StratMC Documentation

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StratMC

StratMC is a statistical framework for reconstructing past Earth system change using sediment-hosted proxy data. It is built on the Python probabilistic programming library PyMC, which provides a flexible toolbox for constructing Bayesian models and sampling their posteriors using Markov chain Monte Carlo (MCMC) methods.

Using geochemical proxy observations and geological age constraints from multiple stratigraphic sections, StratMC simultaneously infers the global proxy signal recorded by all sections and builds an age model for each section. For a complete description of the model, see Edmonsond & Dyer (submitted to *Geoscientific Model Development*).

The StratMC Python package can be *installed* from PyPI using the pip package installer. The *API Reference* catalogs built-in functions for processing data, running the inference model, and plotting the results. For example notebooks, refer to the online package documentation (https://stratmc.readthedocs.io/).

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CHAPTER

ONE

INSTALLATION

If you're new to Python, we recommend using Anaconda to install Python on your machine. You can then manage packages from the terminal using conda.

To create a new conda environment for StratMC, run:

```
conda create --name stratmc_env
```

Before installing StratMC, activate the new environment and install pip:

```
conda activate stratmc_env
conda install pip
```

You can then install StratMC and its dependencies using pip (note that the --pre flag is required to install the current version, which is a pre-release), or by compiling directly from the GitHub repository:

1.1 PIP

```
pip install stratmc --pre
```

1.2 Latest (unstable)

pip install git+https://github.com/sedmonsond/stratmc

1.3 Installing on Apple Silicon

On Apple Silicon machines (M1 chip or later), sampling is significantly faster when the Apple Accelerate BLAS library is used, rather than the default OpenBLAS library. After installing StratMC in a new conda environment, run:

```
conda install -c conda-forge numpy">=1.17.0,<2" "libblas=*=*accelerate"
```

QUICK START GUIDE

Here, we provide a basic example of importing data and running the inference model. More complex examples are available on the example notebooks page.

- 1. Fill out proxy data and age constraint tables according to the data formatting specifications.
- 2. Pre-process your data for model construction with <code>load_data()</code>

3. Build a pymc.model.core.Model with build_model(sample_data, age_data, proxies = ['proxy'])

```
from stratmc.model import build_model
model, gp = build_model(sample_data, age_data, proxies = ['d13c'])
```

4. Sample the model posterior using a JAX-assisted MCMC sampling algorithm with get_trace(model, gp, ages).

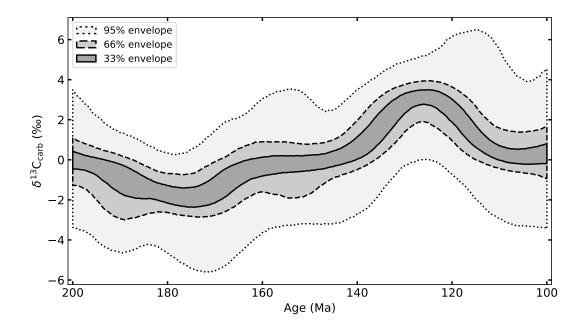
```
import pymc as pm
from stratmc.inference import get_trace

# array of ages at which to sample the posterior proxy curve
predict_ages = np.linspace(lower_age, upper_age, number_ages)

trace = get_trace(model, gp, predict_ages)
```

5. Plot and analyze the results with the *stratmc.plotting* library.

```
from stratmc import plotting
plotting.proxy_inference(sample_data, age_data, trace)
```



DATA TABLE FORMAT

The inference model requires two inputs: proxy data for multiple stratigraphic sections and age constraints (at least a minimum and maximum age for each section). Proxy data and age constraints should be saved in separate .csv files formatted according to the tables below.

3.1 Stratigraphic proxy data

The table below describes the values expected in the data table (.csv file) with proxy data for each section. Each entry corresponds to a single sample. Optional parameters that you do not wish to specify should be left blank, and will be replaced with the default value when the data are loaded with <code>load_data()</code> in <code>stratmc.data</code>.

Parameter	Description
section	Name of the section this data belongs to (type string).
height	Height of sample in section (in meters). For sections where stratigraphic position instead is described by depth , leave blank.
depth	Depth of sample in core (in meters). For sections where stratigraphic position instead is described by height , leave blank.
proxy	Proxy value for sample (replace column header with name of proxy).
proxy_std	$1-\sigma$ uncertainty of proxy measurement (in column header, proxy must match name of the column with the associated proxy value). If not provided, defaults to 0.1.
offset_group	Only required if custom groups of samples share an offset term in the model (otherwise, all samples from the same section will share an offset term). Set to the same value (string or float) for all samples from the same group.
noise_group	Only required if custom groups of samples share a noise term in the model (otherwise, all samples from the same section will share a noise term). Set to the same value (string or float) for all samples from the same group.
Exclude?	Whether to exclude sample from the inference (True or False). Optional; defaults to False if not provided.

3.2 Age constraints

The table below describes the values expected in the data table (.csv file) with age constraints for each section. Each entry corresponds to a single age constraint from one of the sections included in the Stratigraphic proxy data table. Optional parameters that you do not wish to specify should be left blank, and will be replaced with the default value when the data are loaded with <code>load_data()</code> in <code>stratmc.data</code>.

Parameter	Description
section	Name of the section this data belongs to (type string). Must match the corresponding
, , ,	section in the Chemostratigraphic Data table.
height Height of age constraint in section (in meters). For sections where stratigra instead is described by depth , leave blank.	
depth	Depth of age constraint in core (in meters). For sections where stratigraphic position instead is described by height , leave blank.
age	Age (in Myr).
age_std	$1-\sigma$ age uncertainty (in Myr).
name	Name of age constraint (type string). Only required if one of shared? is True.
shared? Whether the age constraint is shared between multiple sections (and should have age in all sections where it is present – i.e., a correlative age constraint) (True Shared constraints must have the same name. Optional; defaluts to False.	
<pre>intermediate detrital?</pre>	Whether the age constraint is an intermediate (i.e., in the middle of a section) detrital age, which provides a maximum age for all overlying samples but does not constrain the age of underlying samples (True or False. Optional; defaults to False.
<pre>intermediate intrusive?</pre>	Whether the age constraint is an intermediate (i.e., in the middle of a section) intrusive age, which provides a minimum age for all underlying samples but does not constrain the age of overlying samples (True or False). Optional; defaults to False.
distribution_type	
param_1_name	Name of parameter for custom distribution; only required if using a distribution other than Normal. If the custom distribution has no parameters, leave blank.
param_1	Value of parameter for custom distribution; only required if using a distribution other than Normal. If the custom distribution has no parameters, leave blank.
param_2_name	Name of parameter for custom distribution; only required if using a distribution other than Normal. If the custom distribution has 0 or 1 parameters, leave blank.
param_2	Value of parameter for custom distribution; only required if using a distribution other than Normal. If the custom distribution has 0 or 1 parameters, leave blank.
Exclude?	Whether to exclude age constraint from the inference (True or False). Optional; defaults to False.

API REFERENCE

4.1 Loading and processing data

Functions for importing and processing proxy and age constraint data.

load_data	Import and pre-process proxy data and age constraints from .csv files formatted according to the <i>Data table formatting</i> guidelines.
combine_data	Helper function for merging pandas.DataFrame objects containing proxy observations or age constraints.
load_object	Custom load command for pickle (.pkl) object (variables can be saved as .pkl files with save_object()).
load_trace	Custom load command for NetCDF file containing a trace (arviz.InferenceData object saved with save_trace()).
save_object	Save variable as a pickle (.pkl) object.
save_trace	Save trace (arviz.InferenceData object) as a NetCDF file.
combine_traces	Helper function for combining multiple arviz. InferenceData objects (saved as NetCDF files) that contain prior and posterior samples for the same inference model (sampled with <code>get_trace()</code> in <code>stratmc.inference</code>).
drop_chains	Remove a subset of chains from a arviz. InferenceData object.
thin_trace	Remove a subset of draws from a arviz. InferenceData object.
accumulation_rate	Calculate apparent sediment accumulation rate between successive samples (if method = 'successive') or every possible sample pairing (method = 'all').
clean_data	Helper function for cleaning sample data before running an inversion.
depth_to_height	Helper function for converting depth in core to height in section.
combine_duplicates	Helper function for combining multiple proxy measurements from the same stratigraphic horizon.

stratmc.data.accumulation_rate(full_trace, sample_df, ages_df, method='all', age_model='posterior', include_age_constraints=True, **kwargs)

Calculate apparent sediment accumulation rate between successive samples (if method = 'successive') or

every possible sample pairing (method = 'all').

Note that if method = 'all', rate is returned in mm/year, and duration is returned in years. If method = 'successive', rate is returned in m/Myr, and duration is returned in Myr. Input data are assumed to have units of meters and millions of years. Used as input to sadler_plot() and accumulation_rate_stratigraphy() in stratmc.plotting.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing all proxy data.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints from all sections.

method: str, optional

Whether to calculate accumulation rates between every possible sample pairing ('all'), or between successive samples ('successive'); defaults to 'all'.

age_model: str, optional

Whether to calculate accumulation rates using the posterior or prior age model for each section; defaults to 'posterior'.

include_age_constraints: bool, optional

Whether to include radiometric age constraints in accumulation rate calculations; defaults to True.

sections: list(str) or numpy.array(str), optional

List of sections to include. Defaults to all sections in sample_df.

Returns

rate_df: pandas.DataFrame

pandas. DataFrame containing sediment accumulation rates and associated durations.

stratmc.data.clean_data(sample_df, ages_df, proxies, sections)

Helper function for cleaning sample data before running an inversion. Sets Exclude? to True for samples with no relevant proxy observations, removes sections where all samples have been excluded, and drops excluded age constraints.

Parameters

sample df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

proxies: str or list(str)

Tracers to include in the inference.

sections: list(str) or numpy.array(str)

List of sections to include in the inference (as named in sample_df and ages_df).

Returns

sample_df: pandas.DataFrame

pandas.DataFrame containing cleaned proxy data for all sections.

ages df: pandas.DataFrame

pandas.DataFrame containing cleaned age constraint data for all sections.

stratmc.data.combine_data(dataframes)

Helper function for merging pandas.DataFrame objects containing proxy observations or age constraints. Data are merged using the section and height columns.

Parameters

dataframes: list(pandas.DataFrame)

List of pandas. DataFrame objects to merge.

Returns

merged_data: pandas.DataFrame

pandas.DataFrame containing merged data.

stratmc.data.combine_duplicates(sample_df, proxies, proxy_sigma_default=0.1)

Helper function for combining multiple proxy measurements from the same stratigraphic horizon. For each horizon with multiple proxy values, replaces the proxy value with the mean, and replaces the standard deviation with the combined uncertainty (proxy_std values summed in quadrature) for all measurements. The standard deviation of the population of proxy values for each horizon is stored in the proxy_population_std column of sample_df (in <code>build_model()</code>, the uncertainty of each proxy observation is modeled as the proxy_std and proxy_population_std values summed in quadrature).

Parameters

sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

proxies: list(str)

List of proxies to include in the inference.

proxy_sigma_default: float or dict{float}, optional

Measurement uncertainty (1σ) to use for proxy observations if not specified in proxy_std column of sample_df. To set a different value for each proxy, pass a dictionary with proxy names as keys. Defaults to 0.1.

