Cosmology Population Monte Carlo

CosmoPMC v1.2

User’s manual

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CosmoPMC (Cosmology Population Monte Carlo) is a Bayesian sampling method to explore the likelihood of various cosmological probes. The sampling engine is implemented with the package `pmclib`. It is called Population Monte Carlo (PMC), which is a novel technique to sample from the posterior \cite{Cappé2008}. PMC is an adaptive importance sampling method which iteratively improves the proposal to approximate the posterior. This code has been introduced, tested and applied to various cosmology data sets in \cite{Wraith2009}. Results on the Bayesian evidence using PMC are discussed in \cite{Kilbinger2010}.

1.1. Importance sampling

One of the main goals in Bayesian inference is to obtain integrals of the form

\[
\pi(f) = \int f(x)\pi(x)dx
\]

over the posterior distribution \(\pi\) which depends on the \(p\)-dimensional parameter \(x\), where \(f\) is an arbitrary function with finite expectation under \(\pi\). Of interest are for example the parameter mean (\(f = \text{id}\)) or confidence regions \(S\) with \(f = 1_S\) being the indicator function of \(S\). The Bayesian evidence \(E\), used in model comparison techniques, is obtained by setting \(f = 1\), but instead of \(\pi\) using the unnormalised posterior \(\pi' = L \cdot P\) in \(1\), with \(L\) being the likelihood and \(P\) the prior.

The evaluation of \(1\) is challenging because the posterior is in general not available analytically, and the parameter space can be high-dimensional. Monte-Carlo methods to approximate the above integrals consist in providing a sample \(\{x_n\}_{n=1..N}\) under \(\pi\), and approximating \(1\) by the estimator

\[
\hat{\pi}(f) = \frac{1}{N} \sum_{n=1}^{N} f(x_n).
\]

Markov Chain Monte Carlo (MCMC) produces a Markov chain of points for which \(\pi\) is the limiting distribution. The popular and widely-used package cosmomc \texttt{(http://cosmologist.info/cosmomc; Lewis & Bridle 2002)} implements MCMC exploration of the cosmological parameter space.

Importance sampling on the other hand uses the identity

\[
\pi(f) = \int f(x)\pi(x)dx = \int f(x) \frac{\pi(x)}{q(x)} q(x) dx
\]
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where \( q \) is any probability density function with support including the support of \( \pi \). A sample \( \{x_n\} \) under \( q \) is then used to obtain the estimator

\[
\hat{\pi}(f) = \frac{1}{N} \sum_{n=1}^{N} f(x_n) w_n; \quad w_n = \frac{\pi(x_n)}{q(x_n)}.
\]

(4)

The function \( q \) is called the proposal or importance function, the quantities \( w_n \) are the importance weights. Population Monte Carlo (PMC) produces a sequence \( q^t \) of importance functions \( (t = 1 \ldots T) \) to approximate the posterior \( \pi \). Details of this algorithm are discussed in Wraith et al. (2009).

The package CosmoPMC provides a C-code for sampling and exploring the cosmological parameter space using Population Monte Carlo. The code uses MPI to parallelize the calculation of the likelihood function. There is very little overhead and on a massive cluster the reduction in wall-clock time can be enormous. Included in the package are post-processing, plotting and various other analysis scripts and programs. It also provides a Markov Chain Monte-Carlo sampler.

1.2. This manual

This manual describes the code CosmoPMC, and can be obtained from www.cosmopmc.info. CosmoPMC is the cosmology interface to the Population Monte Carlo (PMC) engine pmclib. Documentation on the PMC library can be found at the same url. The cosmology module of CosmoPMC can be used as stand-alone program, it has the name nicaea (http://www2.iap.fr/users/kilbinge/nicaea).

Warning: Use undocumented features of the code at your own risk!

2. Installing CosmoPMC

2.1. Software requirements

CosmoPMC has been developed on GNU/Linux and Darwin/FreeBSD systems and should run on those architectures. Required are:

- C-compiler (e.g. gcc, icc)
- PMCLIB (Sect. 2.2)
- GSL (http://www.gnu.org/software/gsl), version 1.15 or higher
- FFTW (http://www.fftw.org)
- Message Parsing Interface (MPI) (http://www-unix.mcs.anl.gov/mpi) for parallel calculations
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Optional:

- **csh**, for post-processing, auxiliary scripts; recommended
- **perl** [http://www.perl.org](http://www.perl.org), for post-processing, auxiliary scripts; recommended
- **yorick** [http://yorick.sourceforge.net](http://yorick.sourceforge.net), post-processing, mainly plotting
- **python** [http://www.python.org](http://www.python.org), for running the configuration script
- **R** [http://www.r-project.org](http://www.r-project.org), post-processing

To produce 1D and 2D marginal posterior plots with scripts that come with CosmoPMC, either **yorick** or **R** are required.

Necessary for CMB anisotropies support:

- Fortran compiler (e.g. **ifort**)
- **Intel Math Kernel** libraries [http://software.intel.com/en-us/intel-mkl](http://software.intel.com/en-us/intel-mkl)
- **CAMB** [http://camb.info, http://cosmologist.info/cosmomc](http://camb.info, http://cosmologist.info/cosmomc)
- WMAP data and likelihood code [http://lambda.gsfc.nasa.gov](http://lambda.gsfc.nasa.gov)

2.2. Download and install **pmclib**

The package **pmclib** can be downloaded from the CosmoPMC site [http://www.cosmopmc.info](http://www.cosmopmc.info).

