collect random grouping factor indicators as `numpy` integer arrays that can be read by Tensorflow. Returns vertical concatenation of GF arrays from each element of **Y**.

Parameters

- **Y** – `pandas` table or `list` of `pandas` tables; response data.
- **rangf_names** – `list` of `str`; names of columns containing random grouping factor levels (order is preserved, changing the order will change the resulting array).
- **rangf_map** – `list` of `dict`; map for each random grouping factor from levels to unique indices.

Returns

cdr.data.**get_time_windows**(*X*, *Y*, *series_ids*, *forward=False*, *window_length=128*, *t_delta_cutoff=None*, *verbose=True*)

Compute row indices in **X** of initial and final impulses for each element of **y**. Assumes time series are already sorted by **series_ids**.

Parameters

- **X** – `pandas` `DataFrame`; impulse (predictor) data.
- **Y** – `pandas` `DataFrame`; response data.
- **series_ids** – `list` of `str`; column names whose jointly unique values define unique time series.
- **forward** – `bool`; whether to compute forward windows (future inputs) or backward windows (past inputs, used if **forward** is `False`).
- **window_length** – `int`; maximum size of time window to consider. If `np.inf`, no bound on window size.
- **t_delta_cutoff** – `float` or `None`; maximum distance in time to consider (can help improve training stability on data with large gaps in time). If `0` or `None`, no cutoff.
- **verbose** – `bool`; whether to report progress to stderr

Returns

2-tuple of `numpy` vectors; first and last impulse observations (respectively) for each response in **y**

cdr.data.**preprocess_data**(*X*, *Y*, *formula_list*, *series_ids*, *filters=None*, *history_length=128*, *future_length=0*, *t_delta_cutoff=None*, *all_interactions=False*, *verbose=True*, *debug=False*)

Preprocess CDR data.

Parameters

- **X** – list of `pandas` tables; impulse (predictor) data.
- **Y** – list of `pandas` tables; response data.
- **formula_list** – `list` of `Formula`; CDR formula for which to preprocess data.
- **series_ids** – `list` of `str`; column names whose jointly unique values define unique time series.
- **filters** – `list`; list of key-value pairs mapping column names to filtering criteria for their values.
- **history_length** – `int`; maximum number of history (backward) observations.

- **future_length** – int; maximum number of future (forward) observations.
- **t_delta_cutoff** – float or None; maximum distance in time to consider (can help improve training stability on data with large gaps in time). If 0 or None, no cutoff.
- **all_interactions** – bool; add powerset of all conformable interactions.
- **verbose** – bool; whether to report progress to stderr
- **debug** – bool; print debugging information

Returns
7-tuple; predictor data, response data, filtering mask, response-aligned predictor names, response-aligned predictors, 2D predictor names, and 2D predictors

cdr.data.**s**(*df*)

Rescale pandas series or data frame by its standard deviation

Parameters
df – pandas Series or DataFrame; input date

Returns
pandas Series or DataFrame; rescaled data

cdr.data.**split_cdr_outputs**(*outputs*, *lengths*)

Takes a dictionary of arbitrary depth containing CDR outputs with their labels as keys and splits each output into a list of outputs with lengths corresponding to **lengths**. Useful for aligning CDR outputs to response files, since multiple response files can be provided, which are underlyingly concatenated by CDR. Recursively modifies the dict in place.

Parameters

- **outputs** – dict of arbitrary depth with numpy arrays at the leaves; the source CDR outputs
- **lengths** – array-like vector of lengths to split the outputs into

Returns
dict; same key-val structure as **outputs** but with each leaf split into a list of len(lengths) vectors, one for each length value.

cdr.data.**z**(*df*)

Z-transform pandas series or data frame

Parameters
df – pandas Series or DataFrame; input date

Returns
pandas Series or DataFrame; z-transformed data

6.4 cdr.formula module

class cdr.formula.**Formula**(*bform_str*, *standardize=True*)

Bases: object

A class for parsing R-style mixed-effects CDR model formula strings and applying them to CDR data matrices.

Parameters
bform_str – str; an R-style mixed-effects CDR model formula string

`ablate_impulses`(*impulse_ids*)

Remove impulses in **impulse_ids** from fixed effects (retaining in any random effects).

Parameters
impulse_ids – `list` of `str`; impulse ID's

Returns
`None`

`apply_formula`(*X*, *Y*, *X_in_Y_names=None*, *all_interactions=False*, *series_ids=None*)

Extract all data and compute all transforms required by the model formula.

Parameters

- **X** – list of `pandas` tables; impulse data.
- **Y** – list of `pandas` tables; response data.
- **X_in_Y_names** – `list` or `None`; List of column names for response-aligned predictors (predictors measured for every response rather than for every input) if applicable, `None` otherwise.
- **all_interactions** – `bool`; add powerset of all conformable interactions.
- **series_ids** – `list` of `str` or `None`; list of ids to use as grouping factors for lagged effects. If `None`, lagging will not be attempted.

Returns
triple; transformed **X**, transformed **y**, response-aligned predictor names

`apply_op`(*op*, *arr*)

Apply op **op** to array **arr**.

Parameters

- **op** – `str`; name of op.
- **arr** – `numpy` or `pandas` array; source data.

Returns
`numpy` array; transformed data.

`apply_op_2d`(*op*, *arr*, *time_mask*)

Apply op to 2D predictor (predictor whose value depends on properties of the response).

Parameters

- **op** – `str`; name of op.
- **arr** – `numpy` or array; source data.
- **time_mask** – `numpy` array; mask for padding cells

Returns
`numpy` array; transformed data

`apply_ops`(*impulse*, *X*)

Apply all ops defined for an impulse

Parameters

- **impulse** – `Impulse` object; the impulse.
- **X** – list of `pandas` tables; table containing the impulse data.

Returns
pandas table; table augmented with transformed impulse.

apply_ops_2d(*impulse*, *X_2d_predictor_names*, *X_2d_predictors*, *time_mask*)

Apply all ops defined for a 2D predictor (predictor whose value depends on properties of the response).

Parameters

- **impulse** – Impulse object; the impulse.
- **X_2d_predictor_names** – list of str; names of 2D predictors.
- **X_2d_predictors** – numpy array; source data.
- **time_mask** – numpy array; mask for padding cells

Returns
2-tuple; list of new predictor name, numpy array of predictor values

static bases(*family*)

Get the number of bases of a spline kernel.

Parameters
family – str; name of IRF family

Returns
int or None; number of bases of spline kernel, or None if **family** is not a spline.

build(*bform_str*, *standardize=True*)

Construct internal data from formula string

Parameters
bform_str – str; source string.

Returns
None

categorical_transform(*X*)

Get transformed formula with categorical predictors in **X** expanded.

Parameters
X – list of pandas tables; input data.

Returns
Formula; transformed Formula object

compute_2d_predictor(*predictor_name*, *X*, *first_obs*, *last_obs*, *history_length=128*, *future_length=None*, *minibatch_size=50000*)

Compute 2D predictor (predictor whose value depends on properties of the most recent impulse).