Returns

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data with duplicates combined.

stratmc.data.combine_traces(trace_list)

Helper function for combining multiple arviz.InferenceData objects (saved as NetCDF files) that contain prior and posterior samples for the same inference model (sampled with $get_trace()$ in stratmc.inference). The arviz.InferenceData objects are concatenated along the chain dimension such that if two traces with 8 chains each are concatenated, the new combined trace will have 16 chains.

Parameters

trace list: list(str)

List of paths to arviz. InferenceData objects (saved as NetCDF files) to be merged.

Returns

combined_trace: arviz.InferenceData

New arviz.InferenceData object containing the prior and posterior draws for all traces in trace_list.

stratmc.data.depth_to_height(sample_df, ages_df)

Helper function for converting depth in core to height in section.

Parameters

sample df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

Returns

sample df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections, with depth in core converted to height in section.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections, with depth in core converted to height in section.

stratmc.data.drop_chains(full_trace, chains)

Remove a subset of chains from a arviz. InferenceData object.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

chains: list or np.array of int

Indices of chains to remove from full_trace.

Returns

full_trace_clean: arviz.InferenceData

Copy of full_trace without the chains specified in chains.

```
stratmc.data.load_data(sample_file, ages_file, proxies=['d13c'], proxy_sigma_default=0.1, drop_excluded_samples=False, drop_excluded_ages=True)
```

Import and pre-process proxy data and age constraints from .csv files formatted according to the *Data table formatting* guidelines. To combine data from different .csv files, load each file separately and then combine the DataFrames with *combine_data()*.

If sample_file.csv includes multiple proxy observations from the same stratigraphic horizon (for a given proxy), then all measurements marked Exclude? = False will be combined using combine_duplicates().

Parameters

sample_file: str

Path to .csv file containing proxy data for all sections (without '.csv' extension).

ages file: str

Path to .csv file containing age constraints for all sections (without '.csv' extension).

proxies: str or list(str), optional

Tracer names (must match column headers in sample_file.csv); defaults to 'd13c'.

proxy_sigma_default: float or dict{float}, optional

Measurement uncertainty (1σ) to use for proxy observations if not specified in proxy_std column of sample_df. To set a different value for each proxy, pass a dictionary with proxy names as keys. Defaults to 0.1.

drop_excluded_samples: bool, optional

Whether to remove samples with Exclude? = True from the sample_df; defaults to

False. If excluded samples are not dropped, their ages will be passively tracked within the inference model (but they will not be considered during the proxy signal reconstruction).

drop_excluded_ages: bool, optional

Whether to remove ages with Exclude? = True from the ages_df; defaults to True.

Returns

sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

stratmc.data.load_object(path)

Custom load command for pickle (.pkl) object (variables can be saved as .pkl files with save_object()).

Parameters

path: str

Path to saved .pkl file (without the '.pkl' extension).

Returns

var:

Variable saved in path.

stratmc.data.load_trace(path)

Custom load command for NetCDF file containing a trace (arviz.InferenceData object saved with save_trace()).

Parameters

path: str

Path to saved NetCDF file (without the '.nc' extension).

Returns

trace: arviz.InferenceData

Trace saved as NetCDF file.

stratmc.data.save_object(var, path)

Save variable as a pickle (.pkl) object.

Parameters

var:

Variable to be saved.

path: str

Location (including the file name, without '.pkl' extension) to save var.

stratmc.data.save_trace(trace, path)

Save trace (arviz.InferenceData object) as a NetCDF file.

Parameters

trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from <code>build_model()</code> in <code>stratmc.model</code> (the output of <code>get_trace()</code> in <code>stratmc.inference()</code>.

path: str

Location (including the file name, without '.nc' extension) to save trace.

stratmc.data.thin_trace(full_trace, drop_freq=2)

Remove a subset of draws from a arviz.InferenceData object. Only applies to groups associated with the posterior (the prior draws will not be affected).

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

drop_freq: int

Frequency of draw removal. For example, 2 will remove every other draw, while 4 will remove every fourth draw.

Returns

thinned trace: arviz.InferenceData

Thinned version of full_trace.

4.2 Statistical model

Functions for building a proxy signal inference model.

build_model	Create a proxy signal (i.e., carbon isotope) inference model.
superposition	Helper function for explicitly enforcing stratigraphic su- perposition (any given sample must be younger than the underlying sample) for a group of radiometric age con- straints.
<pre>intermediate_detrital_potential</pre>	Helper function for enforcing detrital age constraints (maximum age constraint for all overlying samples; no constraint on underlying samples) in the middle of a section.
<pre>intermediate_intrusive_potential</pre>	Helper function for enforcing intrusive age constraints (minimum age constraint for all underlying samples; no constraint on overlying samples) in the middle of a section.
transformed_initval	Helper function to retrieve the transformed initial values for a random variable in a pymc.model.core.Model object.

```
stratmc.model. \textbf{build_model}(sample\_df, ages\_df, proxies=['d13c'], proxy\_sigma\_default=0.1, \\ approximate=False, hsgp\_m=15, hsgp\_c=1.3, ls\_dist='Wald', ls\_min=0, \\ ls\_mu=20, ls\_lambda=50, ls\_sigma=50, var\_sigma=10, white\_noise\_sigma=0.1, \\ gp\_mean\_mu=None, gp\_mean\_sigma=None, offset\_type='section', \\ offset\_prior='Laplace', offset\_alpha=0, offset\_beta=1, offset\_sigma=1, \\ offset\_mu=0, offset\_b=2, noise\_type='section', noise\_prior='HalfCauchy', \\ noise\_beta=1, noise\_sigma=1, noise\_nu=1, jitter=0.001, proxy\_observed=True, \\ **kwargs)
```

Create a proxy signal (i.e., carbon isotope) inference model.

Note that while excluded samples (Exclude? is True in sample_df) do not affect the proxy signal reconstruction, their ages are passively tracked within the inference model (if other samples from the same sections are included).

Parameters

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections. Load from .csv file using load_data() in stratmc.data.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections. Load from .csv file using load_data() in stratmc.data.

sections:: list(str) or numpy.array(str), optional

List of sections to include in the inference model. Defaults to all sections in sample_df.

proxies: str or list(str), optional

Column or columns containing proxy data in sample_df. Defaults to 'd13c'.

proxy sigma default: float or dict{float}, optional

Measurement uncertainty (1σ) to use for proxy observations if not specified in proxy_std column of sample_df. To set a different value for each proxy, pass a dictionary with proxy names as keys. Defaults to 0.1.

approximate: bool, optional

Build model with an unapproximated latent GP (pymc.gp.Latent) if False, or a Hilbert space Gaussian process approximation (pymc.gp.HSGP) if True; defaults to False. If using the HSGP approximation, also pass the hsgp_m and hsgp_c parameters (the defaults are unlikely to work well for all problems). Appropriate values for m and c can be estimated using approx_hsgp_hyperparams().

hsgp m: int or dict{int}, optional

Number of basis vectors to use in the HSGP approximation (see pymc.gp.HSGP). Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 15.

hsgp_c: float or dict{float}, optional

Proportion extension factor for the HSGP approximation (see pymc.gp.HSGP). Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 1.3.

ls_dist: str or dict{str}, optional

Prior distribution for the lengthscale hyperparameter of the exponential quadratic covariance kernel (pymc.gp.cov.ExpQuad); set to Wald (pymc.Wald) or HalfNormal (pymc. HalfNormal). Defaults to Wald with mu = 20 and lambda = 50. To change mu and lambda, pass the ls_mu and ls_lambda parameters. For HalfNormal, the variance defaults to sigma = 50; change by passing ls_sigma. Pass as a dictionary with proxy names as keys to specify a different prior distribution for each proxy.

ls_min: float or dict{float}, optional

Minimum value for the lengthscale hyperparameter of the pymc.gp.cov.ExpQuad covariance kernel; shifts the lengthscale prior by ls_min. Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 0.

ls_mu: float or dict{float}, optional

Mean (*mu*) of the pymc.gp.cov.ExpQuad lengthscale prior if ls_dist = `Wald`. Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 20.

ls_lambda: float or dict{float}, optional

Relative precision (*lam*) of the pymc.gp.cov.ExpQuad lengthscale hyperparameter prior if ls_dist = `Wald`. Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 50.

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ls_sigma: float or dict{float}, optional

Scale parameter (*sigma*) of the pymc.gp.cov.ExpQuad lengthscale hyperparameter prior if ls_dist = `HalfNormal`. Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 50.

var_sigma: float or dict{float}, optional

Scale parameter (*sigma*) of the covariance kernel variance hyperparameter prior, which is a pymc.HalfNormal distribution. Pass as a dictionary with proxy names as keys to specify a different value for each proxy. Defaults to 10.

white_noise_sigma: float or dict{float}, optional

Amplitude of white noise component of GP covariance function. Defaults to 0.1. Should be equal to or less than the proxy measurement uncertainty; use a smaller value for proxies with low-amplitude signals (e.g., Sr isotopes). Pass as a dictionary with proxy names as keys to specify a different value for each proxy.

gp_mean_mu: float or dict{float}, optional

Mean (*mu*) of the GP mean function prior, which is a pymc.Normal distribution. Defaults to the mean of the observations for each proxy. Pass as a dictionary with proxy names as keys to specify a different value for each proxy.

gp_mean_sigma: float or dict{float}, optional

Standard deviation (*sigma*) of the GP mean function prior, which is a pymc.Normal distribution. Defaults to twice the standard deviation of the observations for each proxy. Pass as a dictionary with proxy names as keys to specify a different value for each proxy.

offset type: str or dict{str}, optional

Parameterize offset such that all samples from the same section have the same offset (set to section), or such that custom sample groups share an offset term (set to groups, and specify the group for each sample and proxy with a offset_group_proxy column in sample_df). To omit the offset term, set to none. Defaults to section. Pass as a dictionary with proxy names as keys to specify a different offset type for each proxy.

offset_prior: str or dict{str}, optional

Type of distribution to use for the offset prior. Pass as a string to use the same prior for all proxies, or as a dict of string (with proxy names as keys) to specify a different prior distribution for each proxy. Defaults to Laplace (pymc.Laplace) with mu = 0 and b = 2. mu and b can be changed by passing offset_mu and offset_b. To use other types of priors, pass the name of a distribution from pymc.distributions, along with parameter values in offset_params. Pass as a dictionary with proxy names as keys to specify a different prior for each proxy.

offset_params: dict{float} or dict{dict{float}}, optional

Only required if using a custom offset_prior. Pass as a dictionary to use the same parameters for all proxies, or as a dictionary of dictionaries (with proxy names as keys) to specify different parameters for each proxy. Keys are param_1_name, param_1, param_2_name, and param_2 (with parameter names corresponding to those required for the specified pymc. distributions object). If only one parameter is required, use np.nan for param_2_name and param_2.

noise_type: str or dict{str}, optional

Parameterize noise as per-section (set to section) or per-group (set to groups, and specify the group for each sample and proxy with a noise_group_proxy column in sample_df). Defaults to section. Pass as a dictionary with proxy names as keys to specify a different noise type for each proxy.

noise prior: str or dict(str), optional

Type of distribution to use for the noise prior. Pass as a string to use the same prior for all

proxies, or as a dict of string (with proxy names as keys) to specify a different prior distribution for each proxy. Defaults to HalfCauchy (pymc.HalfCauchy) with beta = 1. beta can be changed by passing noise_beta. Other implemented priors (note that noise must be positive-only) are HalfNormal (pymc.HalfNormal; defaults to noise_sigma = 1) and HalfStudentT (pymc.HalfStudentT; defaults to noise_nu = 1 and noise_sigma = 1).

superposition dict: dict{list(str)}, optional

Optional; dictionary specifying superposition relationships between different sections. Should only be used when superposition is not implicitly enforced by the age constraints; for example, when sections share the same minimum and maximum age constraints, but are from geological formations with a known stratigraphic relationship. Dictionary keys are section names, and the value for each key is a list of sections that must be older (stratigraphically lower).

jitter: float, optional

Value of jitter passed to pymc.gp.Latent.prior(). Defaults to 0.001.

proxy_observed: bool, optional

Whether to pass observed values to the likelihood function; defaults to True. Only set to False to generate synthetic observations from the model prior in synthetic_observations_from_prior() in stratmc.synthetics.