After downloading, unpack the gzipped tar archive

```
> tar xzf pmclib_x.y.tar.gz
```

This creates the **pmclib** root directory **pmclib_x.y**. **pmclib** uses **waf** [http://code.google.com/p/waf](http://code.google.com/p/waf) instead of configure/make to compile and build the software. Change to that directory and type

```
> ./waf --local configure
```

See **./waf --help** for options. The packages **lua**, **hdf5** and **lapack** are optionally linked with **pmclib** but are not necessary to run CosmoPMC. Corresponding warnings of missing files can be ignored. Instead of a local installation (indicated by **--local**), a install prefix can be specified with **--prefix=PREFIX** (default `/usr/local`).
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2.3. Patch pmclib

For CosmoPMC v1.2 and pmclib v1.x, a patch of the latter is necessary. From http://www.cosmopmc.info, download patch_pmclib_1.x_1.2.tar.gz and follow the instructions in the readme file readme_patch_pmclib_1.x_1.2.txt.

2.4. Download and install CosmoPMC

The newest version of CosmoPMC can be downloaded from the site http://www.cosmopmc.info.

First, unpack the gzipped tar archive

> tar xzf CosmoPMC_v1.2.tar.gz

This creates the the CosmoPMC root directory CosmoPMC_v1.2. Change to that directory and run

> [python] ./configure.py

This (poor man’s) configure script copies the file Makefile.no_host to Makefile.host and sets host-specific variables and flags as given by the command-line arguments. For a complete list, see `configure.py --help`.

Alternatively, you can copy by hand the file Makefile.no_host to Makefile.host and edit it. If the flags in this file are not sufficient to successfully compile the code, you can add more flags by rerunning configure.py, or by manually editing Makefile.main. Note that a flag in Makefile.main is overwritten if the same flag is present in Makefile.host.

To compile the code, run

> make; make clean

On success, symbolic links to the binary executables (in ./exec) will be set in ./bin.

It is convenient to define the environment variable COSMOPMC and to set it to the main CosmoPMC directory. For example, in the C-shell:

> setenv COSMOPMC /path/to/CosmoPMC_v1.2

This command can be placed into the startup file (e.g. ~/.cshrc for the C-shell). One can also add $COSMOPMC/bin to the PATH environment variable.
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Examples

To get familiar with CosmoPMC, use the examples which are contained in the package. Simply change to one of the subdirectories in $COSMOPMC/Demo/MC_Demo and proceed on to the point Run below.

User-defined runs

To run different likelihood combinations, or your own data, the following two steps are necessary to set up a CosmoPMC run.

1. Data and parameter files
   
   Create new directory with
   
   newdir.pmc.sh
   
   When asked, enter the likelihood/data type. More than one type can be chosen by adding the corresponding (bit-coded) type id’s. Symbolic links to corresponding files in $COSMOPMC/data are set, and parameter files from $COSMOPMC/par_files are copied to the new directory on request.
   
   If necessary, copy different or additional data and/or parameter files to the present directory.

2. Configuration file
   
   Create the PMC configuration file config.pmc. Examples for existing data modules can be found in $COSMOPMC/Demo/MC_Demo, see also Sect. 5 for details.
   
   In some cases, information about the galaxy redshift distribution(s) have to be provided, and the corresponding files copied (see $COSMOPMC/Demo for example files ‘nofz*’).

Run

Type

> $COSMOPMC/bin/cosmo_pmc.pl -n NCPU

...to run CosmoPMC on NCPU CPUs. See $cosmo_pmc.pl -h for more options. Depending on the type of initial proposal (Sect. 3.2), a maximum-search is started followed by a Fisher matrix calculation. After that, PMC is started. Fig. 1 shows a flow chart of the script’s actions.
Diagnostics

Check the files perplexity and enc. If the perplexity reaches values of 0.8 or larger, and if the effective number of components (ENC) is not smaller than 1.5, the posterior has very likely been explored sufficiently. Those and other files are updated during run-time and can be monitored while PMC is running. See Sect. [3.3.1] for more details.

Results

The text file iter_{niter-1}/mean contains mean and confidence levels. The file iter_{niter-1}/all_contour2d.pdf shows the 1d- and 2d-marginals. Plots can be redone or refined, or created from other than the last iteration with plot_contour2d.pl. Note that in the default setting, the posterior plots are not smoothed. See Sect. [6.1.1] for more details, and for information on the alternative script plot_confidence.R.

3.2. CosmoPMC in detail

This section describes in more detail how PMC is run, and which decisions the user has to make before starting and after stopping a PMC run.

Initial proposal The choice of the initial proposal, used during the first PMC iteration, is of great importance for a successful PMC run. The following options are implemented, determined by the key ‘sinitial’ in the configuration file (see Sect. [5]):

1. **sinitial = fisher_shift** The Fisher matrix is used as the covariance of a multi-variate Gaussian/Student-t distribution g. A mixture-model is constructed by creating D copies of g. Each copy is displaced from the ML point by a random uniform shift, and its variance is stretched by random uniform factor.

2. **sinitial = fisher_eigen** A mixture-model is constructed in a similar way as the first case, with the difference that the shift from the ML point is now performed along the major axes of the Fisher ellipsoid. Note that if the Fisher matrix is diagonal, the shift of each component only concerns one parameter.

3. **sinitial = file** The initial proposal is read from a file (of mix_mvdens format), e.g. from a previous PMC run.

4. **sinitial = random_pos** Mixture-model components with random variance (up to half the box size) and random positions. This case should only be used if the posterior is suspected to be multi-modal, or the calculation of the Fisher matrix fails.

In many cases, a mixture of multi-variate Gaussians as the proposal is the best choice. For that, set the degrees-of-freedom (ν) parameter df to -1. For a posterior with heavy tails, a Student-t
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Figure 1: Flow chart for `cosmo_pmc.pl`.

distribution might be more suited. The degrees of freedom \( \nu \) can be chosen freely; \( \nu = 3 \) is a common choice. For \( \nu \rightarrow \infty \), a Gaussian distribution is reached asymptotically.