Parameters

- **predictor_name** – str; name of predictor
- **X** – pandas table; input data
- **first_obs** – pandas Series or 1D numpy array; row indices in X of the start of the series associated with each regression target.
- **last_obs** – pandas Series or 1D numpy array; row indices in X of the most recent observation in the series associated with each regression target.
- **minibatch_size** – int; minibatch size for computing predictor, can help with memory footprint

Returns
2-tuple; new predictor name, `numpy` array of predictor values

initialize_nns()

Initialize a dictionary mapping ids to metadata for all NN components in this CDR model

Returns
`dict`; mapping from NN `str` id to `NN` object storing metadata for that NN.

insert_impulses(*impulses*, *irf_str*, *rangf=None*)

Insert impulses in **impulse_ids** into fixed effects and all random terms.

Parameters
impulse_ids – `list` of `str`; impulse ID's

Returns
`None`

static irf_params(*family*)

Return list of parameter names for a given IRF family.

Parameters
family – `str`; name of IRF family

Returns
`list` of `str`; parameter names

static is_LCG(*family*)

Check whether a kernel is LCG.

Parameters
family – `str`; name of IRF family

Returns
`bool`; whether the kernel is LCG (linear combination of Gaussians)

pc_transform(*n_pc*, *pointers=None*)

Get transformed formula with impulses replaced by principal components.

Parameters

- **n_pc** – `int`; number of principal components in transform.
- **pointers** – `dict`; map from source nodes to transformed nodes.

Returns
`list` of `IRFNode`; tree forest representing current state of the transform.

process_ast(*t*, *terms=None*, *has_intercept=None*, *ops=None*, *rangf=None*, *impulses_by_name=None*, *interactions_by_name=None*, *under_irf=False*, *under_interaction=False*)

Recursively process a node of the Python abstract syntax tree (AST) representation of the formula string and insert data into internal representation of model formula.

Parameters

- **t** – AST node.
- **terms** – `list` or `None`; CDR terms computed so far, or `None` if no CDR terms computed.
- **has_intercept** – `dict`; map from random grouping factors to boolean values representing whether that grouping factor has a random intercept. `None` is used as a key to refer to the population-level intercept.

- **ops** – list; names of ops computed so far, or None if no ops computed.
- **rangf** – str or None; name of rangf for random term currently being processed, or None if currently processing fixed effects portion of model.

Returns
None

process_irf(*t*, *input_irf*, *ops=None*, *rangf=None*, *nn_inputs=None*, *impulses_by_name=None*, *interactions_by_name=None*)

Process data from AST node representing part of an IRF definition and insert data into internal representation of the model.

Parameters

- **t** – AST node.
- **input_irf** – IRFNode, Impulse, InterationImpulse, or NNImpulse object; child IRF of current node
- **ops** – list of str, or None; ops applied to IRF. If None, no ops applied
- **rangf** – str or None; name of rangf for random term currently being processed, or None if currently processing fixed effects portion of model.
- **nn_inputs** – tuple or None; tuple of input impulses to neural network IRF, or None if not a neural network IRF.

Returns
IRFNode object; the IRF node

re_transform(*X*)

Get transformed formula with regex predictors expanded based on matches to the columns in **X**.

Parameters
X – list of pandas tables; input data.

Returns
Formula; transformed Formula object

remove_impulses(*impulse_ids*)

Remove impulses in **impulse_ids** from the model (both fixed and random effects).

Parameters
impulse_ids – list of str; impulse ID's

Returns
None

response_names()

Get list of names modeled response variables.

Returns
list of str; names modeled response variables.

responses()

Get list of modeled response variables.

Returns
list of Impulse; modeled response variables.

`to_lmer_formula_string`(*z=False*, *correlated=True*)

Generate an `lme4`-style LMER model string representing the structure of the current CDR model. Useful for 2-step analysis in which data are transformed using CDR, then fitted using LME.

Parameters

- **z** – `bool`; z-transform convolved predictors.
- **correlated** – `bool`; whether to use correlated random intercepts and slopes.

Returns
`str`; the LMER formula string.

`to_string`(*t=None*)

Stringify the formula, using **t** as the RHS.

Parameters
t – `IRFNode` or `None`; IRF node to use as RHS. If `None`, uses root IRF associated with `Formula` instance.

Returns
`str`; stringified formula.

`unablate_impulses`(*impulse_ids*)

Insert impulses in **impulse_ids** into fixed effects (leaving random effects structure unchanged).

Parameters
impulse_ids – `list` of `str`; impulse ID's

Returns
`None`

`class` cdr.formula.**IRFNode**(*family=None*, *impulse=None*, *p=None*, *irfID=None*, *coefID=None*, *ops=None*, *fixed=True*, *rangf=None*, *nn_impulses=None*, *nn_config=None*, *impulses_as_inputs=True*, *inputs_to_add=None*, *inputs_to_drop=None*, *param_init=None*, *trainable=None*, *response_params_list=None*)

Bases: `object`

Data structure representing a node in a CDR IRF tree. For more information on how the CDR IRF structure is encoded as a tree, see the reference on CDR IRF trees.

Parameters

- **family** – `str`; name of IRF kernel family.
- **impulse** – `Impulse` object or `None`; the impulse if terminal, else `None`.
- **p** – `IRFNode` object or `None`; the parent IRF node, or `None` if no parent (parent nodes can be connected after initialization).
- **irfID** – `str` or `None`; string ID of node if applicable. If `None`, automatically-generated ID will discribe node's family and structural position.
- **coefID** – `str` or `None`; string ID of coefficient if applicable. If `None`, automatically-generated ID will discribe node's family and structural position. Only applicable to terminal nodes, so this property will not be used if the node is non-terminal.
- **ops** – `list` of `str`, or `None`; ops to apply to IRF node. If `None`, no ops.
- **fixed** – `bool`; Whether node exists in the model's fixed effects structure.
- **rangf** – `list` of `str`, `str`, or `None`; names of any random grouping factors associated with the node.

- **nn_impulses** – tuple or None; tuple of input impulses to neural network IRF, or None if not a neural network IRF.
- **nn_config** – dict or None; dictionary of settings for NN IRF component.
- **impulses_as_inputs** – bool; whether to include impulses in input of a neural network IRF.
- **inputs_to_add** – list of Impulse/NNImpulse or None; list of impulses to add to input of neural network IRF.
- **inputs_to_drop** – list of Impulse/NNImpulse or None; list of impulses to remove from input of neural network IRF (keeping them in output).
- **param_init** – dict; map from parameter names to initial values, which will also be used as prior means.
- **trainable** – list of str, or None; trainable parameters at this node. If None, all parameters are trainable.
- **response_params_list** – list of 2-tuple of str, or None; Response distribution parameters modeled by this IRF, with each parameter represented as a pair (DIST_NAME, PARAM_NAME). DIST_NAME can be None, in which case the IRF will apply to any distribution parameter matching PARAM_NAME.

ablate_impulses(*impulse_ids*)

Remove impulses in **impulse_ids** from fixed effects (retaining in any random effects).

Parameters
impulse_ids – list of str; impulse ID's

Returns
None

add_child(*t*)

Add child to this node in the IRF tree

Parameters
t – IRFNode; child node.

Returns
IRFNode; child node with updated parent.

add_interactions(*response_interactions*)

Add a ResponseInteraction object (or list of them) to this node.