Returns

model: PyMC model

pymc.model.core.Model object.

gp: pymc.gp.Latent or pymc.gp.HSGP

Gaussian process prior for the model. pymc.gp.Latent if approximate = True, or pymc.gp.HSGP if approximate = False.

stratmc.model.intermediate_detrital_potential(detrital_age_dist, detrital_age_dist_name,

maximum_age_dist_name, minimum_age_dist_name, sample_age_dist_sorted, sample_age_dist, sample_age_dist_name, sample_heights, detrital_height, model, section, interval, sf1_name, sf2_name, shared_radiometric_age_dist=True)

Helper function for enforcing detrital age constraints (maximum age constraint for all overlying samples; no constraint on underlying samples) in the middle of a section.

Parameters

detrital_age_dist: pymc.distributions

Detrital age distribution.

detrital_age_dist_name: str

Name of detrital_age_dist in model.

maximum_age_dist_name: str

Name of distribution for underlying maximum age constraint in model.

minimum_age_dist_name: str

Name of distribution for overlying minimum age constraint in model.

sample age dist sorted: pymc.distribtions

Sorted and scaled sample age distribitions.

sample_age_dist: pymc.distributions

Unsorted and unscaled sample age distributions.

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sample age dist name: str

Name of sample_age_dist in the pymc.Model object.

sample_heights: np.array

Array of heights for samples in the current interval.

detrital_height: float

Height of detrital age constraint.

model: pymc.Model

pymc.model.core.Model object associated with the input distributions.

section: str

Name of the current section.

interval: int

Current interval number.

sf1 name: str

Name of the distribution associated with scaling factor 1 in model.

sf2 name: str

Name of the distribution associated with scaling factor 2 in model.

shared_radiometric_age_dist: bool, optional

Whether the radiometric age distributions are part of a single object (versus initiated as separate distributions). Defaults to True.

stratmc.model.intermediate_intrusive_potential(intrusive_age_dist, intrusive_age_dist_name,

maximum_age_dist_name, minimum_age_dist_name, sample_age_dist_sorted, sample_age_dist, sample_age_dist, sample_age_dist_name, sample_heights, intrusive_height, model, section, interval, sfl_name, sf2_name, shared_radiometric_age_dist=True, **kwargs)

Helper function for enforcing intrusive age constraints (minimum age constraint for all underlying samples; no constraint on overlying samples) in the middle of a section.

Parameters

intrusive_age_dist: pymc.distributions

Intrusive age distribution.

intrusive_age_dist_name: str

Name of intrusive_age_dist in model.

maximum_age_dist_name: str

Name of distribution for underlying maximum age constraint in model.

minimum age dist name: str

Name of distribution for overlying minimum age constraint in model.

sample_age_dist_sorted: pymc.distribtions

Sorted and scaled sample age distribitions.

sample age dist: pymc.distributions

Unsorted and unscaled sample age distributions.

sample_age_dist_name: str

Name of sample_age_dist in the pymc.Model object.

sample_heights: np.array

Array of heights for samples in the current interval.

intrusive height: float

Height of intrusive age constraint.

model: pymc.Model

pymc.model.core.Model object associated with the input distributions.

section: str

Name of the current section.

interval: int

Current interval number.

sf1 name: str

Name of the distribution associated with scaling factor 1 in model.

sf2 name: str

Name of the distribution associated with scaling factor 2 in model.

shared_radiometric_age_dist: bool, optional

Whether the radiometric age distributions are part of a single object (versus initiated as separate distributions). Defaults to True.

stratmc.model.superposition(age_dist, age_dist_names, model, section_age_df, section)

Helper function for explicitly enforcing stratigraphic superposition (any given sample must be younger than the underlying sample) for a group of radiometric age constraints.

Parameters

age_dist: pymc.distribtions

pymc.distributions object for the radiometric ages (must be in stratigraphic order).

age_dist_name: str

Name of age_dist in model.

model: pymc.Model

pymc.model.core.Model object associated with the distributions in age_dist.

section_age_df: pandas.DataFrame

pandas.DataFrame containing age constraints for section.

section: str

Name of the section containing the radiometric age constraints.

stratmc.model.transformed_initval(var_name, model)

Helper function to retrieve the transformed initial values for a random variable in a pymc.model.core.Model object.

Parameters

var_name: str

Name of variable to be transformed (as specified in model).

model: PyMC model

pymc.model.core.Model object that contains the target random variable.

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4.3 Inference

Functions for sampling the inference model, checking for convergence, and processing the results.

get_trace	Sample the prior and posterior distributions for a pymc. model.core.Model returned by build_model() in stratmc.model.
extend_age_model	Extend age models to a different set of proxy observa- tions using posterior sample ages from an existing infer- ence.
<pre>interpolate_proxy</pre>	Use interpolated sample ages from <code>extend_age_model()</code> to calculate proxy values at a given set of ages (e.g., to plot 68 and 95% confidence intervals over time for a new proxy using <code>interpolated_proxy_inference()</code> in <code>stratmc.plotting()</code> .
age_range_to_height	Use the posterior age model for each section to find the stratigraphic interval (with uncertainty) corresponding to a given age range.
map_ages_to_section	Helper function for section_proxy_signal() in stratmc.plotting.
count_samples	Helper function for proxy_data_density() in stratmc.plotting.
find_gaps	Helper function for proxy_data_gaps() in stratmc. plotting.
calculate_lengthscale_stability	Compute the posterior standard deviation of the pymc. gp.cov.ExpQuad covariance kernel lengthscale as additional chains are considered (i.e., for 1 to <i>N</i> chains).
calculate_proxy_signal_stability	Compute the residuals between the median inferred proxy signal when all <i>N</i> chains are considered compared to when 1 to <i>N-1</i> chains are considered.

stratmc.inference.age_range_to_height(full_trace, sample_df, ages_df, lower_age, upper_age, **kwargs)

Use the posterior age model for each section to find the stratigraphic interval (with uncertainty) corresponding to a given age range. If sections is not provided, returns height estimates for every section that overlaps the target age range. To visualize the stratigraphic intervals, use section_age_range() in stratmc.plotting.

Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

lower age: float

Lower bound (youngest age) of the target age interval.

upper_age: float

Upper bound (oldest age) of the target age interval.

sections: list(str) or numpy.array(str), optional

List of sections included in the original inference; only required if not all sections in sample_df were included.

Returns

height_range_df: pandas.DataFrame

Summary statistics for the base and top height of the target age interval (maximum likelihood estimate, median, and 68% and 95% confidence intervals) for each section.

stratmc.inference.calculate_lengthscale_stability(full_trace, **kwargs)

Compute the posterior standard deviation of the pymc.gp.cov.ExpQuad covariance kernel lengthscale as additional chains are considered (i.e., for 1 to N chains). When the posterior has been sufficiently explored, the standard deviation will stabilize; if it has not stabilized, then additional chains should be run. Helper function for $lengthscale_stability()$ in stratmc.plotting.

To consider chains from multiple traces associated with the same inference model, first combine the traces (saved as NetCDF files) using *combine_traces()* in *stratmc.data*.

Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Name of the proxy; only required if multiple proxies were included in the inference model.

Returns

gp_ls_std: np.array of float

Posterior standard deviation of the covariance kernel lengthscale posterior; entries correspond to number of chains considered (first entry is 1 chain, last entry is all *N* chains).

stratmc.inference.calculate_proxy_signal_stability(full_trace, **kwargs)

Compute the residuals between the median inferred proxy signal when all N chains are considered compared to when 1 to N-I chains are considered. When the posterior has been sufficiently explored, the residuals will stabilize and approach zero; if they have not stabilized, then additional chains should be run. Helper function for $proxy_signal_stability()$ in stratmc.plotting.

To consider chains from multiple traces associated with the same inference model, first combine the traces (saved as NetCDF files) using <code>combine_traces()</code> in <code>stratmc.data</code>.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Name of the proxy; only required if multiple proxies were included in the inference model.

Returns

median_residuals: np.array of float

Residuals between the median inferred proxy value (at each time in ages passed to $get_trace()$) calculated using 1 to N-1 chains versus all N chains. Shape is (chains x ages).

stratmc.inference.count_samples(full_trace, time_grid=None)

Helper function for *proxy_data_density()* in *stratmc.plotting*. Counts the number of observations within discrete time bins (based on the posterior sample ages).

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Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

time_grid: np.array, optional

Time bin edges; if not provided, defaults to the ages array passed to get_trace().

Returns

sample_counts: np.array

Number of observations in each time bin, summed over all posterior draws such that the average number of observations is sample_counts/n.

grid_centers: np.array

Time bin centers.

grid_widths: np.array

Time bin widths.

n: int

Number of posterior draws in full_trace.

stratmc.inference.extend_age_model(full_trace, sample_df, ages_df, new_proxies, new_proxy_df=None, **kwargs)

Extend age models to a different set of proxy observations using posterior sample ages from an existing inference. For instance, extend an age model built using C isotope data to new S isotope data collected from different stratigraphic horizons in the same sections. Note that the age of stratigraphic horizons that were included in sample_df (but marked Exclude? = True) is already passively tracked within the model; this function is only required to estimate the age of observations that were not in sample_df when the inference was run. To estimate ages for new measurements of the same proxy, place the new data in a different column (e.g., 'd13c_new').

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame with proxy data used during the inference step (as input to build_model() in stratmc.model).

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints used during the inference step (as input to build_model() in stratmc.model).

new_proxies: str or list(str)

New proxy(s) to construct age models for.

new_proxy_df: pandas.DataFrame, optional

pandas.DataFrame containing new proxy observations. Optional; if not provided, uses sample_df (assumes that observations for the new proxy are in the same DataFrame as the original proxy observations).

sections: list(str) or numpy.array(str), optional

List of sections included in the inference; only required if not all sections in sample_df were included.

Returns

interpolated_df: pandas.DataFrame

pandas.DataFrame with interpolated age draws and sample age summary statistics (maximum likelihood estimate, median, and 68% and 95% confidence intervals) for each new proxy observation.

stratmc.inference.find_gaps(full_trace, time_grid=None)

Helper function for *proxy_data_gaps()* in *stratmc.plotting*. Counts the number of draws from the posterior where there are no observations within discrete time bins (based on the posterior sample ages).

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

time_grid: np.array, optional

Time bin edges; if not provided, defaults to the ages array passed to get_trace().

Returns

age_gaps: np.array of int

Number of posterior draws where there are no observations; each entry corresponds to an age bin (corresponding to grid_centers and grid_widths).

grid centers: np.array

Time bin centers.

grid_widths: np.array

Time bin widths.

n: int

Number of posterior draws in full_trace.

```
stratmc.inference.get_trace(model, gp, ages, sample_df, ages_df, proxies=['d13c'], approximate=False, name=", chains=8, draws=1000, tune=2000, prior_draws=1000, target_accept=0.9, sampler='numpyro', nuts_kwargs=None, jitter=0.001, seed=None, save=True, postprocessing_backend=None, **kwargs)
```

Sample the prior and posterior distributions for a pymc.model.core.Model returned by build_model() in stratmc.model. By default, uses pymc.sampling.jax.sample_numpyro_nuts() to sample the posterior; change sampler to 'blackjax` to use pymc.sampling.jax.sample_blackjax_nuts().