If the Fisher matrix has to be calculated for the initial proposal, the script `cosmo_pmc.pl` calls `max_post` and `go_fishing` to estimate the maximum-likelihood point and the Hessian at that point, respectively. The script `config_pmc_to_max_and_fish.pl` can be used to create the corresponding configuration files from the PMC config file for manual calls of `max_post` and `go_fishing`.

**Updating the proposal** The PMC algorithm automatically updates the proposal after each iteration, no user interference is necessary.
The method to update the proposal is a variant of the Expectation-Maximization algorithm (EM, Dempster et al. 1977). It leads to an increase of the perplexity and an increase of ESS. Detailed descriptions of this algorithm in the case of multi-variate Gaussian and Student-t distributions can be found in Cappé et al. (2008) and Wraith et al. (2009).

**Dead components** A component can ‘die’ during the updating if the number of points sampled from that component is less than \( \text{MINCOUNT} = 20 \), or its weight is smaller than the inverse total number of sample points \( 1/N \). There are two possibilities to proceed. First, the component is ‘buried’, its weight set to zero so that no points are sampled from it in subsequent iterations. Alternatively, the component can be revived. In this case, it is placed near the component \( \phi_{d_0} \) which has maximum weight, and it is given the same covariance as \( \phi_{d_0} \).

The first case is the standard method used in Wraith et al. (2009). The second method tries to cure cases where the majority of components die. This can happen if they start too far off from the high-density posterior region. Often, only one component remains to the end, not capable of sampling the posterior reliably.

Both options can be chosen using the config file (Sect. 5) key `sdead comp = {bury|revive}`.

**Errors** If an error occurs during the calculation of the likelihood, the error is intercepted and the likelihood is set to zero. Thus, the parameter vector for which the error occurs is attributed a zero importance weight and does not contribute to the final sample. An error message is printed to `stderr` (unless CosmoPMC is run with the option `-q`) and PMC continues with the next point. An error can be due to cosmological reasons, e.g. a redshift is probed which is larger than the maximum redshift in a loitering Universe. Further, a parameter could be outside the range of a fitting formulae, e.g. a very small scalar spectral index in the dark matter transfer function.

Usually, the errors printed to `stderr` during PMC sampling can be ignored.

**Random numbers** The GSL random number generator is used to generate random variables. It is initialised with a seed reading the current time, to produce different (pseudo-) random numbers at each call. The seed is written to the log file. Using the option `'-s SEED'`, a user-specified seed can be defined. This is helpful if a run is to be repeated with identical results.

### 3.3. Output files

Each iteration \( i \) produces a number of output files which are stored in subdirectories `iter_i` of the CosmoPMC starting directory. Files which are not specific to a single iteration are placed in the starting directory.
3.3.1. Diagnostics

Unlike in MCMC, with adaptive importance sampling one does not have to worry about convergence. In principle, the updating process can be stopped at any time. There are however diagnostics to indicate the quality and effectiveness of the sampling.

Perplexity and effective sample size

The perplexity $p$ is defined in eq. (18) of Wraith et al. (2009). The range of $p$ is $[0; 1]$, and will approach unity if the proposal and posterior distribution are close together, as measured by the Kullback-Leibler divergence. The initial perplexity is typically very low ($< 0.1$) and should increase from iteration to iteration. Final values of 0.99 and larger are not uncommon, but also for $p$ of about 0.6-0.8 very accurate results can be obtained. If $p$ is smaller than say 0.1, the PMC sample is most likely not representative of the posterior. Intermediate values for $p$ are not straight-forward to interpret.

Closely related to the perplexity is the effective sample size ESS, which lies in the range $[1; N]$. It is interpreted as the number of sample point with zero weight (Liu & Chen 1995). A large perplexity is usually accompanied by a high ESS. For a successful PMC run, ESS is much higher than the acceptance rate of a Monte Carlo Markov chain, which is typically between 0.15 and 0.25.

The file perplexity contains the iteration $i$, perplexity $p$, ESS for that iteration, and the total ESS. This file is updated after each iteration and can therefore be used to monitor a PMC run.

If there are points with very large weights, they can dominate the other points whose normalised weights will be small. Even a few sample points might dominate the sum over weights and result in a low perplexity. The perplexity is the most sensitive quantity to those high-weight points, much more than e.g. the mean, the confidence intervals or the evidence.

Effective number of proposal components

The proposal $q^i$ provides useful information about the performance of a PMC run. For example, the effective number of components, defined in complete analogy to ESS,

$$\text{ENC} = \left( \sum_{d=1}^{D} \left( \alpha_d^i \right)^2 \right)^{-1},$$

is an indication of components with non-zero weight. If ENC is close to unity, the number of remaining components to sample the posterior is likely to be too small to provide a representative sample. For a badly chosen initial proposal, this usually happens already at the first few iterations. By monitoring the file enc which is updated each iteration, an unsuccessful PMC run can be aborted.
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The effective number of components can also be determined from any proposal file (mix_mvdens format) with the script `neff_proposal.pl`. An additional diagnostic is the evolution of the proposal components with iteration. This illustrates whether the components spread out nicely across the high-posterior region and reach a more or less stationary behaviour, or whether they stay too concentrated at one point. The scripts `proposal_mean.pl` (or `proposal_var.pl`) read in the proposal information $q'$ and plot the means (variances) as function of iteration $t$.

3.3.2. Results

**PMC samples** iter/*pmcsim*

This file contains the sample points. The first column is the (unnormalised) importance weight (log), the second column denotes the component number from which the corresponding point was sampled. Note that the $n_{\text{clip}}$ points with highest weights are not considered in subsequent calculations (of moments, perplexity, evidence etc.). The next $p$ columns are the $p$-dimensional parameter vector. Optionally, $n_{\text{ded}}$ numbers of deduced parameters follow.