Parameters
response_interaction – ResponseInteraction or list of ResponseInteraction; response interaction(s) to add

Returns
None

add_rangf(*rangf*)

Add random grouping factor name to this node.

Parameters
rangf – str; random grouping factor name

Returns
None

`atomic_irf_by_family()`

Get map from IRF kernel family names to list of IDs of IRFNode instances belonging to that family.

Returns
`dict` from `str` to `list` of `str`; IRF IDs by family.

`atomic_irf_param_init_by_family()`

Get map from IRF kernel family names to maps from IRF IDs to maps from IRF parameter names to their initialization values.

Returns
`dict`; parameter initialization maps by family.

`atomic_irf_param_trainable_by_family()`

Get map from IRF kernel family names to maps from IRF IDs to lists of trainable parameters.

Returns
`dict`; trainable parameter maps by family.

`bases()`

Get the number of bases of node.

Returns
`int` or `None`; number of bases of node, or `None` if node is not a spline.

`categorical_transform(X, expansion_map=None)`

Generate transformed copy of node with categorical predictors in **X** expanded. Recursive. Returns a tree forest representing the current state of the transform. When run from ROOT, should always return a length-1 list representing a single-tree forest, in which case the transformed tree is accessible as the 0th element.

Parameters

- **X** – list of `pandas` tables; input data.
- **expansion_map** – `dict`; Internal variable. Do not use.

Returns
`list` of `IRFNode`; tree forest representing current state of the transform.

`coef2impulse()`

Get map from coefficient IDs dominated by node to lists of corresponding impulses.

Returns
`dict`; map from coefficient IDs to lists of corresponding impulses.

`coef2terminal()`

Get map from coefficient IDs dominated by node to lists of corresponding terminal IRF nodes.

Returns
`dict`; map from coefficient IDs to lists of corresponding terminal IRF nodes.

`coef_by_rangf()`

Get map from random grouping factor names to associated coefficient IDs dominated by node.

Returns
`dict`; map from random grouping factor names to associated coefficient IDs.

`coef_id()`

Get coefficient ID for this node.

Returns
`str` or `None`; coefficient ID, or `None` if non-terminal.

`coef_names()`

Get list of names of coefficients dominated by node.

Returns
`list` of `str`; names of coefficients dominated by node.

`depth()`

Get depth of node in tree.

Returns
`int`; depth

`fixed_coef_names()`

Get list of names of fixed coefficients dominated by node.

Returns
`list` of `str`; names of fixed coefficients dominated by node.

`fixed_interaction_names()`

Get list of names of fixed interactions dominated by node.

Returns
`list` of `str`; names of fixed interactions dominated by node.

`formula_terms()`

Return data structure representing formula terms dominated by node, grouped by random grouping factor. Key `None` represents the fixed portion of the model (no random grouping factor).

Returns
`dict`; map from random grouping factors to data structure representing formula terms. Data structure contains 2 fields, `'impulses'` containing impulses and `'irf'` containing IRF Nodes.

`has_coefficient(`*rangf*`)`

Report whether **rangf** has any coefficients in this subtree

Parameters
rangf – Random grouping factor

Returns
`bool`: Whether **rangf** has any coefficients in this subtree

`has_composed_irf()`

Check whether node dominates any IRF compositions.

Returns
`bool`, whether node dominates any IRF compositions.

`has_irf(`*rangf*`)`

Report whether **rangf** has any IRFs in this subtree

Parameters
rangf – Random grouping factor

Returns
`bool`: Whether **rangf** has any IRFs in this subtree

`impulse2coef()`

Get map from impulses dominated by node to lists of corresponding coefficient IDs.

Returns
`dict`; map from impulses to lists of corresponding coefficient IDs.

impulse2terminal()

Get map from impulses dominated by node to lists of corresponding terminal IRF nodes.

Returns
dict; map from impulses to lists of corresponding terminal IRF nodes.

impulse_names(*include_interactions=False*, *include_nn=False*, *include_nn_inputs=True*)

Get list of names of impulses dominated by node.

Parameters

- **include_interactions** – bool; whether to return impulses defined by interaction terms.
- **include_nn** – bool; whether to return NN transformations of impulses.
- **include_nn_inputs** – bool; whether to return input impulses to NN transformations.

Returns
list of str; names of impulses dominated by node.

impulse_set(*include_interactions=False*, *include_nn=False*, *include_nn_inputs=True*, *out=None*)

Get set of impulses dominated by node.

Parameters

- **include_interactions** – bool; whether to return impulses defined by interaction terms.
- **include_nn** – bool; whether to return NN transformations of impulses.
- **include_nn_inputs** – bool; whether to return input impulses to NN transformations.

:param set or None; initial dictionary to modify.

Returns
list of Impulse; impulses dominated by node.

impulses(*include_interactions=False*, *include_nn=False*, *include_nn_inputs=True*)

Get alphabetically sorted list of impulses dominated by node.

Parameters

- **include_interactions** – bool; whether to return impulses defined by interaction terms.
- **include_nn** – bool; whether to return NN transformations of impulses.
- **include_nn_inputs** – bool; whether to return input impulses to NN transformations.

Returns
list of Impulse; impulses dominated by node.

impulses_by_name(*include_interactions=False*, *include_nn=False*, *include_nn_inputs=True*)

Get dictionary mapping names of impulses dominated by node to their corresponding impulses.

Parameters

- **include_interactions** – bool; whether to return impulses defined by interaction terms.
- **include_nn** – bool; whether to return NN transformations of impulses.
- **include_nn_inputs** – bool; whether to return input impulses to NN transformations.

Returns
list of Impulse; impulses dominated by node.

impulses_from_response_interaction()

Get list of any impulses from response interactions associated with this node.

Returns
list of Impulse; impulses dominated by node.

interaction_by_rangf()

Get map from random grouping factor names to associated interaction IDs dominated by node.

Returns
dict; map from random grouping factor names to associated interaction IDs.

interaction_names()

Get list of names of interactions dominated by node.

Returns
list of str; names of interactions dominated by node.

interactions()

Return list of all response interactions used in this subtree, sorted by name.

Returns
list of ResponseInteraction

interactions2inputs()

Get map from IDs of ResponseInteractions dominated by node to lists of IDs of their inputs.

Returns
dict; map from IDs of ResponseInteractions nodes to lists of their inputs.

irf_by_rangf()

Get map from random grouping factor names to IDs of associated IRF nodes dominated by node.

Returns
dict; map from random grouping factor names to IDs of associated IRF nodes.

irf_id()

Get IRF ID for this node.

Returns
str or None; IRF ID, or None if terminal.

irf_to_formula(*rangf=None*)

Generates a representation of this node's impulse response kernel in formula string syntax

Parameters
rangf – random grouping factor for which to generate the stringification (fixed effects if rangf==None).

Returns
str; formula string representation of node

is_LCG()

Check the non-parametric type of a node's kernel, or return None if parametric.

Parameters
family – str; name of IRF family

Returns
str or None; name of kernel type if non-parametric, else ``None.

`local_name()`

Get descriptive name for this node, ignoring its position in the IRF tree.

Returns
`str`; name.

`name()`

Get descriptive name for this node.

Returns
`str`; name.