After the posterior has been sampled, runs <code>check_inference()</code> in <code>stratmc.tests</code> to check that superposition is never violated in the posterior. Any chains with superposition violations are removed from the trace with <code>drop_chains()</code> before it is returned (if <code>save = True</code>, both the original and 'cleaned' traces are saved to the <code>traces</code> subfolder), and a warning is issued. See <code>check_inference()</code> for details; superposition issues are rare, and typically are related to minor violations of detrital or intrusive age constraints.

Problems during sampling, including frequent divergences or minor violations of limiting age constraints, might be resolved by increasing the number of tune steps and/or increasing target_accept (which decreases the step size).

Parameters

model: PyMC model

pymc.model.core.Model object returned by build_model() in stratmc.model.

gp: pymc.gp.Latent

Gaussian process prior (pymc.gp.Latent or pymc.gp.HSGP) returned by build_model() in stratmc.model.

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ages: numpy.array(float)

array of ages at which to sample the posterior distribution of the proxy signal.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas. DataFrame containing age constraints for all sections.

sections:: list(str) or numpy.array(str), optional

List of sections to include in the inference model. Defaults to all sections in sample_df.

proxies: str or list(str), optional

List of proxies included in the model. Defaults to 'd13c'.

approximate: bool, optional

Set to True if the Hilbert space GP approximation (pymc.gp.HSGP) was used in build_model(); defaults to False.

name: str, optional

Prefix for the saved NetCDF file with the inference results (suffix is timestamp for function call).

chains: int, optional

Number of Markov chains to sample in parallel; defaults to 8.

draws: int, optional

Number of samples per chain to draw from the posterior; defaults to 1000.

tune: int, optional

Number of iterations to tune; defaults to 1000.

prior_draws: int, optional

Number of samples to draw from the prior; defaults to 1000.

target_accept: float, optional

Between 0 and 1 (exclusive). During tuning, the sampler adapts the proposals such that the average acceptance probability is equal to target_accept; higher values for target_accept typically lead to smaller step sizes. Defaults to 0.9.

sampler: str, optional

Which NUTS algorithm to use to sample the posterior ('numpyro' or 'blackjax'); defaults to 'numpyro'.

nuts_kwargs: dict, optional

Dictionary of keyword arguments passed to NumPyro NUTS sampler (see pymc.sampling.jax.sample_numpyro_nuts() and numpyro.infer.hmc.NUTS) or blackjax NUTS sampler (see pymc.sampling.jax.sample_blackjax_nuts()).

jitter: float, optional

Value of jitter passed to pymc.gp.Latent.conditional(). Defaults to 0.001. Changing this value may help if a linear algebra error is encountered during posterior predictive sampling.

postprocessing_backend: str, optional

Use the cpu' or 'gpu' for postprocessing. Defaults to 'None'.

seed: int, optional

Random seed for sampler.

save: bool, optional

Whether to save the trace (to 'traces' subfolder in the current directory); defaults to True.

Returns

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples.

stratmc.inference.interpolate_proxy(interp_df, proxy, ages)

Use interpolated sample ages from <code>extend_age_model()</code> to calculate proxy values at a given set of ages (e.g., to plot 68 and 95% confidence intervals over time for a new proxy using <code>interpolated_proxy_inference()</code> in <code>stratmc.plotting()</code>.

Parameters

interp_df: pandas.DataFrame

pandas.DataFrame with proxy data and interpolated ages from extend_age_model().

proxy: str

Tracer to interpolate.

ages: list(float) or numpy.array(float)

Target ages at which to interpolate proxy values.

Returns

interpolated_proxy_df: pandas.DataFrame

pandas.DataFrame with interpolated proxy values and summary statistics (maximum likelihood estimate, median, and 68% and 95% confidence intervals) at each age in ages.

Helper function for <code>section_proxy_signal()</code> in <code>stratmc.plotting</code>. Maps the ages array passed to <code>get_trace()</code> to height in each section using the most likely posterior age models.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

include_radiometric_ages: bool, optional

Whether to consider radiometric ages when calculating the most likely posterior age model for each section: defaults to False.

sections: list(str) or numpy.array(str), optional

List of sections included in the inference; only required if not all sections in sample_df were included.

Returns

age_model_df: pandas.DataFrame

pandas. DataFrame with interpolated heights at each age in the ages vector that was passed to $get_trace()$.

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4.4 Plotting

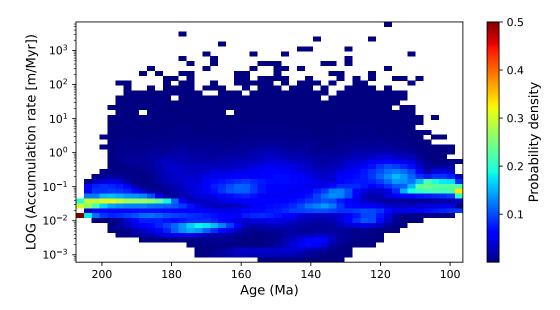
Functions for plotting the input data, inference results, and convergence/stability metrics.

chains are considered compared to when 1 to N-1 chains

proxy_strat	Plot stratigraphic data (proxy observations and age constraints) for each section.
proxy_inference	Plot the inferred proxy signal over time.
<pre>interpolated_proxy_inference</pre>	Plot interpolated proxy signal over time (by extending the posterior section age models to a new proxy not included in the inference model) using interpolated age models from <code>extend_age_model()</code> and interpolated proxy values from <code>interpolate_proxy()</code> in <code>stratmc.inference</code> .
age_height_model	Generate a posterior age-height plot for each section.
section_proxy_signal	Map the posterior proxy signal back to height in each section (using its most likely posterior age model), and plot alongside the proxy observations (plotted by most likely posterior age).
covariance_hyperparameters	Plot prior and posterior distributions for the lengthscale (ℓ) and variance (σ) hyperparameters of the pymc.gp. cov.ExpQuad Gaussian process covariance kernel:
section_summary	For a given section, plot posterior estimates of sample age, sedimentation rate, noise, and offset.
noise_summary	Plot posterior noise distributions for each section or group of samples (depending on noise_type used in build_model()) for a given proxy.
offset_summary	Plot posterior offset distributions for each section or group of samples (depending on offset_type used in build_model()).
section_proxy_residuals	Plot the residuals between the observed proxy values for each section and the inferred proxy signal (using the posterior section age models to map the signal back to height in section).
sample_ages	Plot sample age prior and posterior distributions for a given section.
sample_ages_per_chain	Plot sample age posterior distributions for a given section, with separate distributions for each chain.
age_constraints	For a given section, plot prior and posterior age distri- butions for all depositional age constraints (and limiting age constraints that provide a minimum or maximum age for the entire section).
limiting_age_constraints	For a given section, plot prior and posterior age distribu- tions for all intermediate limiting (i.e., detrital and intru- sive ages in the middle of a section) age constraints.
sadler_plot	Plot accumulation rate against duration.
accumulation_rate_stratigraphy	Plot the probability density of sediment accumulation rates (calculated between successive samples) through time.
section_age_range	Plot the stratigraphic interval corresponding to a given age range (based on the posterior section age models).
proxy_data_gaps	For a set of discrete time bins, shows the number of draws from the posterior where there are no proxy observations (i.e., where there are temporal <i>gaps</i> in the proxy data).
proxy_data_density	Plot the mean number proxy observations in discrete time bins (averaged over all posterior draws).
lengthscale_traceplot lengthscale_stability	Generate trace plot (parameter value vs. Plot the posterior standard deviation of the pymc.gp.
4.4. Plotting	cov.ExpQuad covariance kernel lengthscale when 1 through N chains are considered
proxy_signal_stability	through <i>N</i> chains are considered. 27 Plot the sum (over all time slices) of the residuals be-
proxy_signar_stability	tween the median inferred proxy signal when all N chains are considered compared to when 1 to N-1 chains

stratmc.plotting.accumulation_rate_stratigraphy(full_trace, sample_df, ages_df, age_bins=50, age_bin_edges=[], rate_bins=50, rate_bin_edges=[], rate_scale='log', include_age_constraints=True, cmap='jet', figsize=(8, 4), **kwargs)

Plot the probability density of sediment accumulation rates (calculated between successive samples) through time. Probability density for each age bin sums to 1. Unless a sections argument is passed, includes accumulation rates for all sections.



Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

age_bins: int, optional

Number of bin edges for age data (if age_bin_edges not provided). Defaults to 50.

rate_bins: int, optional

Number of bin edges for rate data (if rate_bin_edges not provided). Defaults to 50.

age_bin_edges: list(float) or numpy.array(float), optional

List or array of bin edges for the age data.

rate_bin_edges: list(float) numpy.array(float), optional

List or array of bin edges for the rate data.

rate_scale: str, optional

Scaling for rate ('linear' or 'log'). Defaults to 'log'.

include age constraints: bool, optional

Include age constraints in sedimentation rate calculations. Defaults to True.

sections: list(str) or numpy.array(str), optional

Section(s) to include. If not provided, combines data from all sections in sample_df.

Returns

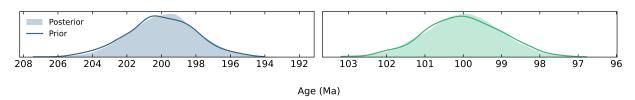
fig: matplotlib.pyplot.figure

Figure with accumulation rate probability density through time.

stratmc.plotting.age_constraints(full_trace, section, cmap='viridis', **kwargs)

For a given section, plot prior and posterior age distributions for all depositional age constraints (and limiting age constraints that provide a minimum or maximum age for the entire section). To plot intermediate limiting ages (i.e., detrital and intrusive age constraints in the middle of a section), use <code>limiting_age_constraints()</code>.

Section: 1



Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

section: str

Name of target section.

cmap: str, optional

Name of seaborn color palette to use for age distributions. Defaults to 'viridis'.

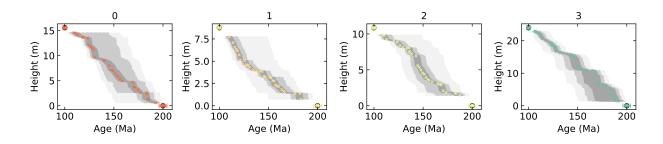
Returns

fig: matplotlib.pyplot.figure

Figure with prior and posterior depositional age constraint distributions.

stratmc.plotting.age_height_model(sample_df, ages_df, full_trace, include_excluded_samples=True, plot_samples=True, cmap='Spectral', legend=False, **kwargs)

Generate a posterior age-height plot for each section.



Parameters

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

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ages df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sections: list(str) or numpy.array(str), optional

List of sections to plot. Defaults to all sections in sample_df.

cmap: str, optional

Name of seaborn color palette to use for sections. Defaults to 'Spectral'.

legend: bool, optional

Generate a legend. Defaults to False.

include_excluded_samples: bool, optional

Whether to consider excluded samples (Exclude? is True in sample_df) whose ages were passively tracked in the inference model. Defaults to True.

plot_samples: bool, optional

Plot proxy observations by most likely posterior age. Defaults to True.