**Proposals** iter/*proposal*

The proposal used for the importance sampling in iteration $i$ is in mix_mvdens format (Sect. A.3). The final proposal, updated from the sample of the last iteration, is `proposal_fin`

**Mean and confidence intervals** iter/*mean*

This file contains mean and one-dimensional, left- and right-sided confidence levels (c.l.). A c.l. of $p\%$ is calculated by integrating the one dimensional normalised marginal posterior starting from the mean in positive or negative direction, until a density of $p\%/2$ is reached. PMC outputs c.l.’s for $p = 63.27\%$, $95.45\%$ and $99.73\%$. With the program `cl_one_sided` one-sided c.l.’s can be obtained.

For post-processing, the program [meanvar_sample] outputs the same information (mean and c.l.) from an existing PMC sample, including possible deduced parameters.

**Resampled PMC simulations** iter[/niter-1]/sample

If `cosmo_pmc.pl` has been run with the option `-p`, the directory of the final iteration contains the file of parameter vectors `sample`, which is resampled from the PMC simulation `pmcsim`, taking into account the importance weights. The resampled points all have unit weight. Resampling is a post-processing step, it is performed by calling the R script `sample_from_pmcsimu.R` from `cosmo_pmc.pl`; this can also be done manually with any `pmcsim` simulation.
3. Running CosmoPMC

Histograms iter_i/chi_j, iter_i/chi_j_k
One- and two-dimensional histograms are written at each iteration to the text files chi_j and chi_j_k, respectively, where j and k, j < k, are parameter indices. Those histograms can be used to create 1d- and 2d-marginals, using the script `plot_contour2d.pl`. The bin number is set by the config entry nbinhist.

In post-processing, use `histograms_sample` to produce histograms from a PMC sample. This can be useful if deduced parameters have been added to the sample.

Covariance iter_i/covar*.fin
The parameter covariance and inverse covariance are printed to the files covar.fin and, respectively, covarinv.fin. The addition “+ded” in the file name indicates the inclusion of deduced parameters. The covariance matrices are in “mvdens”-format (see Sect. A.3).

Evidence evidence
This file contains the Bayesian evidence as a function of iteration. Before the first iteration, the Laplace approximation using the Fisher matrix is printed to `evidence_fisher` if the file fisher exists. At each iteration i, iter_i/evidence_covarinv contains the Laplace approximation of the evidence from the inverse covariance matrix of the sample iter_i/pmcsim.

3.3.3. Deduced parameters
Deduced parameters can be part of a PMC simulation. These parameters are not sampling parameters, but they are deduced from the main parameters. For example, if Ω_m and Ω_Λ are sampling parameters of a non-flat model, the curvature Ω_K = Ω_m + Ω_Λ can be a deduced parameter.

In most cases, deduced parameters are ignored while running CosmoPMC. They are usually added to the PMC simulation after the sampling, for example using a script. In the case of galaxy clustering, `add_deduced_halomodel` adds deduced parameters which depend on the sampling parameters but also on the underlying cosmology and halo model.

A PMC simulation with deduced parameters added can be used as input to `histograms_sample` to create the histogram files, now including the deduced parameters. These can then in turn be read by `plot_contour2d.pl` to produce 1d- and 2d-marginals, including the deduced parameters. Alternatively, the PMC simulation with added parameters can be resampled using `sample_from_pmcsimu.R` from which plots can be created by `plot_confidence.R`
3.3.4. Other files

**Maximum-posterior parameter**  
\[ \text{max\_logP} \]

\[ \text{max\_post} \]

stores its estimate of the maximum posterior in this file.

**Fisher matrix**  
\[ \text{fisher} \]

The final result of \[ \text{go\_fishing} \] the Fisher matrix in mvdens (Sect. A.3) format.

**Log files**  
\[ \text{log\_max\_post, log\_fish, log\_pmc} \]

\[ \text{max\_post, go\_fishing} \] and \[ \text{cosmo\_pmc} \] each produce their corresponding log file.

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The cosmology part of CosmoPMC is essentially the same as the stand-alone package \[ \text{nicaea} \]

This excludes the external program \[ \text{camb} \] and the WMAP likelihood library, which are called by CosmoPMC for CMB anisotropies. Further, CosmoPMC contains a wrapper layer to communicate between the PMC sampling and the cosmology modules.

4.1. Basic calculations

A number of routines to calculate cosmological quantities are included in the code. These are

- Background cosmology: Hubble parameter, distances, geometry
- Linear perturbations: growth factor, transfer function, cluster mass function, linear 3D power spectra
- Non-linear evolution: fitting formulae for non-linear power spectra (Peacock & Dodds [1996] Smith et al. [2003]), emulators (Heitmann et al. [2009] [2010] Lawrence et al. [2010]), halo model
- Galaxy clustering: HOD model
- Cosmic shear: convergence power spectrum, second-order correlation functions and derived second-order quantities, third-order aperture mass skewness
- CMB anisotropies via \[ \text{camb} \].