`nns_by_key(nns_by_key=None)`

Get a dict mapping NN keys to objects associated with them.

Parameters
keys – `dict` or `None`; dictionary to modify. Empty if `None`.

Returns
`dict`; map from string keys to `list` of associated `IRFNode` and/or `NNImpulse` objects.

`node_table()`

Get map from names to nodes of all nodes dominated by node (including self).

Returns
`dict`; map from names to nodes of all nodes dominated by node.

`nonparametric_coef_names()`

Get list of names of nonparametric coefficients dominated by node. :return: `list` of `str`; names of spline coefficients dominated by node.

`static pointers2namemmaps(p)`

Get a map from source to transformed IRF node names.

Parameters
p – `dict`; map from source to transformed IRF nodes.

Returns
`dict`; map from source to transformed IRF node names.

`re_transform(X, expansion_map=None)`

Generate transformed copy of node with regex-matching predictors in **X** expanded. Recursive. Returns a tree forest representing the current state of the transform. When run from ROOT, should always return a length-1 list representing a single-tree forest, in which case the transformed tree is accessible as the 0th element.

Parameters

- **X** – list of `pandas` tables; input data.
- **expansion_map** – `dict`; Internal variable. Do not use.

Returns
`list` of `IRFNode`; tree forest representing current state of the transform.

`remove_impulses(impulse_ids)`

Remove impulses in **impulse_ids** from the model (both fixed and random effects).

Parameters
impulse_ids – `list` of `str`; impulse ID's

Returns
None

`supports_non_causal()`

Check whether model contains only IRF kernels that lack the causality constraint t >= 0.

Returns
`bool`: whether model contains only IRF kernels that lack the causality constraint t >= 0.

`terminal()`

Check whether node is terminal.

Returns
`bool`; whether node is terminal.

`terminal2coef()`

Get map from IDs of terminal IRF nodes dominated by node to lists of corresponding coefficient IDs.

Returns
`dict`; map from IDs of terminal IRF nodes to lists of corresponding coefficient IDs.

`terminal2impulse()`

Get map from terminal IRF nodes dominated by node to lists of corresponding impulses.

Returns
`dict`; map from terminal IRF nodes to lists of corresponding impulses.

`terminal_names()`

Get list of names of terminal IRF nodes dominated by node.

Returns
`list` of `str`; names of terminal IRF nodes dominated by node.

`terminals()`

Get list of terminal IRF nodes dominated by node.

Returns
`list` of `IRFNode`; terminal IRF nodes dominated by node.

`terminals_by_name()`

Get dictionary mapping names of terminal IRF nodes dominated by node to their corresponding nodes.

Returns
`dict`; map from node names to nodes

`unablate_impulses(`*impulse_ids*`)`

Insert impulses in **impulse_ids** into fixed effects (leaving random effects structure unchanged).

Parameters
impulse_ids – `list` of `str`; impulse ID's

Returns
None

`unary_nonparametric_coef_names()`

Get list of names of non-parametric coefficients with no siblings dominated by node. Because unary splines are non-parametric, their coefficients are fixed at 1. Trainable coefficients are therefore perfectly confounded with the spline parameters. Splines dominating multiple coefficients are excepted, since the same kernel shape must be scaled in different ways.

Returns
`list` of `str`; names of unary spline coefficients dominated by node.

class cdr.formula.**Impulse**(*name*, *ops=None*, *is_re=False*)

Bases: object

Data structure representing an impulse in a CDR model.

Parameters

- **name** – str; name of impulse
- **ops** – list of str, or None; ops to apply to impulse. If None, no ops.
- **is_re** – bool; whether impulse is a regular expression search pattern

categorical(*X*)

Checks whether impulse is categorical in a dataset

Parameters
X – list pandas tables; data to to check.

Returns
bool; True if impulse is categorical in **X**, False otherwise.

expand_categorical(*X*)

Expand any categorical predictors in **X** into 1-hot columns.

Parameters
X – list of pandas tables; input data

Returns
2-tuple of pandas table, list of Impulse; expanded data, list of expanded Impulse objects

expand_re(*X*)

Expand any regular expression predictors in **X** into a sequence of all matching columns.

Parameters
X – list of pandas tables; input data

Returns
list of Impulse; list of expanded Impulse objects

get_matcher()

Return a compiled regex matcher to compare to data columns

Returns
re object

is_nn_impulse()

Type check for whether impulse represents an NN transformation of impulses.

Returns
False

name()

Get name of term.

Returns
str; name.

class cdr.formula.**ImpulseInteraction**(*impulses*, *ops=None*)

Bases: object

Data structure representing an interaction of impulse-aligned variables (impulses) in a CDR model.

Parameters

- **impulses** – list of Impulse; impulses to interact.
- **ops** – list of str, or None; ops to apply to interaction. If None, no ops.

expand_categorical(*X*)

Expand any categorical predictors in **X** into 1-hot columns.

Parameters
X – list of pandas tables; input data.

Returns
3-tuple of pandas table, list of ImpulseInteraction, list of list of Impulse; expanded data, list of expanded ImpulseInteraction objects, list of lists of expanded Impulse objects, one list for each interaction.

expand_re(*X*)

Expand any regular expression predictors in **X** into a sequence of all matching columns.

Parameters
X – list of pandas tables; input data

Returns
2-tuple of list of ImpulseInteraction, list of list of Impulse; list of expanded ImpulseInteraction objects, list of lists of expanded Impulse objects, one list for each interaction.

impulses()

Get list of impulses dominated by interaction.

Returns
list of Impulse; impulses dominated by interaction.

is_nn_impulse()

Type check for whether impulse represents an NN transformation of impulses.

Returns
False

name()

Get name of interation impulse.

Returns
str; name.

class cdr.formula.**NN**(*nodes*, *nn_type*, *rangf=None*, *nn_key=None*, *nn_config=None*)

Bases: object

Data structure representing a neural network within a CDR model.

Parameters

- **nodes** – list of IRFNode, and/or NNImpulse objects; nodes associated with this NN
- **nn_type** – str; name of NN type ('irf' or 'impulse').
- **rangf** – str or list of str; random grouping factors for which to build random effects for this NN.
- **nn_type** – str or None; key uniquely identifying this NN node (constructed automatically if None).
- **nn_config** – dict or None; map of NN config fields to their values for this NN node.

all_impulse_names()

Get list of all impulse names associated with this NN component.

Returns
list of str: All impulse names associated with this NN component.

input_impulse_names()

Get list of input impulse names associated with this NN component.

Returns
list of str: Input impulse names associated with this NN component.

name()

Get name of NN.

Returns
str; name.

output_impulse_names()

Get list of output impulse names associated with this NN component (NN IRF only).

Returns
list of str: Output impulse names associated with this NN component.

class cdr.formula.**NNImpulse**(*impulses*, *impulses_as_inputs=True*, *inputs_to_add=None*, *inputs_to_drop=None*, *nn_config=None*)

Bases: object

Data structure representing a feedforward neural network transform of one or more impulses in a CDR model.

Parameters

- **impulses** – list of Impulse; impulses to transform.
- **impulses_as_inputs** – bool; whether to include impulses as NN inputs.
- **inputs_to_add** – list of Impulse or None; extra impulses to add to NN input.
- **inputs_to_drop** – list of Impulse or None; output impulses to drop from NN input.
- **nn_config** – dict or None; map of NN config fields to their values for this NN node.

expand_categorical(*X*)

Expand any categorical predictors in **X** into 1-hot columns.