Returns

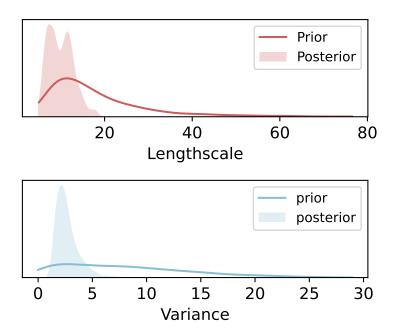
fig: matplotlib.pyplot.figure

Figure with age-height models for each section.

stratmc.plotting.covariance_hyperparameters(full_trace, figsize=(4, 3.5), **kwargs)

Plot prior and posterior distributions for the lengthscale (ℓ) and variance (σ) hyperparameters of the pymc . gp . cov . ExpQuad Gaussian process covariance kernel:

$$k(x, x') = \sigma^2 \exp\left[-\frac{(x - x')^2}{2\ell^2}\right]$$



Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Tracer to plot model parameters for (each proxy has a different covariance kernel); only required if more than one proxy was included in the inference.

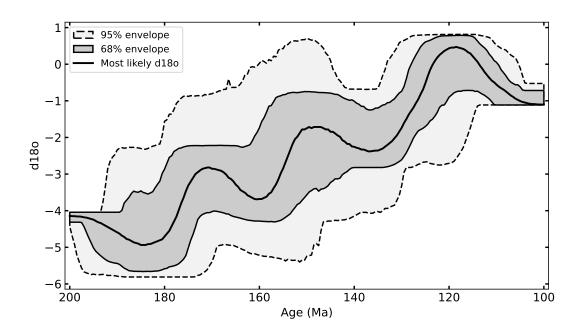
Returns

fig: matplotlib.pyplot.figure

Figure with prior and posterior model parameters.

stratmc.plotting.interpolated_proxy_inference(interpolated_df, interpolated_proxy_df, proxy, legend=True, plot_samples=False, plot_mle=True, orientation='horizontal', section_legend=False, marker_size=20, section_cmap='Spectral', **kwargs)

Plot interpolated proxy signal over time (by extending the posterior section age models to a new proxy not included in the inference model) using interpolated age models from <code>extend_age_model()</code> and interpolated proxy values from <code>interpolate_proxy()</code> in <code>stratmc.inference</code>.



Parameters

interpolated_df: pandas.DataFrame

pandas.DataFrame with interpolated age draws and sample age summary statistics from extend_age_model() in stratmc.inference.

interpolated_proxy_df: pandas.DataFrame

pandas.DataFrame with interpolated proxy values and summary statistics at target ages from <code>interpolate_proxy()</code> in <code>stratmc.inference</code>.

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proxy: str

Name of new proxy (must match column name in interpolated_proxy_df).

legend: bool, optional

Generate a legend. Defaults to True.

plot samples: bool, optional

Plot proxy observations by most likely posterior age. Defaults to False.

plot mle: bool, optional

Plot the maximum likelihood estimate. Defaults to True.

orientation: str, optional

Orientation of figure ('horizontal' or 'vertical'). Defaults to 'horizontal'.

marker_size: int, optional

Size of markers if plot_samples is True. Defaults to 20.

section_legend: bool, optional

Include section names in the legend (if plot_samples is True). Defaults to False.

section cmap: str, optional

Name of seaborn color palette to use for sections (if plot_samples is True). Defaults to 'Spectral'.

Returns

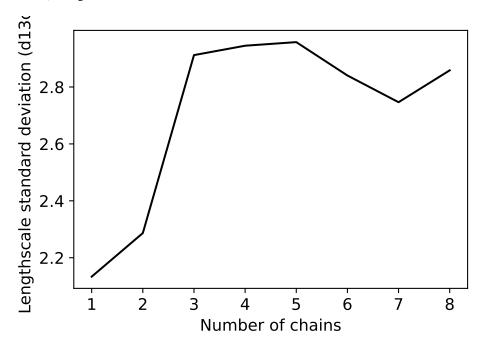
fig: matplotlib.pyplot.figure

Figure with interpolated proxy signal over time.

stratmc.plotting.lengthscale_stability(full_trace, figsize=(5, 3.5), **kwargs)

Plot the posterior standard deviation of the pymc.gp.cov.ExpQuad covariance kernel lengthscale when 1 through N chains are considered. When the posterior has been sufficiently explored, the standard deviation will stabilize; if it has not stabilized, then additional chains should be run.

To consider chains from multiple traces associated with the same inference model, first combine the traces (saved as NetCDF files) using <code>combine_traces()</code> in <code>stratmc.data</code>.



full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

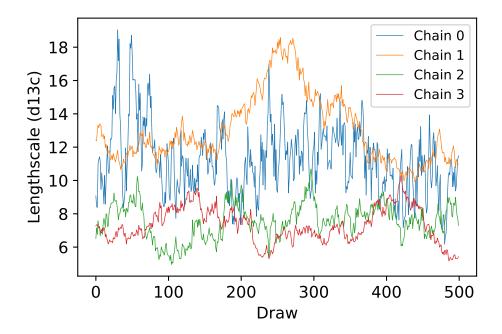
Returns

fig: matplotlib.pyplot.figure

Figure showing the standard deviation of the covariance kernel lengthscale hyperparameter posterior for 1 through N chains.

stratmc.plotting.lengthscale_traceplot(full_trace, chains=None, legend=True, figsize=(5, 3.5), **kwargs)

Generate trace plot (parameter value vs. step in Markov chain) for the pymc.gp.cov.ExpQuad covariance kernel lengthscale. By default, includes all chains; to plot the draws for only a subset of chains, past list of chain indices to chains. Use to check for posterior multimodality.



Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

chains: list(int) or numpy.array(int); optional

Indices of chains to plot; optional (defaults to all chains).

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

legend: bool, optional

Generate a legend. Defaults to True.

Returns

fig: matplotlib.pyplot.figure

Figure with lengthscale trace plot.

stratmc.plotting.limiting_age_constraints(full_trace, sample_df, ages_df, section, cmap='viridis', **kwargs)

For a given section, plot prior and posterior age distributions for all intermediate limiting (i.e., detrital and intrusive ages in the middle of a section) age constraints. To plot depositional age constraints (and limiting age constraints that provide a minimum or maximum age for the entire section), use age_constraints().

Section: 1 Detrital 0 Detrital 1 Intrusive 0 Posterio Prior 445.0 442.5 440.0 437.5 435.0 430 425 420 430 425 420 415 405 435 410

Age (Ma)

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

section: str

Name of target section.

cmap: str, optional

Name of seaborn color palette to use for age distributions. Defaults to 'viridis'.

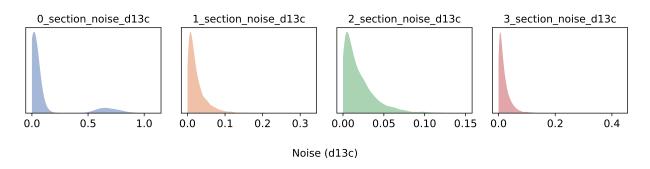
Returns

fig: matplotlib.pyplot.figure

Figure with prior and posterior limiting age constraint distributions.

stratmc.plotting.noise_summary(full_trace, **kwargs)

Plot posterior noise distributions for each section or group of samples (depending on noise_type used in <code>build_model()</code>) for a given proxy. If multiple proxies were included in the inference, pass a proxy argument to specify which noise terms to plot.



full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace in stratmc.inference.

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

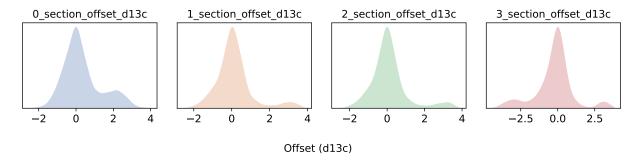
Returns

fig: matplotlib.pyplot.figure

Figure with noise distributions for each section or group of samples.

stratmc.plotting.offset_summary(full_trace, **kwargs)

Plot posterior offset distributions for each section or group of samples (depending on offset_type used in build_model()). If multiple proxies were included in the inference, pass a proxy argument to specify which offset terms to plot.



Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

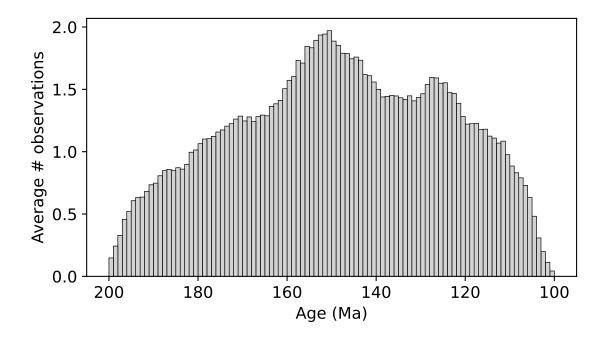
Returns

fig: matplotlib.pyplot.figure

Figure with offset distributions for each section or group of samples.

$\verb|stratmc.plotting.proxy_data_density| (full_trace, time_grid=None, figsize=(6, 3.5), **kwargs)|$

Plot the mean number proxy observations in discrete time bins (averaged over all posterior draws). This plot can be used to determine where proxy observations are relatively sparse, and additional observations may improve the inference.



full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

time_grid: np.array, optional

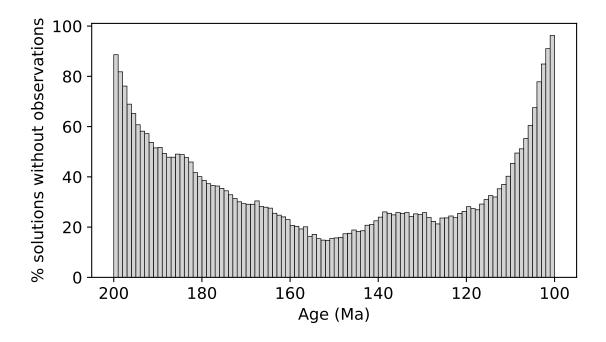
Time bin edges; if not provided, defaults to the ages array passed to get_trace().

Returns

fig: matplotlib.pyplot.figure

Figure with bar plot of mean number of observations in each time bin.

For a set of discrete time bins, shows the number of draws from the posterior where there are no proxy observations (i.e., where there are temporal *gaps* in the proxy data). This plot can be used to determine where additional observations are needed to improve the inference.



full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

time_grid: np.array, optional

Time bin edges; if not provided, defaults to the ages array passed to get_trace().

yaxis: str, optional

Set y-axis to percentage of posterior draws without observations ('percentage') or to the number of posterior draws without observations ('count'). Defaults to 'percentage'.