[http://www2.iap.fr/users/kilbinge/nicaea](http://www2.iap.fr/users/kilbinge/nicaea)
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Table 1: Extrapolation of the power spectra

| snonlinear   | $k_{\text{max}}$ | $n_{\text{ext}}$ |
|--------------|------------------|------------------|
| linear       | $333.6 \, h \, \text{Mpc}^{-1}$ | $n_s - 4$ |
| pd96         | $333.6 \, h \, \text{Mpc}^{-1}$ | $-2.5$ |
| smith03, smith03.de | $333.6 \, h \, \text{Mpc}^{-1}$ | Eq. (61), Smith et al. (2003) |
| coyote10     | $2.416 \, \text{Mpc}^{-1}$ | no extrapolation |

4.1.1. Density parameters

Both the density parameters ($\Omega_X = \rho_X/\rho_c$) and the physical density parameters ($\omega_X = \Omega_X h^2$) are valid input parameters for sampling with PMC. Internally, the code uses non-physical density parameters ($\Omega_X$). All following rules hold equivalently for both classes of parameters. Note that physical and non-physical density parameters can not be mixed, e.g. $\Omega_c$ and $\omega_K$ on input causes the program to abort.

The parameter for massive neutrinos, $\Omega_{\nu,\text{mass}}$, is not contained in the matter density $\Omega_m = \Omega_c + \Omega_b$.

A parameter which is missing from the input list is assigned the default value, found in the corresponding cosmology parameter file (cosmo.par), unless there is an inconsistency with other input parameters. E.g., if $\Omega_{\text{de}}$ and $\Omega_K$ are input parameters, $\Omega_m$ is assigned the value $\Omega_m = 1 - \Omega_{\text{de}} - \Omega_K - \Omega_{\nu,\text{mass}}$, to keep the curvature consistent with $\Omega_K$.

A flat Universe is assumed, unless (a) both $\Omega_m$ and $\Omega_{\text{de}}$, or (b) $\Omega_K$ are given as input parameter.

4.1.2. Matter power spectrum

Usually, models of the non-linear power spectrum have a limited validity range in $k$ and/or redshift. For small $k$, each model falls back to the linear power spectrum, which goes as $P_{\delta}(k) \propto k^{n_s}$. For large $k$, the extrapolation as a power law $P_{\delta}(k) \propto n_{\text{ext}}$ is indicated in Table 4.1.2.

See for more details on the models.

The Coyote emulator In the coyote10 case, the power spectrum is zero for $k > k_{\text{max}}$. The same is true for redshifts larger than the maximum of $z_{\text{max}} = 1$. See Eifler (2011) for an alternative approach.

The Hubble constant $h$ can not be treated as a free parameter. For a given cosmology, it has to be fixed to match the CMB first-peak constraint $\ell_A = \pi d_{ls}/r_s = 302.4$, where $d_{ls}$ is the distance to last scattering, and $r_s$ is the sound horizon. This can be done with the function set_H0_Coyote, see Demo/lensingdemo.c for an example. When doing sampling with non-physical density
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parameters, \( h \) has to be set at each sample point. Alternatively, the physical density parameters can be sampled, where \( h \) is set internally to match the CMB peak.

4.1.3. Likelihood

Each cosmological probe has its own log-likelihood function. The log-likelihood function is called from a wrapping routine, which is the interface to the PMC sampler. In general, within this function the model vector is computed using the corresponding cosmology routine. The exception are the WMAP-modules where the \( C_\ell \)'s are calculated using \texttt{camb} and handed over to the log-likelihood function as input.

4.2. Cosmic shear

CosmoPMC implements second- and third-order weak lensing observables.

4.2.1. Second-order

The basic second-order quantities in real space for weak gravitational lensing are the two-point correlation functions \( \xi_{\pm} \) (2PCF) (e.g.\cite{kaiser1992}),

\[
\xi_{\pm}(\theta) = \frac{1}{2\pi} \int_0^\infty d\ell \ell P_\kappa(\ell) J_0(\ell \theta) \tag{6}
\]

Data corresponding to both functions (\texttt{slensdata=xipm}) as well as only one of them (\texttt{xip}, \texttt{xim}) can be used. The aperture-mass dispersion (\cite{schneider1998})

\[
\langle M_{\text{ap}}^2(\theta) \rangle = \frac{1}{2\pi} \int_0^\infty d\ell \ell P_\kappa(\ell) \hat{U}^2(\ell \theta) \tag{7}
\]

is supported for two filter functions \( U_\theta(\theta) = u(\theta/\theta)\theta^2 \) \cite{schneider1998,crittenden2002}.

- polynomial (\texttt{map2poly}): \( u(x) = \frac{9}{\pi}(1 - x^2) \left( \frac{1}{3} - x^2 \right) H(1 - x) \); \cite{kaiser1992}.

- Gaussian (\texttt{map2gauss}): \( u(x) = \frac{1}{2\pi} \left( 1 - \frac{x^2}{2} \right) e^{-x^2/2} \). \cite{kaiser1992}.

The top-hat shear dispersion \cite{kaiser1992}

\[
\langle |\gamma|^2 \rangle_{E,B}(\theta) = \frac{1}{2\pi} \int_0^\infty d\ell \ell P_\kappa(\ell) \frac{4J_1(\ell \theta)}{(\ell \theta)^2} \tag{10}
\]

is used with \texttt{slensdata = gsq}.
Pure E-/B-mode separating functions (Schneider & Kilbinger 2007) are chosen with slensdata = decomp_eb. For the lack of analytical expressions for filter functions to obtain these real-space statistics from the convergence power spectrum, they are calculated by integrating over the 2PCF. The integral is performed over the finite angular interval \([\theta_{\text{min}}, \theta_{\text{max}}]\). The prediction for the E-mode is

\[
E = \frac{1}{2} \int_{\theta_{\text{min}}}^{\theta_{\text{max}}} \, d\theta \, \theta \left[ T_+ (\theta) \xi_+ (\theta) \pm T_- (\theta) \xi_- (\theta) \right].
\] (11)

Two variants of filter functions are implemented: The ‘optimized’ E-/B-mode function \(F \& K\) (2010) for which the real-space filter functions are Chebyshev polynomials of the second kind,

\[
T_+ (x) = \frac{2\theta - \theta_{\text{max}} - \theta_{\text{min}}}{\theta_{\text{max}} - \theta_{\text{min}}} = \sum_{n=0}^{N-1} a_n U_n (x); \quad U_n (x) = \frac{\sin((n + 1) \arccos x)}{\sin(\arccos x)}.
\] (12)

The coefficients \(a_n\) have been optimized with respect to signal-to-noise and the \(\Omega_m - \sigma_8\) Fisher matrix. The function \(E\) is defined as a function of the lower angular limit \(\theta_{\text{min}}\). The ratio \(\eta\) of lower to upper limit, \(\eta = \theta_{\text{min}}/\theta_{\text{max}}\) is fixed.