Parameters
X – list of pandas tables; input data.

Returns
3-tuple of pandas table, list of NNImpulse, list of list of Impulse; expanded data, list of expanded NNImpulse objects, list of lists of expanded Impulse objects, one list for each interaction.

expand_re(*X*)

Expand any regular expression predictors in **X** into a sequence of all matching columns.

Parameters
X – list of pandas tables; input data

Returns
2-tuple of list of ImpulseInteraction, list of list of Impulse; list of expanded ImpulseInteraction objects, list of lists of expanded Impulse objects, one list for each interaction.

impulses()

Get list of output impulses dominated by NN.

Returns
list of Impulse; impulses dominated by NN.

is_nn_impulse()

Type check for whether impulse represents an NN transformation of impulses.

Returns
True

name()

Get name of NN impulse.

Returns
str; name.

class cdr.formula.**ResponseInteraction**(*responses*, *rangf=None*)

Bases: object

Data structure representing an interaction of response-aligned variables (containing at least one IRF-convolved impulse) in a CDR model.

Parameters

- **responses** – list of terminal IRFNode, Impulse, and/or ImpulseInteraction objects; responses to interact.
- **rangf** – str or list of str; random grouping factors for which to build random effects for this interaction.

add_rangf(*rangf*)

Add random grouping factor name to this interaction.

Parameters
rangf – str; random grouping factor name

Returns
None

contains_member(*x*)

Check if object is a member of the set of responses belonging to this interaction

Parameters
x – IRFNode, Impulse, and/or ImpulseInteraction object; object to check.

Returns
bool; whether x is a member of the set of responses

dirac_delta_responses()

Get list of response-aligned Dirac delta variables dominated by interaction.

Returns
list of Impulse and/or ImpulseInteraction objects; Dirac delta variables dominated by interaction.

irf_responses()

Get list of IRFs dominated by interaction.

Returns
list of IRFNode objects; terminal IRFs dominated by interaction.

name()

Get name of interation impulse.

Returns
str; name.

nn_impulse_responses()

Get list of NN impulse terms dominated by interaction.

Returns
list of NNImpulse objects; NN impulse terms dominated by interaction.

replace(*old*, *new*)

Replace an old input with a new one

Parameters

- **old** – IRFNode, Impulse, and/or ImpulseInteraction object; response to remove.
- **new** – IRFNode, Impulse, and/or ImpulseInteraction object; response to add.

Returns
None

responses()

Get list of variables dominated by interaction.

Returns
list of IRFNode, Impulse, and/or ImpulseInteraction objects; impulses dominated by interaction.

cdr.formula.**pythonize_string**(*s*)

Convert string to valid python variable name

Parameters
s – str; source string

Returns
str; pythonized string

cdr.formula.**standardize_formula_string**(*s*)

Standardize a formula string, removing notational variation. IRF specifications C(...) are sorted alphabetically by the IRF call name e.g. Gamma(). The order of impulses within an IRF specification is preserved.

Parameters
s – str; the formula string to be standardized

Returns
str; standardization of **s**

6.5 cdr.io module

cdr.io.**read_tabular_data**(*X_paths*, *Y_paths*, *series_ids*, *categorical_columns=None*, *sep=' '*, *verbose=True*)

Read impulse and response data into pandas dataframes and perform basic pre-processing.

Parameters

- **X_paths** – str or list of str; path(s) to impulse (predictor) data (multiple tables are concatenated). Each path may also be a ;-delimited list of paths to files containing predictors with different timestamps, where the predictors in each file are all timestamped with respect to the same reference point.
- **Y_paths** – str or list of str; path(s) to response data (multiple tables are concatenated). Each path may also be a ;-delimited list of paths to files containing different response variables with different timestamps, where the response variables in each file are all timestamped with respect to the same reference point.
- **series_ids** – list of str; column names whose jointly unique values define unique time series.
- **categorical_columns** – list of str; column names that should be treated as categorical.
- **sep** – str; string representation of field delimiter in input data.
- **verbose** – bool; whether to log progress to stderr.

Returns

2-tuple of list(pandas DataFrame); (impulse data, response data). X and Y each have one element for each dataset in X_paths/Y_paths, each containing the column-wise concatenation of all column files in the path.

6.6 cdr.kwargs module

class cdr.kwargs.**Kwarg**(*key*, *default_value*, *dtypes*, *descr*, *aliases=None*, *default_value_cdrnn='same'*, *suppress=False*)

Bases: object

Data structure for storing keyword arguments and their docstrings.

Parameters

- **key** – str; Key
- **default_value** – Any; Default value
- **dtypes** – list or class; List of classes or single class. Members can also be specific required values, either None or values of type str.
- **descr** – str; Description of kwarg
- **default_value_cdrnn** – Any; Default value for CDRNN if distinct from CDR. If 'same', CDRNN uses **default_value**.
- **suppress** – bool; Whether to print documentation for this kwarg. Useful for hiding deprecated or little-used kwargs in order to simplify autodoc output.

dtypes_str()

String representation of dtypes permitted for kwarg.

Returns

str; dtypes string.

get_type_name(*x*)

String representation of name of a dtype

Parameters

x – dtype; the dtype to name.

Returns
str; name of dtype.

in_settings(*settings*)

Check whether kwarg is specified in a settings object parsed from a config file.

Parameters
settings – settings from a ConfigParser object.

Returns
bool; whether kwarg is found in **settings**.

kwarg_from_config(*settings*, *is_cdrnn=False*)

Given a settings object parsed from a config file, return value of kwarg cast to appropriate dtype. If missing from settings, return default.

Parameters

- **settings** – settings from a ConfigParser object or dict.
- **is_cdrnn** – bool; whether this is for a CDRNN model.

Returns
value of kwarg

static type_comparator(*a*, *b*)

Types precede strings, which precede None

Parameters

- **a** – First element
- **b** – Second element

Returns
-1, 0, or 1, depending on outcome of comparison

cdr.kwargs.**cdr_kwarg_docstring**()

Generate docstring snippet summarizing all CDR kwargs, dtypes, and defaults.

Returns
str; docstring snippet

cdr.kwargs.**docstring_from_kwarg**(*kwarg*)

Generate docstring from CDR keyword argument object.

Parameters
kwarg – Keyword argument object.

Returns
str; docstring.

cdr.kwargs.**plot_kwarg_docstring**()

Generate docstring snippet summarizing all plotting kwargs, dtypes, and defaults.

Returns
str; docstring snippet

6.7 cdr.model module

6.8 cdr.opt module

6.9 cdr.plot module

cdr.plot.**plot_heatmap**(*m*, *row_names*, *col_names*, *outdir='.'*, *filename='eigenvectors.png'*, *plot_x_inches=7*, *plot_y_inches=5*, *cmap='Blues'*)

Plot a heatmap. Used in CDR for visualizing eigenvector matrices in principal components models.

