Diagnostics

Diagnostics

`diag.diag` is a class to unify various diagnostics methods and provide a consistent interface for diagnostics.

Compute the widely applicable information criterion.

Estimates the expected log pointwise predictive density (elpd) using WAIC. Also calculates the WAIC's standard error and the effective number of parameters. Read more theory here https://arxiv.org/abs/1507.04544 and here https://arxiv.org/abs/1004.2316

Parameters

pointwise: bool If True the pointwise predictive accuracy will be returned. Defaults to `stats.ic_pointwise` rcParam. var_name : str, optional The name of the variable in log_likelihood groups storing the pointwise log likelihood data to use for waic computation. scale: str Output scale for WAIC. Available options are:

- `log` : (default) log-score
- `negative_log` : -1 * log-score
- `deviance` : -2 * log-score

A higher log-score (or a lower deviance or negative log_score) indicates a model with better predictive accuracy. dask_kwargs : dict, optional Dask related kwargs passed to :func:~`arviz.wrap_xarray_ufunc`.

Returns

ELPDData object (inherits from :class:`pandas.Series`) with the following row/attributes: elpd_waic: approximated expected log pointwise predictive density (elpd) se: standard error of the elpd p_waic: effective number parameters n_samples: number of samples n_data_points: number of data points warning: bool True if posterior variance of the log predictive densities exceeds 0.4 waic_i: :class:`~xarray.DataArray` with the pointwise predictive accuracy, only if pointwise=True scale: scale of the elpd

The returned object has a custom print method that overrides pd.Series method.

```
bi.dist.WAIC(
self,
pointwise=None,
var_name=None,
scale=None,
dask_kwargs=None,
)
```

Plot autocorrelation of the MCMC chains.

Args: *args, **kwargs: Additional arguments for arviz.plot_autocorr

Returns: fig: Autocorrelation plot

```
bi.dist.autocor(
self,
*args,
**kwargs,
)
```

Compare models based on their expected log pointwise predictive density (ELPD).

The ELPD is estimated either by Pareto smoothed importance sampling leave-one-out cross-validation (LOO) or using the widely applicable information criterion (WAIC). We recommend loo. Read more theory here - in a paper by some of the leading authorities on model comparison dx.doi.org/10.1111/1467-9868.00353

Parameters

compare_dict: dict of {str: InferenceData or ELPDData} A dictionary of model names and :class:`arviz.InferenceData` or `ELPDData`. ic: str, optional Method to estimate the ELPD, available options are "loo" or "waic". Defaults to `rcParams["stats.information_criterion"]`. method: str, optional Method used to estimate the weights for each model. Available options are:

- 'stacking' : stacking of predictive distributions.
- 'BB-pseudo-BMA' : pseudo-Bayesian Model averaging using Akaike-type weighting. The weights are stabilized using the Bayesian bootstrap.
- 'pseudo-BMA': pseudo-Bayesian Model averaging using Akaike-type weighting, without Bootstrap stabilization (not recommended).

For more information read https://arxiv.org/abs/1704.02030 b_samples: int, optional default = 1000 Number of samples taken by the Bayesian bootstrap estimation. Only useful when method = 'BB-pseudo-BMA'. Defaults to `rcParams["stats.ic_compare_method"]`. alpha: float, optional The shape parameter in the Dirichlet distribution used for the Bayesian bootstrap. Only useful when method = 'BB-pseudo-BMA'. When alpha=1 (default), the distribution is uniform on the simplex. A smaller alpha will keeps the final weights more away from 0 and 1. seed: int or np.random.RandomState instance, optional If int or RandomState, use it for seeding Bayesian bootstrap. Only useful when method = 'BB-pseudo-BMA'. Default None the global :mod:`numpy.random` state is used. scale: str, optional Output scale for IC. Available options are:

- `log` : (default) log-score (after Vehtari et al. (2017))
- `negative_log` : -1 * (log-score)
- `deviance` : -2 * (log-score)

A higher log-score (or a lower deviance) indicates a model with better predictive accuracy. var_name: str, optional If there is more than a single observed variable in the `InferenceData`, which should be used as the basis for comparison.

Returns

A DataFrame, ordered from best to worst model (measured by the ELPD). The index reflects the key with which the models are passed to this function. The columns are: rank: The rank-order of the models. 0 is the best. elpd: ELPD estimated either using (PSIS-LOO-CV `elpd_loo` or WAIC `elpd_waic`). Higher ELPD indicates higher out-of-sample predictive fit ("better" model). If `scale` is `deviance` or `negative_log` smaller values indicates higher out-of-sample predictive fit ("better" model). pIC: Estimated effective number of parameters. elpd_diff: The difference in ELPD between two models. If more than two models are compared, the difference is computed relative to the top-ranked model, that always has a elpd_diff of 0.

weight: Relative weight for each model. This can be loosely interpreted as the probability of each model (among the compared model) given the data. By default the uncertainty in the weights estimation is considered using Bayesian bootstrap. SE: Standard error of the ELPD estimate. If method = BB-pseudo-BMA these values are estimated using Bayesian bootstrap. dSE: Standard error of the difference in ELPD between each model and the top-ranked model. It's always 0 for the top-ranked model. warning: A value of 1 indicates that the computation of the ELPD may not be reliable. This could be indication of WAIC/LOO starting to fail see http://arxiv.org/abs/1507.04544 for details. scale: Scale used for the ELPD.