The second variant are the so-called COSEBIs (Complete Orthogonal Sets of E-/B-mode Integrals; Schneider et al. 2010). We implement their ‘logarithmic’ filter functions,

\[
T_{+}^{\log} (\theta) = T_+ \left( x = \frac{2\theta - \theta_{\text{max}} - \theta_{\text{min}}}{\theta_{\text{max}} - \theta_{\text{min}}} \right) = \sum_{j=0}^{n+1} c_{nj} z^j = N_n \prod_{j=1}^{n+1} (z - r_n).
\] (13)

The coefficients \(c_{nj}\) are fixed by integral conditions that assure the E-/B-mode decomposition of the 2PCF on a finite angular integral. They are given by a linear system of equations, which is given in Schneider et al. (2010). To solve this system, a very high numerical accuracy is needed. The Mathematica notebook file $\$\$COSMOPMC/par_files/COSEBIs/cosebi.nb$, adapted from Schneider et al. (2010), can be run to obtain the coefficients for a given \(\theta_{\text{min}}\) and \(\theta_{\text{max}}\). An output text file is created with the zeros \(r_n\) and amplitudes \(N_n\). The file name is cosebi_tlog_rN_[Nmax]_[thmin]_[thmax], where \(Nmax\) is the number of COSEBI modes, \(th\)\(\text{min}\) and \(th\)\(\text{max}\) are the minimum and maximum angular scale \(\theta_{\text{min}}\) and \(\theta_{\text{max}}\), respectively. For a given \(\theta_{\text{min}}\) and \(\theta_{\text{max}}\), specified with the config entries \(th\)\(\text{min}\) and \(th\)\(\text{max}\), CosmoPMC reads the corresponding text file from a directory that is specified by \(\text{path}\). A sample of files with various scales are provided in $\$\$COSMOPMC/par_files/COSEBIs$.

The COSEBIs are discrete numbers, they are specified by an integer mode number \(n\).

In both cases of pure E-/B-mode separating statistics, the function \(T_-\) is calculated from \(T_+\) according to Schneider et al. (2002).

The additional flag \texttt{decomp_eb_filter} decides between different filter functions:
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| decomp Eb_filter | Reference | Filter function type | $\eta$ |
|------------------|-----------|----------------------|--------|
| FK10_SN          | Fu & Kilbinger (2010) | optimized Signal-to-noise | 1/50   |
| FK10_FoM_eta10   | Fu & Kilbinger (2010) | optimized Fisher matrix | 1/10   |
| FK10_FoM_eta50   | Fu & Kilbinger (2010) | optimized Fisher matrix | 1/50   |
| COSEBIs_log      | Schneider et al. (2010) | logarithmic         |        |

The convergence power spectrum $P_\kappa$ with covariance matrix can be used with the flag `s lensdata = pkappa`.

### 4.2.2. Third-order

We implement the aperture-mass skewness (Pen et al. 2003; Jarvis et al. 2004; Schneider et al. 2005) with the Gaussian filter (eq. ??). There are two cases:

- `s lensdata = map3gauss`
  The ‘generalised’ skewness $\langle M^3_{ap} \rangle (\theta_1, \theta_2, \theta_3)$ (Schneider et al. 2005) with three filter scales.

- `s lensdata = map3gauss_diag`
  The ‘diagonal’ skewness $\langle M^3_{ap} \rangle (\theta)$ using a single aperture filter scale.

TODO: equations

### 4.2.3. Second- plus third-order

A joint data vector of second- and third-order observables can be used in CosmoPMC. The covariance is interpreted as a joint block matrix, with the second-order and third-order auto-covariances on the diagonal, and the cross-correlation on the off-diagonal blocks. The possible scenarios are:

- `s lensdata = map2gauss_map3gauss`
  Gaussian aperture-mass dispersion and generalised skewness.

- `s lensdata = map2gauss_map3gauss_diag`
  Gaussian aperture-mass dispersion and diagonal skewness.

- `s lensdata = decomp Eb_map3gauss`
  Log-COSEBIs and generalised aperture-mass skewness. The flag `decomp Eb_filter` has to be set to `COSEBIs_log`.

- `s lensdata = decomp Eb_map3gauss_diag`
  Log-COSEBIs and diagonal aperture-mass skewness. The flag `decomp Eb_filter` has to be set to `COSEBIs_log`.
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The first two cases use the same filter for second- and third-order, and provide therefore a consistent measure for both orders. The last two cases use the optimal E-/B-mode function known for second order.

4.2.4. Covariance

The covariance matrix is read from a file, and the inverse is calculated in CosmoPMC. The matrix has to be positive definite. An Anderson-Hartlap debiasing factor is multiplied to the inverse (Anderson 2003; Hartlap et al. 2007), which is specified with the config entry corr.inv cov. This can also be used to rescale the covariance, e.g. to take into account a different survey area. Set this value to unity if no correction is desired.