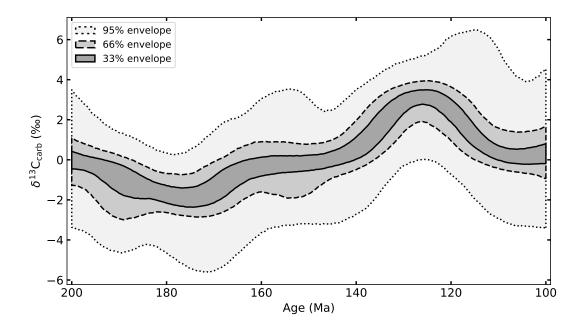
Returns

fig: matplotlib.pyplot.figure

Figure with bar plot of number of posterior draws with gaps for each time bin.

stratmc.plotting.proxy_inference(sample_df, ages_df, full_trace, legend=True, plot_constraints=False, plot_samples=False, plot_excluded_samples=False, plot_mean=False, plot_mle=False, orientation='horizontal', marker_size=20, section_legend=False, section_cmap='Spectral', **kwargs')

Plot the inferred proxy signal over time.



sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Tracer to plot; only required if more than one proxy was included in the inference.

legend: bool, optional

Generate a legend. Defaults to True.

plot_constraints: bool, optional

Plot age constraints for each section as dashed lines. Defaults to False.

plot_samples: bool, optional

Plot proxy observations by most likely posterior age. Defaults to False.

plot_excluded_samples: bool, optional

Plot proxy observations that were excluded from the inference (Exclude? is True in sample_df). Defaults to False.

plot_mean: bool, optional

Plot the mean as a dashed line. Defaults to False.

plot_mle: bool, optional

Plot the maximum likelihood estimate. Defaults to False.

orientation: str, optional

Orientation of figure ('horizontal' with age on the x-axis, or 'vertical' with age on the y-axis). Defaults to 'horizontal'.

marker size: int, optional

Size of markers if plot_samples is True. Defaults to 20.

section_legend: bool, optional

Include section names in the legend (if plot_samples is True). Defaults to False.

section cmap: str, optional

Name of seaborn color palette to use for sections (if plot_samples is True). Defaults to 'Spectral'.

Returns

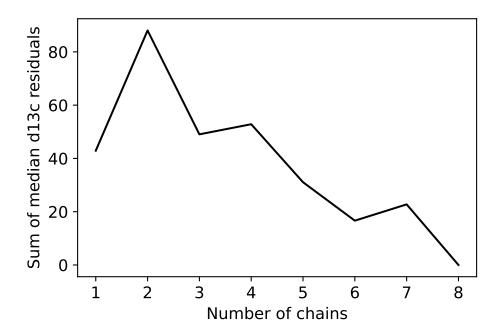
fig: matplotlib.pyplot.figure

Figure with the proxy signal inference.

stratmc.plotting.proxy_signal_stability(full_trace, figsize=(5, 3.5), **kwargs)

Plot the sum (over all time slices) of the residuals between the median inferred proxy signal when all N chains are considered compared to when 1 to N-I chains are considered. When the posterior has been sufficiently explored, the residuals will stabilize and approach zero; if they have not stabilized, then additional chains should be run.

To consider chains from multiple traces associated with the same inference model, first combine the traces (saved as NetCDF files) using <code>combine_traces()</code> in <code>stratmc.data</code>.



Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

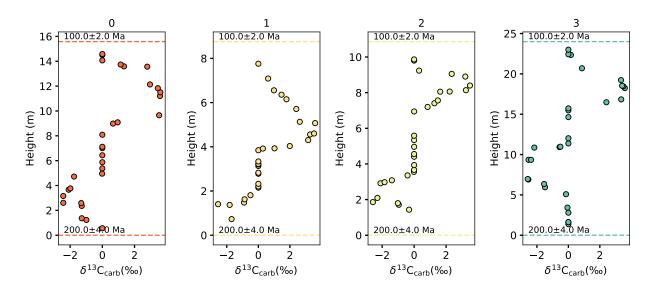
Returns

fig: matplotlib.pyplot.figure

Figure showing the stability of the proxy signal inference.

stratmc.plotting.proxy_strat(sample_df, ages_df, proxy='d13c', plot_constraints=True, plot_excluded_samples=False, cmap='Spectral', legend=False, **kwargs)

Plot stratigraphic data (proxy observations and age constraints) for each section.



Parameters

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

proxy: str, optional

Name of proxy. Defaults to 'd13c'.

sections: list(str) or numpy.array(str), optional

List of sections to plot. Defaults to all sections in sample_df.

plot_constraints: bool, optional

Whether to plot age constraints as dashed lines. Ages are printed above dashed lines by defalut; to turn off age labels, pass print_ages = False.

plot excluded samples: bool, optional

Whether to plot proxy observations for excluded samples (Exclude? is True in sample_df) as red dots. Defaults to False.

cmap: str, optional

Name of seaborn color palette to use for sections. Defaults to 'Spectral'.

legend: bool, optional

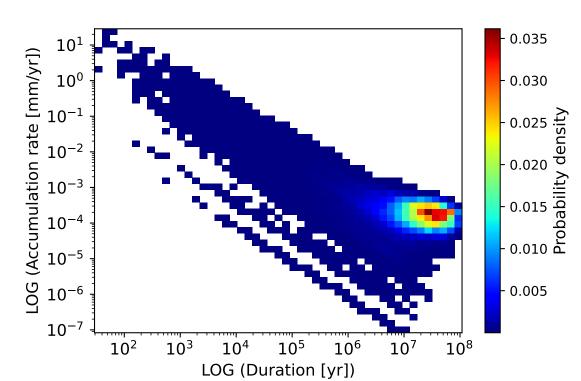
Generate a legend. Defaults to False.

Returns

fig: matplotlib.pyplot.figure

Figure with observations for each section.

stratmc.plotting.sadler_plot(full_trace, sample_df, ages_df, method='density', duration_bins=50, rate_bins=50, scale='log', include_age_constraints=True, density_cmap='jet', section_cmap='Spectral', figsize=(6, 4), **kwargs')



Plot accumulation rate against duration.

Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

method: str, optional

Plot as a 2D histogram ('density') or as a scatter plot ('scatter'). The density plot will combine data for all sections in sections, while a scatter plot will assign a unique color to each section. Defaults to 'density'.

duration_bins: int, optional

Number of bin edges to use for the duration data. Defaults to 50.

rate_bins: int, optional

Number of bin edges to use for the rate data. Defaults to 50.

scale: str, optional

Scaling for x- and y-axes ('linear' or 'log'). Defaults to 'log'.

sections: list(str) numpy.array(str), optional

List of target sections. Defaults to all sections in sample_df.

include_age_constraints: bool, optional

Include age constraints in sedimentation rate calculations. Defaults to False.

density_cmap: str, optional

Name of matplotlib colormap to use for probability density if method is 'density'. Defaults to 'jet'.

section cmap: str, optional

Name of seaborn color palette to use for sections if method is 'scatter'. Defaults to 'Spectral'.

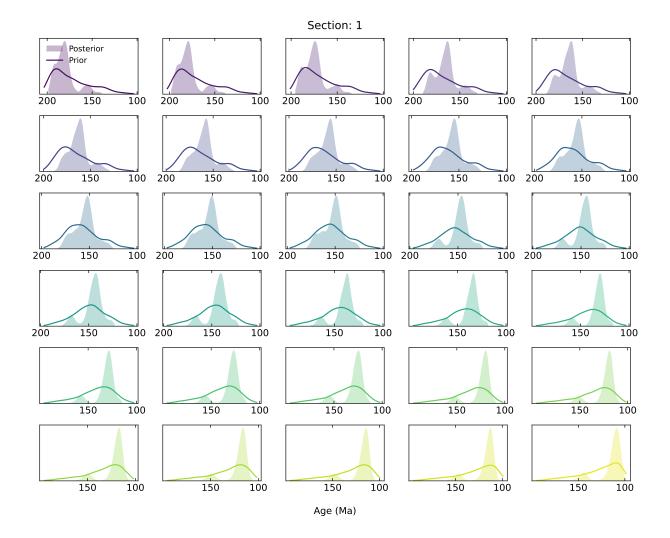
Returns

fig: matplotlib.pyplot.figure

Figure with sediment accumulation rate plotted against duration.

stratmc.plotting.sample_ages(full_trace, sample_df, section, plot_excluded_samples=False, cmap='viridis')

Plot sample age prior and posterior distributions for a given section. Each subplot contains posterior distributions for a different sample.



Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples

from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

section: str

Name of target section.

plot_excluded_samples: bool, optional

Plot age distributions for proxy observations that were excluded from the inference (Exclude? is True in sample_df). Defaults to False.

cmap: str, optional

Name of seaborn color palette to use for age distributions. Defaults to 'viridis'.

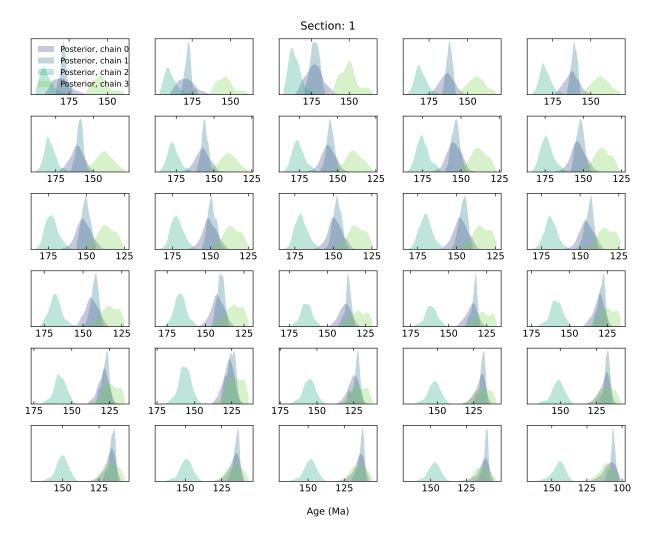
Returns

fig: matplotlib.pyplot.figure

Figure with prior and posterior sample age distributions.

stratmc.plotting.sample_ages_per_chain(full_trace, sample_df, section, chains=None, plot_prior=False, plot_excluded_samples=False, legend=True, cmap='viridis')

Plot sample age posterior distributions for a given section, with separate distributions for each chain. Each subplot contains posterior distributions for a different sample. Use to check for posterior multimodality (in this example, each chain has explored a different mode of the posterior age distributions).



full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

section: str

Name of target section.

chains: list(int) or numpy.array(int); optional

Indices of chains to include; optional (defaults to all chains).

plot_prior: bool, optional

Plot prior distributions for sample ages. Defaults to False.

plot_excluded_samples: bool, optional

Plot age distributions for proxy observations that were excluded from the inference (Exclude? is True in sample_df). Defaults to False.

legend: bool, optional

Generate a legend. Defaults to True.

cmap: str, optional

Name of seaborn color palette to use for different chains. Defaults to 'viridis'.

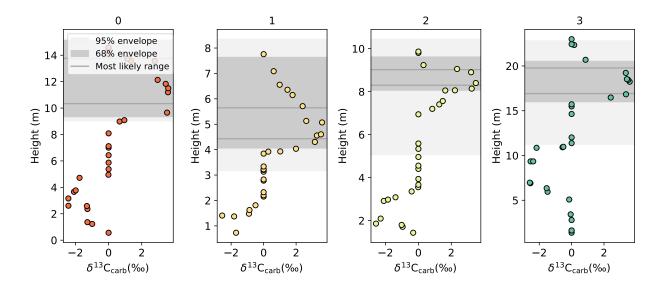
Returns

fig: matplotlib.pyplot.figure

Figure with per-chain posterior sample age distributions.

stratmc.plotting.section_age_range(full_trace, sample_df, ages_df, lower_age, upper_age, legend=True, section_cmap='Spectral', **kwargs)

Plot the stratigraphic interval corresponding to a given age range (based on the posterior section age models). If sections is not provided, includes each section that overlaps the target age range.



Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

lower_age: float

Lower bound (youngest) of the target age interval.

upper_age: float

Upper bound (oldest) of the target age interval.

legend: bool, optional

Generate a legend. Defaults to True.

cmap: str, optional

Name of seaborn color palette to use for sections. Defaults to 'Spectral'.