References

.. [1] Vehtari, A., Gelman, A. & Gabry, J. Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. Stat Comput 27, 1413–1432 (2017) see https://doi.org/10.1007/s11222-016-9696-4

```
bi.dist.compare(
compare_dict,
ic=None,
method='stacking',
b_samples=1000,
alpha=1,
seed=None,
scale=None,
var_name=None,
)
```

Plot density plots of the posterior distribution.

Args: var_names (list): Variables to include shade (float): Transparency of the filled area *args, **kwargs: Additional arguments for arviz.plot_density

Returns: fig: Density plots

```
bi.dist.density(
self,
var_names=None,
shade=0.2,
*args,
**kwargs,
)
```

Calculate effective sample size (ESS).

Args: *args, **kwargs: Additional arguments for arviz.ess

Returns: ess: Effective sample sizes

```
bi.dist.ess(
self,
*args,
**kwargs,
)
```

Create a forest plot of estimated values.

Args: list: Data to plot (default: self.trace) kind (str): Type of plot (default: "ridgeplot") ess (bool): Include effective sample size var_names (list): Variables to include *args, **kwargs: Additional arguments for arviz.plot_forest

Returns: fig: Forest plot

```
bi.dist.forest(
self,
list=None,
kind='ridgeplot',
ess=True,
var_names=None,
*args,
**kwargs,
)
```

Compute Pareto-smoothed importance sampling leave-one-out cross-validation (PSIS-LOO-CV).

Estimates the expected log pointwise predictive density (elpd) using Pareto-smoothed importance sampling leave-one-out cross-validation (PSIS-LOO-CV). Also calculates LOO's standard error and the effective number of parameters. Read more theory here https://arxiv.org/abs/1507.04544 and here https://arxiv.org/abs/1507.02646

Parameters

pointwise: bool, optional If True the pointwise predictive accuracy will be returned. Defaults to `stats.ic_pointwise` rcParam. var_name : str, optional The name of the variable in log_likelihood groups storing the pointwise log likelihood data to use for loo computation. reff: float, optional Relative MCMC efficiency, `ess / n` i.e. number of effective samples divided by the number of actual samples. Computed from trace by default. scale: str Output scale for loo. Available options are:

- `log` : (default) log-score
- `negative_log` : -1 * log-score
- `deviance` : -2 * log-score

A higher log-score (or a lower deviance or negative log_score) indicates a model with better predictive accuracy.

Returns

ELPDData object (inherits from :class:`pandas.Series`) with the following row/attributes: elpd_loo: approximated expected log pointwise predictive density (elpd) se: standard error of the elpd p_loo: effective number of parameters n_samples: number of samples n_data_points: number of data points warning: bool True if the estimated shape parameter of Pareto distribution is greater than `good_k`. loo_i: :class:`~xarray.DataArray` with the pointwise predictive accuracy, only if pointwise=True pareto_k: array of Pareto shape values, only if pointwise True scale: scale of the elpd good_k: For a sample size S, the thresold is compute as min(1 - 1/log10(S), 0.7)

The returned object has a custom print method that overrides pd.Series method.

```
bi.dist.loo(
self,
pointwise=None,
var_name=None,
reff=None,
scale=None,
)
```

Perform comprehensive model diagnostics.

Creates various diagnostic plots including: - Posterior distributions - Autocorrelation plots - Trace plots - Rank plots - Forest plots

Stores plots in instance variables: self.plot_posterior, self.autocor, self.traces, self.rank, self.forest

```
bi.dist.model_checks(
self,
)
```

Create pairwise plots of the posterior distribution.

Args: var_names (list): Variables to include kind (list): Type of plots ("scatter" and/or "kde") kde_kwargs (dict): Additional arguments for KDE plots marginals (bool): Include marginal distributions point_estimate (str): Point estimate to plot figsize (tuple): Size of the figure *args, **kwargs: Additional arguments for arviz.plot_pair

Returns: fig: Pair plot

```
bi.dist.pair(
self,
var_names=None,
kind=['scatter', 'kde'],
kde_kwargs={'fill_last': False},
marginals=True,
point_estimate='median',
figsize=(11.5, 5),
*args,
**kwargs,
)
```

Summary plot for model comparison.

Models are compared based on their expected log pointwise predictive density (ELPD). This plot is in the style of the one used in [2]_. Chapter 6 in the first edition or 7 in the second.

Notes

The ELPD is estimated either by Pareto smoothed importance sampling leave-one-out cross-validation (LOO) or using the widely applicable information criterion (WAIC). We recommend LOO in line with the work presented by [1]_.