The covariance is either taken to be constant and not dependent on cosmology. In that case, set scov.scaling to cov.const. Or the approximated schemes from Eifler et al. (2009) are adopted, see ? for the implementation. In that scheme, the shot-noise term $D$ is constant, the mixed term $M$ is modulated with $\Omega_m$ and $\sigma_8$ using fitting formulae, and the cosmic-variance term $V$ is proportional to the square of the shear correlation function. This scheme is available for slensdata = xipm. The three covariance terms have to be read individually. The entry covname, which for scov.scaling = cov.const corresponds to the total covariance matrix, now specified the file name of cosmic-variance term, covname $M$ the name of the mixed term, and covname $D$ the name of the shot-noise term.

4.2.5. Reduced shear

The fact that not the shear $\gamma$ but the reduced shear $g = \gamma / (1 - \kappa)$ is observable leads to corrections to the shear power spectrum of a few percent, mainly on small scales. These corrections are either ignored, or modelled to first order according to Kilbinger (2010). This is controlled in the lensing parameter file (cosmo_lens.par). The parameter range where the reduced-shear corrections are valid are indicated in Table 2.

4.2.6. Angular scales

The flag sformat describes the mapping of angular scales (given in the data file) and ‘effective’ scales, where the model predictions of the shear functions are evaluated:

1. sformat = angle_center: The effective scale is the same as given in the data file, $\theta_{\text{eff}} = \theta$.

2. sformat = angle_mean: The model is averaged over a range of scales $[\theta_0, \theta_1]$ given in the data file.
Table 2: Parameter limits where the reduced-shear corrections are valid (from Kilbinger 2010).

| $\alpha$ | Parameter | lower | upper |
|----------|-----------|-------|-------|
| 1        | $\Omega_m$ | 0.22  | 0.35  |
| 2        | $\Omega_{de}$ | 0.33  | 1.03  |
| 3        | $w$        | -1.6  | -0.6  |
| 4        | $\Omega_b$ | 0.005 | 0.085 |
| 5        | $h$        | 0.61  | 1.11  |
| 6        | $\sigma_8$ | 0.65  | 0.93  |
| 7        | $n_s$      | 0.86  | 1.16  |

3. $\text{sformat} = \text{angle}_\text{wlinear}$: The model is the weighted average over a range of scales $[\theta_0, \theta_1]$, where the weight is $w = \theta/\text{arcmin}$.

4. $\text{sformat} = \text{angle}_\text{wquadr}$: The model is the weighted average over a range of scales $[\theta_0, \theta_1]$, where the weight is $w = a_1(\theta/\text{arcmin}) + a_2(\theta/\text{arcmin})^2$.

The first mode (angle_center) should be used for aperture-mass, shear rms and ‘ring’ statistics, since those quantities are not binned, but instead are integrals up to some angular scale $\theta$. For the correlation functions, in particular for wide angular bins, one of the last three modes is preferred. The quadratic weighting (angle_wquadr) corresponds to a weighting of the correlation function by the number of pairs $3$. This mode was used in the COSMOS analysis (Schraback et al. 2010).

4.3. SNIa

The standard distance modulus (schi2mode = chi2_simple) for a supernova with index $i$ is

$$\mu_{B,i} = m_{B,i}^* - \bar{M} + \alpha(s_i - 1) - \beta c_i. \quad (14)$$

where the quantities measured from the light-curve fit are the rest-frame $B$-band magnitude $m_{B,i}^*$, the shape or stretch parameter $s_i$, and the color $c_i$. The universal absolute SNIa magnitude is $\bar{M}$, the linear response parameters to stretch and color are $\alpha$ and $\beta$, respectively. The $\chi^2$-function is

$$\chi^2_{\text{sn}}(p) = \sum_i \frac{[\mu_{B,i}(p) - 5 \log_{10} \left( \frac{d_L(z_i, p)}{10 \text{pc}} \right)]^2}{\sigma^2(\mu_{B,i}) + \sigma_{\text{pv},i}^2 + \sigma_{\text{int}}^2}, \quad (15)$$

where $d_L$ is the luminosity distance and $z_i$ the redshift of object $i$. The contributions to the total error for object $i$ are: (1) The light-curve parameter variance $\sigma^2(\mu_{B,i}) = \theta_2^4 W_w \theta_2$ with the

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4. Cosmology

parameter vector $\theta_2 = (1, \alpha, \beta)$ and the covariance $W_2$ of the data vector $(m_{B,i}^*, s_i, c_i)$. (2) The peculiar velocity uncertainty $\sigma_{pv,i} = 5/\ln 10 \cdot v_p/(c z_i)$. (3) The intrinsic absolute magnitude scatter $\sigma_{\text{int}}$.

The Hubble parameter is absorbed into the absolute magnitude which we define as $M = \bar{M} - 5 \log_{10} h_{70}$.

The form of this log-likelihood function has been used in Astier et al. (2006).

The following variations of the distance modulus and log-likelihood are implemented:

- **schi2mode = chi2_Theta1**: The $\chi^2$ is extended to include photometric zero-point uncertainties, see Kilbinger et al. (2009).
- **schi2mode = chi2_Theta2_d denom fixed**: The parameters $\alpha$ and $\beta$ in the denominator of (15) are fixed and kept constant during the Monte-Carlo sampling.
- **schi2mode = chi2_no_sc**: The stretch and color parameters are ignored, the distance modulus is $\mu_{B,i} = m_{B,i}^* - \bar{M}$.
- **schi2mode = chi2_betaz**: Instead of a single parameter, the color response is redshift-dependent, $\beta \rightarrow \beta + \beta z_i$.
- **chi2_dust**: Intergalactic dust absorption is taken into account in the distance modulus, see Menard et al. (2010).