Parameters

- **m** – 2D numpy array; source data for plot.
- **row_names** – list of str; row names.
- **col_names** – list of str; column names.
- **outdir** – str; output directory.
- **filename** – str; filename.
- **plot_x_inches** – float; width of plot in inches.
- **plot_y_inches** – float; height of plot in inches.
- **cmap** – str; name of matplotlib cmap object (determines colors of plotted IRF).

Returns

None

cdr.plot.**plot_irf**(*plot_x*, *plot_y*, *irf_names*, *lq=None*, *uq=None*, *density=None*, *sort_names=True*, *prop_cycle_length=None*, *prop_cycle_map=None*, *outdir='.'*, *filename='irf_plot.png'*, *irf_name_map=None*, *plot_x_inches=6*, *plot_y_inches=4*, *ylim=None*, *cmap='gist_rainbow'*, *legend=True*, *xlab=None*, *ylab=None*, *use_line_markers=False*, *use_grid=True*, *transparent_background=False*, *dpi=300*, *dump_source=False*)

Plot impulse response functions.

Parameters

- **plot_x** – numpy array with shape (T,1); time points for which to plot the response. For example, if the plots contain 1000 points from 0s to 10s, **plot_x** could be generated as `np.linspace(0, 10, 1000)`.
- **plot_y** – numpy array with shape (T, N); response of each IRF at each time point.
- **irf_names** – list of str; CDR ID's of IRFs in the same order as they appear in axis 1 of **plot_y**.
- **lq** – numpy array with shape (T, N), or None; lower bound of credible interval for each time point. If None, no credible interval will be plotted.
- **uq** – numpy array with shape (T, N), or None; upper bound of credible interval for each time point. If None, no credible interval will be plotted.
- **sort_names** – bool; alphabetically sort IRF names.
- **prop_cycle_length** – int or None; Length of plotting properties cycle (defines step size in the color map). If None, inferred from **irf_names**.

- **prop_cycle_map** – `list` of `int`, or `None`; Integer indices to use in the properties cycle for each entry in **irf_names**. If `None`, indices are automatically assigned.
- **outdir** – `str`; output directory.
- **filename** – `str`; filename.
- **irf_name_map** – `dict` of `str` to `str`; map from CDR IRF ID's to more readable names to appear in legend. Any plotted IRF whose ID is not found in **irf_name_map** will be represented with the CDR IRF ID.
- **plot_x_inches** – `float`; width of plot in inches.
- **plot_y_inches** – `float`; height of plot in inches.
- **ylim** – 2-element `tuple` or `list`; (lower_bound, upper_bound) to use for y axis. If `None`, automatically inferred.
- **cmap** – `str`; name of `matplotlib` `cmap` object (determines colors of plotted IRF).
- **legend** – `bool`; include a legend.
- **xlab** – `str` or `None`; x-axis label. If `None`, no label.
- **ylab** – `str` or `None`; y-axis label. If `None`, no label.
- **use_line_markers** – `bool`; add markers to IRF lines.
- **use_grid** – `bool`; whether to show a background grid.
- **transparent_background** – `bool`; use a transparent background. If `False`, uses a white background.
- **dpi** – `int`; dots per inch.
- **dump_source** – `bool`; Whether to dump the plot source array to a csv file.

Returns

`None`

cdr.plot.**plot_irf_as_heatmap**(*plot_x*, *plot_y*, *irf_names*, *sort_names=True*, *outdir='.'*, *filename='irf_hm.png'*, *irf_name_map=None*, *plot_x_inches=6*, *plot_y_inches=4*, *ylim=None*, *cmap='seismic'*, *xlab=None*, *ylab=None*, *transparent_background=False*, *dpi=300*, *dump_source=False*)

Plot impulse response functions as a heatmap.

Parameters

- **plot_x** – `numpy` array with shape (T,1); time points for which to plot the response. For example, if the plots contain 1000 points from 0s to 10s, **plot_x** could be generated as `np.linspace(0, 10, 1000)`.
- **plot_y** – `numpy` array with shape (T, N); response of each IRF at each time point.
- **irf_names** – `list` of `str`; CDR ID's of IRFs in the same order as they appear in axis 1 of **plot_y**.
- **sort_names** – `bool`; alphabetically sort IRF names.
- **outdir** – `str`; output directory.
- **filename** – `str`; filename.
- **irf_name_map** – `dict` of `str` to `str`; map from CDR IRF ID's to more readable names to appear in legend. Any plotted IRF whose ID is not found in **irf_name_map** will be represented with the CDR IRF ID.

- **plot_x_inches** – float; width of plot in inches.
- **plot_y_inches** – float; height of plot in inches.
- **ylim** – 2-element tuple or list; (lower_bound, upper_bound) to use for y axis. If None, automatically inferred.
- **cmap** – str; name of matplotlib cmap object (determines colors of plotted IRF).
- **xlab** – str or None; x-axis label. If None, no label.
- **ylab** – str or None; y-axis label. If None, no label.
- **transparent_background** – bool; use a transparent background. If False, uses a white background.
- **dpi** – int; dots per inch.
- **dump_source** – bool; Whether to dump the plot source array to a csv file.

Returns
None

cdr.plot.**plot_qq**(*theoretical*, *actual*, *actual_color='royalblue'*, *expected_color='firebrick'*, *outdir='.'*, *filename='qq_plot.png'*, *plot_x_inches=6*, *plot_y_inches=4*, *legend=True*, *xlab='Theoretical'*, *ylab='Empirical'*, *ticks=True*, *as_lines=False*, *transparent_background=False*, *dpi=300*)

Generate quantile-quantile plot.

Parameters

- **theoretical** – numpy array with shape (T,); theoretical error quantiles.
- **actual** – numpy array with shape (T,); empirical errors.
- **actual_color** – str; color for actual values.
- **expected_color** – str; color for expected values.
- **outdir** – str; output directory.
- **filename** – str; filename.
- **plot_x_inches** – float; width of plot in inches.
- **plot_y_inches** – float; height of plot in inches.
- **legend** – bool; include a legend.
- **xlab** – str or None; x-axis label. If None, no label.
- **ylab** – str or None; y-axis label. If None, no label.
- **as_lines** – bool; render QQ plot using lines. Otherwise, use points.
- **transparent_background** – bool; use a transparent background. If False, uses a white background.
- **dpi** – int; dots per inch.

Returns
None

cdr.plot.**plot_surface**(*x*, *y*, *z*, *lq=None*, *uq=None*, *density=None*, *bounds_as_surface=False*, *outdir='.'*, *filename='surface.png'*, *irf_name_map=None*, *plot_x_inches=6*, *plot_y_inches=4*, *xlim=None*, *ylim=None*, *zlim=None*, *plot_type='wireframe'*, *cmap='coolwarm'*, *xlab=None*, *ylab=None*, *zlab='Response'*, *title=None*, *transparent_background=False*, *dpi=300*, *dump_source=False*)

Plot an IRF or interaction surface.