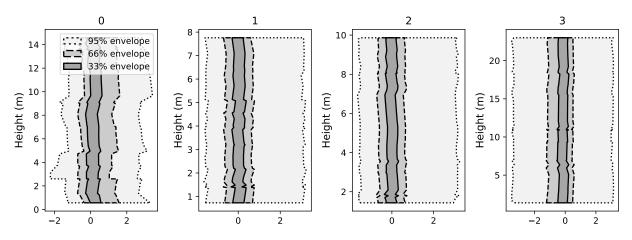
Returns

fig: matplotlib.pyplot.figure

Tracer stratigraphy for each section, with the stratigraphic interval corresponding to the input age range highlighted.

 $stratmc.plotting.section_proxy_residuals(full_trace, sample_df, legend=True, cmap='Spectral', \\ plot_mle=False, include_excluded_samples=False, **kwargs)$

Plot the residuals between the observed proxy values for each section and the inferred proxy signal (using the posterior section age models to map the signal back to height in section). Use to check for stratigraphic trends in the residuals, which may give insight to the processes that cause noisy sections to deviate from the inferred common signal. If multiple proxies were included in the inference, pass a proxy argument.



Residual d13c value (observed - predicted)

Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

legend: bool, optional

Generate a legend. Defaults to True.

cmap: str, optional

Name of seaborn color palette to use for sections. Defaults to 'Spectral'.

plot_mle: bool, optional

Plot the maximum likelihood estimate as a line. Defaults to False.

proxy: str, optional

Target proxy; only required if more than one proxy was included in the inference.

include_excluded_samples: bool, optional

Whether to plot the residuals for samples that were excluded from the inference (Exclude? is True in sample_df). Defaults to False.

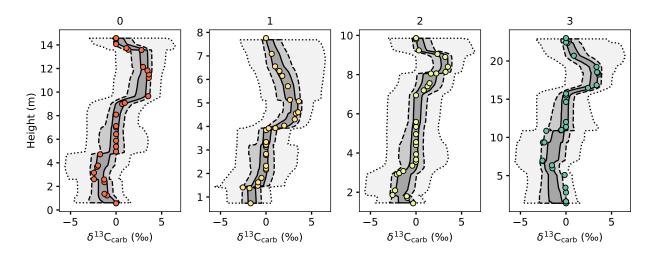
Returns

fig: matplotlib.pyplot.figure

Figure with residuals for each section.

stratmc.plotting.section_proxy_signal(full_trace, sample_df, ages_df, include_radiometric_ages=False, plot_constraints=False, plot_mle=False, yax='height', legend=False, cmap='Spectral', **kwargs)

Map the posterior proxy signal back to height in each section (using its most likely posterior age model), and plot alongside the proxy observations (plotted by most likely posterior age).



Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

include_radiometric_ages: bool, optional

Whether to consider radiometric ages in the posterior age model for each section. Defaults to False.

plot constraints: bool, optional

Plot age constraints for each section as dashed lines. Defaults to False.

plot mle: bool, optional

Plot the maximum likelihood estimate for the proxy signal as a line. Defaults to False.

yax: str, optional

Scale for the y-axis ('height' or 'age'). Defaults to 'height'.

legend: bool, optional

Generate a legend. Defaults to True.

cmap: str, optional

Name of seaborn color palette to use for sections. Defaults to 'Spectral'.

proxy: str, optional

Tracer to plot; only required if more than one proxy was included in the inference.

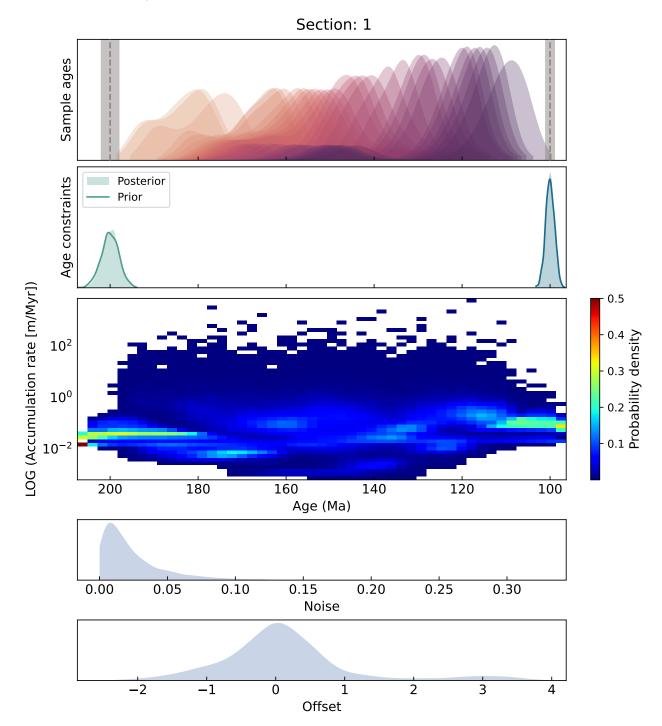
Returns

fig: matplotlib.pyplot.figure

Figure with inferred proxy signal mapped to height in each section.

stratmc.plotting.section_summary(sample_df, ages_df, full_trace, section, plot_excluded_samples=False, plot_noise_prior=False, plot_offset_prior=False, include_age_constraints_sedrate=True, figsize=(8, 9))

For a given section, plot posterior estimates of sample age, sedimentation rate, noise, and offset. Noise and offset terms must be either per-section or global; to plot per-sample noise and offset terms, use <code>noise_summary()</code> and <code>offset_summary()</code>.



sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

section: str

Name of target section.

plot_excluded_samples: bool, optional

Plot age estimates for proxy observations that were excluded from the inference (Exclude? is True in sample_df). Defaults to False.

plot_noise_prior: bool, optional

Plot prior distribution for noise term. Defaults to False.

plot_offset_prior: bool, optional

Plot prior distribution for offset term. Defaults to False.

include_age_constraints_sedrate: bool, optional

Include age constraints in sedimentation rate calculations. Defaults to True.

Returns

fig: matplotlib.pyplot.figure

Figure summarizing posterior sample ages, sedimentation rate, and posterior noise and offset terms for the input section.

4.5 Tools for generating synthetic data

Functions for creating synthetic proxy signals/stratigraphic observations and evaluating model performance for synthetic tests.

make_excursion	Function for generating a synthetic proxy signal that contains a number of user-specified excursions.
synthetic_sections	Function for generating synthetic proxy observations and age constraints using a predefined proxy signal.
synthetic_observations_from_prior	Given age constraints for a set of stratigraphic sections in ages_df, generate synthetic proxy observations by sampling the model prior.
synthetic_signal_from_prior	Draws synthetic signals from the model prior, and returns the signal conditioned over the points in ages.
quantify_signal_recovery	Calculates the likelihood of the true proxy signal (for synthetic tests, where the true signal is known) conditioned on the posterior (default) or prior proxy signal inference.
sample_age_recovery	Calculates the likelihood of the true sample ages (for synthetic tests, where the true age of each sample is known) given draws from the posterior (default) or prior.
sample_age_residuals	Calculates the residual (for each draw) between the true age and the posterior (default) or prior age of each sample.
synthetic_signal_to_df	Helper function for generating artificial sample and age data using <i>synthetic_sections()</i> .

stratmc.synthetics.make_excursion(time, amplitude, baseline=0, rising_time=None, rate_offset=True, excursion_duration=None, min_duration=1, smooth=False, smoothing_factor=10, seed=None)

Function for generating a synthetic proxy signal that contains a number of user-specified excursions.

Parameters

time: numpy.array(float)

Time vector over which to generate proxy signal.

amplitude: float, list(float), or numpy.array(float)

Amplitude of excursion; pass a list or array to generate multiple excursions.

baseline: float, optional

Baseline proxy value. Defaults to 0.

rising_time: float, list(float), or numpy.array(float), optional

Fraction of excursion duration spent on the rising limb (linear increase/decrease toward peak). Must be between 0 and 1. If not provided, randomly generated if rate_offset is True and set to 0.5 if rate_offset is False. Pass a list to specify different rising times for each excursion.

rate_offset: bool, optional

If False, rising and falling limbs of excursion have equal duration. If True, the fraction of the excursion duration spent on the rising limb is set by rising_time. Defaults to False.

excursion_duration: float, list(float), or numpy.array(float), optional

Duration of excursion; pass a list or array to generate multiple excursions. Random if not provided.

min duration: float, optional

Minimum excursion duration if excursion_duration is not provided. Defaults to 1.

smooth: bool, optional

Whether to smooth excursion peaks. Defaults to False.

smoothing_factor: float, optional

Smoothing factor if smooth is True; higher values produce smoother signals. Defaults to 10.

seed: int, optional

Random seed used to generate signal.

Returns

interp proxy: np.array

Tracer signal interpolated to points in the time vector

stratmc.synthetics.quantify_signal_recovery(full_trace, true_signal, proxy='d13c', mode='posterior')

Calculates the likelihood of the true proxy signal (for synthetic tests, where the true signal is known) conditioned on the posterior (default) or prior proxy signal inference. The likelihood is evaluated at each age (the posterior signal and the true signal must be evaluated at the same ages). Provides a measure of signal recovery.

Parameters

full_trace: arviz.InferenceData or list(arviz.InferenceData)

An arviz.InferenceData object containing the full set of prior and posterior samples from <code>get_trace()</code> in <code>stratmc.inference</code>. If passed as a list, the posterior draws for all traces will be combined when calculating <code>posterior_likelihood</code>.

true signal: np.array

True values for the proxy signal, evaluated at the same ages as the posterior signal in full_trace.

proxy: str, optional

Tracer signal to evaluate. Defaults to 'd13c'.

mode: str, optional

Whether to use the posterior or prior to calculate signal recovery. Defaults to 'posterior'.

Returns

posterior_likelihood: np.array

Array of posterior likelihoods (evaluated at each age).

stratmc.synthetics.sample_age_recovery(full_trace, sample_df, sections=None, mode='posterior')

Calculates the likelihood of the true sample ages (for synthetic tests, where the true age of each sample is known) given draws from the posterior (default) or prior. Provides a measure of age model recovery.

Parameters

full trace: arviz.InferenceData or list(arviz.InferenceData)

An arviz.InferenceData object containing the full set of prior and posterior samples from <code>get_trace()</code> in <code>stratmc.inference</code>. If passed as a list, the posterior draws for all traces will be combined when calculating <code>posterior_likelihood</code>.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for synthetic sections.

sections: list(str) or numpy.array(str), optional

List of sections to evaluate. Defaults to all sections in sample_df.

mode: str, optional

Whether to use the posterior or prior age models. Defaults to 'posterior'.

Returns

posterior_likelihood: dict{float} or np.array(float)

Posterior likelihoods for the true age of each sample. Returned as an array if only one section is evaluated, or a dictionary of arrays if multiple sections are evaluated.

stratmc.synthetics.sample_age_residuals(full_trace, sample_df, sections=None, mode='posterior')

Calculates the residual (for each draw) between the true age and the posterior (default) or prior age of each sample.

Parameters

full trace: arviz.InferenceData or list(arviz.InferenceData)

An arviz.InferenceData object containing the full set of prior and posterior samples from <code>get_trace()</code> in <code>stratmc.inference</code>. If passed as a list, the posterior draws for all traces will be combined when calculating <code>age_residuals</code>.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for synthetic sections.

sections: list(str) or numpy.array(str), optional

List of sections to evaluate. Defaults to all sections in sample_df.

mode: str, optional

Whether to use the posterior or prior age models. Defaults to 'posterior'.

Returns

age_residuals: np.array or dict{np.array}

Sample age residuals; shape is (number of samples, number of posterior draws). Returned as an array if only one section is evaluated, or a dictionary of arrays if multiple sections are evaluated.