Parameters

comp_df : pandas.DataFrame Result of the :func:`arviz.compare` method. insample_dev : bool, default False Plot in-sample ELPD, that is the value of the information criteria without the penalization given by the effective number of parameters (p_loo or p_waic). plot_standard_error : bool, default True Plot the standard error of the ELPD. plot_ic_diff : bool, default False Plot standard error of the difference in ELPD between each model and the top-ranked model. order_by_rank : bool, default True If True ensure the best model is used as reference. legend : bool, default False Add legend to figure. figsize : (float, float), optional If `None`, size is (6, num of models) inches. title : bool, default True Show a tittle with a description of how to interpret the plot. textsize : float, optional Text size scaling factor for labels, titles and lines. If `None` it will be autoscaled based on `figsize`. labeller : Labeller, optional Class providing the method `make_label_vert` to generate the labels in the plot titles. Read the :ref:`label_guide` for more details and usage examples. plot_kwargs : dict, optional Optional arguments for plot elements. Currently accepts 'color_ic', 'marker_ic', 'color_insample_dev', 'marker_insample_dev', 'color_dse', 'marker_dse', 'ls_min_ic' 'color_ls_min_ic', 'fontsize' ax : matplotlib_axes or bokeh_figure, optional Matplotlib axes or bokeh figure. backend : {"matplotlib", "bokeh"}, default "matplotlib" Select plotting backend. backend_kwargs : bool, optional These are kwargs specific to the backend being used, passed to :func:`matplotlib.pyplot.subplots` or :class:`bokeh.plotting.figure`. For additional documentation check the plotting method of the backend. show : bool, optional Call backend show function.

Returns

axes : matplotlib_axes or bokeh_figure

See Also

plot_elpd : Plot pointwise elpd differences between two or more models. compare : Compare models based on PSIS-LOO loo or WAIC waic cross-validation. loo : Compute Pareto-smoothed importance sampling leave-one-out cross-validation (PSIS-LOO-CV). waic : Compute the widely applicable information criterion.

References

.. [1] Vehtari et al. (2016). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC https://arxiv.org/abs/1507.04544

.. [2] McElreath R. (2022). Statistical Rethinking A Bayesian Course with Examples in R and Stan, Second edition, CRC Press.

```
bi.dist.plot_compare(
comp_df,
insample_dev=False,
plot_standard_error=True,
plot_ic_diff=False,
order_by_rank=True,
legend=False,
title=True,
figsize=None,
textsize=None,
labeller=None,
plot_kwargs=None,
ax=None,
backend=None,
backend_kwargs=None,
show=None,
)
```

Plot evolution of effective sample size across iterations.

Returns: fig: ESS evolution plot

```
bi.dist.plot_ess(
self,
)
```

Create a trace plot for visualizing MCMC diagnostics.

Args: var_names (list): List of variable names to include kind (str): Type of plot (default: "rank_bars") *args, **kwargs: Additional arguments for arviz.plot_trace

Returns: plot: The trace plot object

```
bi.dist.plot_trace(
self,
var_names=None,
kind='rank_bars',
*args,
```

```
**kwargs,
)
```

Create posterior distribution plots.

Args: figsize (tuple): Size of the figure (width, height)

Returns: fig: Matplotlib figure containing posterior plots

```
bi.dist.posterior(
self,
figsize=(8, 4),
)
```

Visualize prior distributions compared to log probability.

Args: N (int): Number of samples to draw from priors

Returns: fig: Matplotlib figure containing the prior distribution plots

```
bi.dist.prior_dist(
self,
N=100,
)
```

Create rank plots for MCMC chains.

Args: *args, **kwargs: Additional arguments for arviz.plot_rank

Returns: fig: Rank plots

```
bi.dist.rank(
self,
*args,
**kwargs,
)
```

Calculate R-hat statistics for convergence.

Args: *args, **kwargs: Additional arguments for arviz.rhat

Returns: rhat: R-hat values

```
bi.dist.rhat(
self,
*args,
**kwargs,
)
```

Calculate summary statistics for the posterior distribution.

Args: round_to (int): Number of decimal places to round results kind (str): Type of statistics to compute (default: "stats") hdi_prob (float): Probability for highest posterior density interval *args, **kwargs: Additional arguments for arviz.summary

Returns: pd.DataFrame: Summary statistics of the posterior distribution

```
bi.dist.summary(
self,
round_to=2,
kind='stats',
hdi_prob=0.89,
*args,
**kwargs,
)
```

Convert the sampler output to an arviz trace object.

This method prepares the trace for use with arviz diagnostic tools.

Returns: self.trace: The arviz trace object containing the diagnostic data

```
bi.dist.to_az(
self,
backend='numpyro',
sample_stats_name=['target_log_prob', 'log_accept_ratio', 'has_divergence', 'energy'],
)
```

Create trace plots for MCMC chains.

Args: *args, **kwargs: Additional arguments for arviz.plot_trace

Returns: fig: Trace plots

```
bi.dist.traces(
self,
*args,
**kwargs,
)
```