Parameters

- **x** – numpy array with shape (M,N); x locations for each plot point, copied N times.
- **y** – numpy array with shape (M,N); y locations for each plot point, copied M times.
- **z** – numpy array with shape (M,N); z locations for each plot point.
- **lq** – numpy array with shape (M,N), or None; lower bound of credible interval for each plot point. If None, no credible interval will be plotted.
- **uq** – numpy array with shape (M,N), or None; upper bound of credible interval for each plot point. If None, no credible interval will be plotted.
- **bounds_as_surface** – bool; whether to plot interval bounds using additional surfaces. If False, bounds are plotted with vertical error bars instead. Ignored if lq, uq are None.
- **outdir** – str; output directory.
- **filename** – str; filename.
- **irf_name_map** – dict of str to str; map from CDR IRF ID's to more readable names to appear in legend. Any plotted IRF whose ID is not found in **irf_name_map** will be represented with the CDR IRF ID.
- **plot_x_inches** – float; width of plot in inches.
- **plot_y_inches** – float; height of plot in inches.
- **xlim** – 2-element tuple or list or None; (lower_bound, upper_bound) to use for x axis. If None, automatically inferred.
- **ylim** – 2-element tuple or list or None; (lower_bound, upper_bound) to use for y axis. If None, automatically inferred.
- **zlim** – 2-element tuple or list or None; (lower_bound, upper_bound) to use for z axis. If None, automatically inferred.
- **plot_type** – str; name of plot type to generate. One of ["contour", "surf", "trisurf"].
- **cmap** – str; name of matplotlib cmap object (determines colors of plotted IRF).
- **legend** – bool; include a legend.
- **xlab** – str or None; x-axis label. If None, no label.
- **ylab** – str or None; y-axis label. If None, no label.
- **zlab** – str or None; z-axis label. If None, no label.
- **use_line_markers** – bool; add markers to IRF lines.
- **transparent_background** – bool; use a transparent background. If False, uses a white background.
- **dpi** – int; dots per inch.
- **dump_source** – bool; Whether to dump the plot source array to a csv file.

Returns

None

6.10 cdr.signif module

cdr.signif.**correlation_test**(*y*, *x1*, *x2*, *nested=False*, *verbose=True*)

Perform a parametric test of difference in correlation with observations between two prediction vectors, based on Steiger (1980).

Parameters

- **y** – numpy vector; observation vector.
- **x1** – numpy vector; first prediction vector.
- **x2** – numpy vector; second prediction vector.
- **nested** – bool; assume that the second model is nested within the first.
- **verbose** – bool; report progress logs to standard error.

Returns

cdr.signif.**permutation_test**(*a*, *b*, *n_iter=10000*, *n_tails=2*, *mode='loss'*, *agg='mean'*, *nested=False*, *verbose=True*)

Perform a paired permutation test for significance.

Parameters

- **a** – numpy array; first error/loss/prediction matrix, shape (n_item, n_model).
- **b** – numpy array; second error/loss/prediction matrix, shape (n_item, n_model).
- **n_iter** – int; number of resampling iterations.
- **n_tails** – int; number of tails.
- **mode** – str; one of `["mse", "loglik"]`, the type of error used (SE's are averaged while loglik's are summed).
- **agg** – str; aggregation function over ensemble components. E.g., `'mean'`, `'median'`, `'min'`, `'max'`.
- **nested** – bool; assume that the second model is nested within the first.
- **verbose** – bool; report progress logs to standard error.

Returns

6.11 cdr.synth module

class cdr.synth.**SyntheticModel**(*n_pred*, *irf_name*, *irf_params=None*, *coefs=None*, *fn=None*, *interactions=False*, *ranef_range=None*, *n_ranef_levels=None*)

Bases: object

A data structure representing a synthetic "true" model for empirical validation of CDR fits. Contains a randomly generated set of IRFs that can be used to convolve data, and provides methods for sampling data with particular structure and convolving it with the true IRFs in order to generate a response vector.

Parameters

- **n_pred** – int; Number of predictors in the synthetic model.
- **irf_name** – str; Name of IRF kernel to use. One of `['Exp', 'Normal', 'Gamma', 'ShiftedGamma']`.

- **irf_params** – dict or None; Dictionary of IRF parameters to use, with parameter names as keys and numeric arrays as values. Values must each have **n_pred** cells. If None, parameter values will be randomly sampled.
- **coefs** – numpy array or None; Vector of coefficients to use, where len(coefs) == n_pred. If None, coefficients will be randomly sampled.
- **fn** – str or None; Effect shape to use. One of ['quadratic', 'exp', 'logmod', 'linear']. If ``None, linear effects.
- **interactions** – bool; Whether there are randomly sampled pairwise interactions (same bounds as those used for coefs).
- **ranef_range** – float or None; Maximum magnitude of simulated random effects. If 0 or None, no random effects.
- **n_ranef_levels** – int or None; Number of random effects levels. If 0 or None, no random effects.

convolve(*X*, *t_X*, *t_y*, *history_length=None*, *err_sd=None*, *allow_instantaneous=True*, *ranef_level=None*, *verbose=True*)

Convolve data using the model's IRFs.

Parameters

- **X** – numpy array; 2-D array of predictors.
- **t_X** – numpy array; 1-D vector of predictor timestamps.
- **t_y** – numpy array; 1-D vector of response timestamps.
- **history_length** – int or None; Drop preceding events more than history_length steps into the past. If None, no history clipping.
- **err_sd** – float or None; Standard deviation of Gaussian noise to inject into responses. If None, use the empirical standard deviation of the response vector.
- **allow_instantaneous** – bool; Whether to compute responses when t==0.
- **ranef_level** – str or None; Random effects level to use (or None to use population-level effect)
- **verbose** – bool; Verbosity.

Returns

(2-D numpy array, 1-D numpy array); Matrix of convolved predictors, vector of responses

convolve_v2(*X*, *t_X*, *t_y*, *err_sd=None*, *allow_instantaneous=True*, *verbose=True*)

Convolve data using the model's IRFs. Alternate memory-intensive implementation that is faster for small arrays but can exhaust resources for large ones.

Parameters

- **X** – numpy array; 2-D array of predictors.
- **t_X** – numpy array; 1-D vector of predictor timestamps.
- **t_y** – numpy array; 1-D vector of response timestamps.
- **err_sd** – float; Standard deviation of Gaussian noise to inject into responses.
- **allow_instantaneous** – bool; Whether to compute responses when t==0.
- **verbose** – bool; Verbosity.

Returns
(2-D numpy array, 1-D numpy array); Matrix of convolved predictors, vector of responses

`get_curves`(*n_time_units=None*, *n_time_points=None*, *ranef_level=None*)

Extract response curves as an array.

Parameters

- **n_time_units** – `float`; Number of units of time over which to extract curves.
- **n_time_points** – `int`; Number of samples to extract for each curve (resolution of curve)
- **ranef_level** – `str` or `None`; Random effects level to use (or `None` to use population-level effect)

Returns
numpy array; 2-D numpy array with shape `[T, K]`, where `T` is **n_time_points** and `K` is the number of predictors in the model.

`irf`(*x*, *coefs=False*, *ranef_level=None*)

Computes the values of the model's IRFs elementwise over a vector of timepoints.

Parameters

- **x** – numpy array; 1-D array with shape `[N]` containing timepoints at which to query the IRFs.
- **coefs** – `bool`; Whether to rescale responses by coefficients
- **ranef_level** – `str` or `None`; Random effects level to use (or `None` to use population-level effect)

Returns
numpy array; 2-D array with shape `[N, K]` containing values of the model's `K` IRFs evaluated at the timepoints in **x**.