 $\verb|stratmc.synthetics.synthetic_observations_from_prior(|age_vector, |ages_df|, |sample_heights=None, |ages_df|)| | |stratmc.synthetics.synthetic_observations_from_prior(|age_vector, |ages_df|, |sample_heights=None, |ages_df|)| | |stratmc.synthetic_observations_from_prior(|age_vector, |ages_df|, |sample_heights=None, |ages_df|)| | |stratmc.synthetic_observations_from_prior(|age_vector, |ages_df|, |sample_heights=None, |ages_df|, |sample_heights=None, |ages_df|, |ages_df|, |ages_$

uniform_heights=False,
samples_per_section=20, proxies=['d13c'],
proxy_std=0.1, seed=None, ls_dist='Wald',
ls_min=0, ls_mu=20, ls_lambda=50,
ls_sigma=50, var_sigma=10,
white_noise_sigma=0.1, gp_mean_mu=0,
gp_mean_sigma=10, approximate=False,
hsgp_m=15, hsgp_c=1.3, offset_type='section',
offset_prior='Laplace', offset_alpha=0,
offset_beta=1, offset_sigma=1, offset_mu=0,
offset_b=2, noise_type='section',
noise_prior='HalfCauchy', noise_beta=1,
noise_sigma=1, noise_nu=1, jitter=0.001,
**kwargs)

Given age constraints for a set of stratigraphic sections in ages_df, generate synthetic proxy observations by sampling the model prior. Accepts all arguments that can be passed to <code>build_model()</code> in <code>stratmc.model</code>.

Parameters

age_vector: np.array(float)

Vector of ages at which to evaluate synthetic proxy signal(s).

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for synthetic sections.

sample_heights: dict{list(float) or numpy.array(float)}, optional

Sample heights for each stratigraphic section in ages_df; must be a dictionary with section

names as keys. Defaults to None, which results in either uniformly spaced or randomly spaced sample heights (depending on the uniform_heights argument).

uniform_heights: bool, optional

Whether to generate uniformly spaced (set to True) or randomly spaced (set to False) sample heights if dictionary of sample_heights not provided. Defaults to False (randomly spaced samples).

samples per section: int or dict(int), optional

Number of samples per section to generate if sample_heights not provided; either an integer (if the same for all sections) or a dictionary with section names as keys. Defaults to 20.

proxies: list(str), optional

List of proxies to generate synthetic observations for. Defaults to d13c.

proxy_std: float or dict(float), optional

Measurement uncertainty for each proxy; pass a dictionary of floats with the elements of proxies as keys to use a different value for each proxy, or an integer to use the same value for all proxies. Defaults to 0.1.

seed: int, optional

Seed to use while generating synthetic observations.

Returns

signals: dict(float)

Tracers signals drawn from the model prior (evaluated at the points in age_vector) used to generate synthetic observations; dictionary keys are proxies.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for synthetic stratigraphic sections.

prior: arviz.InferenceData

An arviz. InferenceData object containing the prior draw from the model used to generate synthetic observations.

model: pymc.Model

pymc.model.core.Model object used to generate synthetic observations.

```
stratmc.synthetics.synthetic_sections(true\_time, true\_proxy, num\_sections, num\_samples, max\_section\_thickness, proxies=['d13c'], noise=False, noise\_amp=0.1, min\_constraints=2, max\_constraints=3, seed=None, **kwargs)
```

Function for generating synthetic proxy observations and age constraints using a predefined proxy signal.

Parameters

true time: numpy.array(float)

True time vector for input signal.

true_proxy: numpy.array(float) or dict{numpy.array(float)}

True proxy vector for input signal. If generating synthetic data for multiple proxies, pass as a dictionary with proxy names as keys.

num sections: int

Number of synthetic sections to generate.

num_samples: int

Number of samples per synthetic section.

max section thickness: float

Maximum thickness of synthetic sections.

proxies: str or list(str), optional

Column name(s) for synthetic proxy observations in sample_df. Defaults to 'd13c'.

noise: bool, optional

Whether to add white noise to proxy observations. Defaults to False.

noise_amp: float or dict{float}, optional

Amplitude of white noise added to proxy observations (if noise is True). To specify a different noise amplitude for each proxy, pass as a dictionary with proxy names as keys. Defaults to 0.1.

min_constraints: int, optional

Minimum number of age constraints per synthetic section (must be at least 2). Defaults to 2.

max_constraints: int, optional

Maximum number of age constraints per synthetic section. Defaults to 3.

seed: int, optional

Random seed used to generate synthetic sections.

Returns

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for synthetic sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for synthetic sections.

```
stratmc.synthetics.synthetic\_signal\_from\_prior(ages, num\_signals=100, ls\_dist='Wald', ls\_min=0, ls\_mu=20, ls\_lambda=50, ls\_sigma=50, var\_sigma=10, gp\_mean\_mu=0, gp\_mean\_sigma=5, seed=None)
```

Draws synthetic signals from the model prior, and returns the signal conditioned over the points in ages. To generate both signals and synthetic stratigraphic sections, instead use <code>synthetic_observations_from_prior()</code>.

Parameters

ages: numpy.array(float)

Array of ages over which to condition the signal.

num_signals: int, optional

Number of signals to draw from prior. Defaults to 100.

ls dist: str, optional

Prior distribution for the lengthscale hyperparameter of the exponential quadratic covariance kernel (pymc.gp.cov.ExpQuad); set to Wald (pymc.Wald) or HalfNormal (pymc. HalfNormal). Defaults to Wald with mu = 20 and lambda = 50; to change mu and lambda, pass the ls_mu and ls_lambda parameters. For HalfNormal, the variance defaults to sigma = 50; change by passing ls_sigma.

ls_min: float, optional

Minimum value for the lengthscale hyperparameter of the pymc.gp.cov.ExpQuad covariance kernel; shifts the lengthscale prior by ls_min . Defaults to 0.

ls mu: float, optional

Mean (mu) of the pymc.gp.cov.ExpQuad lengthscale prior if ls_dist = `Wald`. Defaults to 20.

ls_lambda: float, optional

Relative precision (*lam*) of the pymc.gp.cov.ExpQuad lengthscale hyperparameter prior if ls_dist = `Wald`. Defaults to 50.

Is sigma: float, optional

Scale parameter (*sigma*) of the pymc.gp.cov.ExpQuad lengthscale hyperparameter prior if ls_dist = `HalfNormal`. Defaults to 50.

var_sigma: float, optional

Scale parameter (*sigma*') of the covariance kernel variance hyperparameter prior, which is a :class: 'pymc.HalfNormal distribution. Defaults to 10.

gp_mean_mu: float, optional

Mean (mu) of the GP mean function prior, which is a pymc. Normal distribution. Defaults to 0.

gp_mean_sigma: float, optional

Standard deviation (sigma) of the GP mean function prior, which is a pymc.Normal distribution. Defaults to 5.

seed: int, optional

Random seed used to generate signals.

Returns

signal: numpy.ndarray(float)

Array with shape ages x number of signals containing the $n = num_signals$ synthetic signals drawn from the prior.

stratmc.synthetics.synthetic_signal_to_df(proxy_vec, heights, section_ages, section_names, ages, age_std, age_heights, age_section_names, proxies=['d13c'])

Helper function for generating artificial sample and age data using *synthetic_sections()*.

Parameters

proxy_vec: np.array(float) or dict{np.array(float)}

Array of proxy observations. Pass as a dictionary if more than one proxy.

heights: np.array(float)

Array of heights corresponding to proxy observations in proxy_vec.

section_ages: np.array(float)

Array of ages corresponding to proxy observations in proxy_vec.

section_names: np.array(str)

Array of section names corresponding to proxy observations in proxy_vec.

ages: np.array(float)

Array of age constraints.

age_std: np.array(float)

Array of uncertainties for each age constraint in ages.

age_heights: np.array(float)

Array of heights for each age constraint in ages.

age_section_names: np.array(str)

Array of section names corresponding to age constraints in ages.

proxies: str or list(str), optional

Name(s) of proxies. Defaults to d13c.

Returns

sample df: pandas.DataFrame

pandas.DataFrame containing proxy data for synthetic sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for synthetic sections.

4.6 Tests and checks

Functions for checking that the inference model is working correctly.

check_inference	Master function (calls each of the functions in the tests module) for checking that superposition is never violated in the posterior.
check_superposition	Check that stratigraphic superposition between all age constriants and samples is respected in the posterior.
check_detrital_ages	Check that detrital age constraints have been enforced in the posterior.
check_intrusive_ages	Check that intrusive age constraints have been enforced in the posterior.

stratmc.tests.check_detrital_ages(full_trace, sample_df, ages_df, quiet=True, **kwargs)

Check that detrital age constraints have been enforced in the posterior.

Parameters

full_trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

sections: list(str) or numpy.array(str), optional

List of sections included in the inference. Defaults to all sections in sample_df.

quiet: bool, optional

Whether to print the section name and chain/draw of each superposition violation; defaults to False.

Returns

bad chains: numpy.array

Array of chain indices where superposition was violated in the posterior.

stratmc.tests.check_inference(full_trace, sample_df, ages_df, quiet=True, **kwargs)

Master function (calls each of the functions in the tests module) for checking that superposition is never violated in the posterior. Returns a list of chain indices where superposition was violated; these chains can be dropped from the trace using $drop_chains()$. Run automatically inside of $get_trace()$ in stratmc.inference.

Because of the likelihood penalty used to manually enforce detrital and intrusive ages in intermediate_detrital_potential() and intermediate_intrusive_potential() (called in build_model()), rare chains may have minor superposition violations when deterital/intrusive ages are present. These chains can simply be discarded. If superposition is frequently violated in a given section, or if

superposition violations are severe, check that the heights for all age constraints in ages_df are correct, and that the reported ages respect superposition. The model can correct for mean ages that are out of superposition, but may fail if the age constraints do not overlap given their 2\$sigma\$ uncertainties.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

sections: list(str) or numpy.array(str), optional

List of sections included in the inference. Defaults to all sections in sample_df.

quiet: bool, optional

Whether to print the type, section name, and chain/draw of each superposition violation; defaults to False.

Returns

bad_chains: numpy.array

Array of chain indices where superposition was violated in the posterior.

stratmc.tests.check_intrusive_ages(full_trace, sample_df, ages_df, quiet=True, **kwargs)

Check that intrusive age constraints have been enforced in the posterior.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

sample_df: pandas.DataFrame

pandas. DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

sections: list(str) or numpy.array(str), optional

List of sections included in the inference. Defaults to all sections in sample_df.

quiet: bool, optional

Whether to print the section name and chain/draw of each superposition violation; defaults to False.

Returns

bad_chains: numpy.array

Array of chain indices where superposition was violated in the posterior.

stratmc.tests.check_superposition(full_trace, sample_df, ages_df, quiet=True, **kwargs)

Check that stratigraphic superposition between all age constriants and samples is respected in the posterior.

Parameters

full trace: arviz.InferenceData

An arviz.InferenceData object containing the full set of prior and posterior samples from get_trace() in stratmc.inference.

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sample_df: pandas.DataFrame

pandas.DataFrame containing proxy data for all sections.

ages_df: pandas.DataFrame

pandas.DataFrame containing age constraints for all sections.

sections: list(str) or numpy.array(str), optional

List of sections included in the inference. Defaults to all sections in sample_df.

quiet: bool, optional

Whether to print the section name and chain/draw of each superposition violation; defaults to False.

Returns

bad_chains: numpy.array

Array of chain indices where superposition was violated in the posterior.

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