`plot_irf`(*n_time_units=None*, *n_time_points=None*, *dir='.'*, *filename='synth_irf.png'*, *plot_x_inches=6*, *plot_y_inches=4*, *cmap='gist_rainbow'*, *legend=False*, *xlab=None*, *ylab=None*, *use_line_markers=False*, *transparent_background=False*)

Plot impulse response functions.

Parameters

- **n_time_units** – `float`; number if time units to use for plotting.
- **n_time_points** – `int`; number of points to use for plotting.
- **dir** – `str`; output directory.
- **filename** – `str`; filename.
- **plot_x_inches** – `float`; width of plot in inches.
- **plot_y_inches** – `float`; height of plot in inches.
- **cmap** – `str`; name of `matplotlib` `cmap` object (determines colors of plotted IRF).
- **legend** – `bool`; include a legend.
- **xlab** – `str` or `None`; x-axis label. If `None`, no label.
- **ylab** – `str` or `None`; y-axis label. If `None`, no label.
- **use_line_markers** – `bool`; add markers to IRF lines.

- **transparent_background** – bool; use a transparent background. If False, uses a white background.

Returns
None

sample_data(*m*, *n=None*, *X_interval=None*, *y_interval=None*, *rho=None*, *align_X_y=True*)

Samples synthetic predictors and time vectors

Parameters

- **m** – int; Number of predictors.
- **n** – int; Number of response query points.
- **X_interval** – str, float, list, tuple, or None; Predictor interval model. If None, predictor offsets are randomly sampled from an exponential distribution with parameter 1. If float, predictor offsets are evenly spaced with interval **X_interval**. If list or tuple, the first element is the name of a scipy distribution to use for sampling offsets, and all remaining elements are positional arguments to that distribution.
- **y_interval** – str, float, list, tuple, or None; Response interval model. If None, response offsets are randomly sampled from an exponential distribution with parameter 1. If float, response offsets are evenly spaced with interval **y_interval**. If list or tuple, the first element is the name of a scipy distribution to use for sampling offsets, and all remaining elements are positional arguments to that distribution.
- **rho** – float; Level of pairwise correlation between predictors.
- **align_X_y** – bool; Whether predictors and responses are required to be sampled at the same points in time.

Returns
(2-D numpy array, 1-D numpy array, 1-D numpy array); Matrix of predictors, vector of predictor timestamps, vector of response timestamps

6.12 cdr.util module

cdr.util.**filter_models**(*names*, *filters=None*, *cdr_only=False*)

Return models contained in **names** that are permitted by **filters**, preserving order in which filters were matched. Filters can be ordinary strings, regular expression objects, or string representations of regular expressions. For a regex filter to be considered a match, the expression must entirely match the name. If filters is zero-length, returns **names**.

Parameters

- **names** – list of str; pool of model names to filter.
- **filters** – list of {str, SRE_Pattern} or None; filters to apply in order. If None, no additional filters.
- **cdr_only** – bool; if True, only returns CDR models. If False, returns all models admitted by **filters**.

Returns
list of str; names in **names** that pass at least one filter, or all of **names** if no filters are applied.

cdr.util.**filter_names**(*names*, *filters*)

Return elements of **names** permitted by **filters**, preserving order in which filters were matched. Filters can be ordinary strings, regular expression objects, or string representations of regular expressions. For a regex filter to be considered a match, the expression must entirely match the name.

Parameters

- **names** – `list` of `str`; pool of names to filter.
- **filters** – `list` of `{str, SRE_Pattern}`; filters to apply in order

Returns

`list` of `str`; names in **names** that pass at least one filter

cdr.util.**get_random_permutation**(*n*)

Draw a random permutation of integers 0 to **n**. Used to shuffle arrays of length **n**. For example, a permutation and its inverse can be generated by calling `p, p_inv = get_random_permutation(n)`. To randomly shuffle an **n**-dimensional vector `x`, call `x[p]`. To un-shuffle `x` after it has already been shuffled, call `x[p_inv]`.

Parameters

n – maximum value

Returns

2-tuple of `numpy` arrays; the permutation and its inverse

cdr.util.**load_cdr**(*dir_path*, *suffix=''*)

Convenience method for reconstructing a saved CDR object. First loads in metadata from `m.obj`, then uses that metadata to construct the computation graph. Then, if saved weights are found, these are loaded into the graph.

Parameters

- **dir_path** – Path to directory containing the CDR checkpoint files.
- **suffix** – `str`; file suffix.

Returns

The loaded CDR instance.

cdr.util.**mae**(*true*, *preds*)

Compute mean absolute error (MAE).

Parameters

- **true** – True values
- **preds** – Predicted values

Returns

`float`; MAE

cdr.util.**mse**(*true*, *preds*)

Compute mean squared error (MSE).

Parameters

- **true** – True values
- **preds** – Predicted values

Returns

`float`; MSE

cdr.util.**names2ix**(*names*, *l*, *dtype=<class 'numpy.int32'>*)

Generate 1D numpy array of indices in **l** corresponding to names in **names**

Parameters

- **names** – list of str; names to look up in **l**
- **l** – list of str; list of names from which to extract indices
- **dtype** – numpy dtype object; return dtype

Returns

numpy array; indices of **names** in **l**

cdr.util.**nested**(*model_name_1*, *model_name_2*)

Check whether two CDR models are nested with 1 degree of freedom

Parameters

- **model_name_1** – str; name of first model
- **model_name_2** – str; name of second model

Returns

bool; True if models are nested with 1 degree of freedom, False otherwise

cdr.util.**pca**(*X*, *n_dim=None*, *dtype=<class 'numpy.float32'>*)

Perform principal components analysis on a data table.

Parameters

- **X** – numpy or pandas array; the input data
- **n_dim** – int or None; maximum number of principal components. If None, all components are retained.
- **dtype** – numpy dtype; return dtype

Returns

5-tuple of numpy arrays; transformed data, eigenvectors, eigenvalues, input means, and input standard deviations

cdr.util.**percent_variance_explained**(*true*, *preds*)

Compute percent variance explained.

Parameters

- **true** – True values
- **preds** – Predicted values

Returns

float; percent variance explained

cdr.util.**reg_name**(*string*)

Standardize a variable name for regularization

Parameters

string – str; input string

Returns

str; transformed string

cdr.util.**sn**(*string*)

Compute a valid scope name version of a string.

Parameters
string – str; input string

Returns
str; transformed string

CHAPTER

SEVEN

CDR VISUALIZER

The CDR Visualizer supports interactive plotting of CDR estimates in your web browser. To run it, you will first need to install the `dash` library using either Anaconda or pip, e.g.:

```
pip install dash
```

Once dash is installed, you can visualize any trained model by running:

```
python -m cdr.viz.app <PATH/TO/CONFIG> -m <MODEL_NAME>
```

where <PATH/TO/CONFIG> and <MODEL_NAME> are respectively replaced by the path to your config file and the name specified in the config for the model you want to visualize. CDR Visualizer is a useful complement to the static plotting tools provided by `cdr.bin.plot` because it permits flexible, fast exploration of the solution space recovered by the model. This tool is currently in early development and many planned features are yet to be implemented.

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