The covariance matrix $W_2$ of the data vector $(m_{B,i}^*, s_i, c_i)$ depends on the parameters $\alpha$ and $\beta$. In a Bayesian framework, this leads to an additional term $\frac{1}{2} \log \det W_2$ in the log-likelihood function. Taking into account this parameter-dependent term leads however to a biased maximum-likelihood estimator, in particular for $\alpha$ and $\beta$. Therefore, it is recommended to not include this term. Use the flag add_logdetCov = 0/1 in the configuration file to disable/enable this term.

4.4. CMB anisotropies

The full CMB anisotropies are handled externally: The $C_\ell$’s are calculated by calling camb (Lewis et al. 2000), the WMAP likelihood function (3rd-, 5th- and 7th-year) is computed using the WMAP public code (Dunkley et al. 2009). The maximum $\ell$ up to which the $C_\ell$’s are calculated and used in the likelihood can be determined in the configuration file. An $\ell_{\text{max}} = 2000$ is recommended for high precision calculations.

The power spectrum from the Sunyaev-Zel’dovich (SZ) effect can be added to the $C_\ell$’s, multiplied with an amplitude $A$ as free parameter. The predicted SZ power spectrum is taken from Komatsu & Seljak (2002). This model has been used in the 3-, 5- and 7-year analyses of the WMAP data (Komatsu et al. 2011).

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4 J. Guy, private communication
5 http://camb.info
6 http://lambda.gsfc.nasa.gov

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Alternatively, the WMAP distance priors (Komatsu et al. 2009) can be employed.

4.5. Galaxy clustering

4.5.1. Halomodel and HOD

The theoretical model of galaxy clustering is the one used in Coupon et al. (2012); see this paper for details of the model and further references.

As the basis to describe galaxy clustering, we implement the halo-model as reviewed in Cooray & Sheth (2002), which accounts for the clustering of dark-matter halos. On top of that, a halo occupation distribution (HOD) function (Berlind & Weinberg 2002; Kravtsov et al. 2004; Zheng et al. 2005) is the prescription of how galaxies populate those halos. This function is the number of galaxies $N$ in a halo of mass $M$. With the flag $\text{hod = berwein02}_\text{excl}$, this number is expressed as the sum of central ($N_c$) plus satellite ($N_s$) galaxies,

$$N(M) = N_c(M) \times [1 + N_s(M)] \ ,$$

with

$$n_c(M) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{\log_{10} M - \log_{10} M_{\min}}{\sigma_{\log M}} \right) \right] ;$$

$$n_s(M) = \begin{cases} (M - M_0)^\alpha & \text{if } M > M_0 \\ 0 & \text{else} \end{cases} ,$$

We further compute the galaxy two-point correlation function $\xi(r)$ and its angular projection $\nu(\theta)$ using the redshift distribution provided by the user, as well as the galaxy number density (for a full description of the model see Coupon et al. 2012). To prevent haloes from overlapping, we implement the halo exclusion formalism as described in Tinker et al. (2005).

For the halo bias, three options are available:

- $\text{shalo\_bias = bias\_sc}$
  
  Bias expansion from the spherical collapse model, see e.g. eq. (68) from Cooray & Sheth (2002).

- $\text{shalo\_bias = bias\_tinker05}$
  
  Bias calibrated with numerical simulations, Tinker et al. (2005) eq. (A1).

- $\text{shalo\_bias = bias\_tinker10}$
  
  Updated bias fitting formula from Tinker et al. (2010), eq. (6) and Table 2.

The mass function describes the number of halos for a given mass and redshift. It is defined as

$$\frac{dn}{d \ln M} = \frac{\bar{n}_0}{M} v f(v) \frac{dv}{d \ln M} \ ,$$

with

$$f(v) = \sqrt{\frac{10}{\sqrt{\pi}}} \frac{1}{v} \exp \left( \frac{-1}{v^2} \right) ,$$

$$\bar{n}_0 = 3 \times 10^5 \ .$$
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where \( \nu(M,z) = \delta_c(z)/[D_s(z)\sigma(M)] \) is a measure of the overdensity with \( \sigma(M) \) being the rms matter fluctuation in a top-hat window containing the mass \( M \). \( \bar{\rho}_0 = \Omega_m \rho_c,0 \) is the mean density of matter at the present day.

The following mass functions are implemented, via the flag smassfct:

- From the spherical/elliptical collapse model:
  \[
  \nu_f(\nu) = A \sqrt{\frac{2}{\pi a^2}} \left[ 1 + (av^2)^p \right] \exp \left( -\frac{av^2}{2} \right),
  \]
  (20)
  - ps: \( p = 0, q = 1 \) \cite{Press & Schechter 1974}
  - st: \( p = 0.3, q = 0.75 \) \cite{Sheth & Tormen 1999}
  - st2: \( p = 0.3, q = 0.707 \) \cite{Sheth & Tormen 1999}

- From numerical simulations:
  \[
  \nu_f(\nu) = f(\sigma) = 0.315 \exp \left[ -|\ln(\sigma - 1 + 0.61)|^{3.8} \right]
  \]
  (21)
  - j01: \cite{Jenkins et al. 2001}

The dark-matter halos have the density profile
\[
\rho(r) = \rho_s \left[ \frac{r}{r_s} \right]^\alpha (1 + r/r_s)^{3-\alpha}.
\]
(22)

For slopes unequal to the \cite{Navarro et al. 1997} value of \( \alpha = 1 \), closed expressions for the Fourier transform of \( \rho \) do not exist, and the code will be slower.

The concentration parameter is given by
\[
c(M,z) = c_0 \left[ \frac{M}{M_*} \right]^{-\beta},
\]
(23)
following \cite{Takada & Jain 2003}. The parameters \( c_0 \) and \( \beta \) can be chosen freely in the halomodel parameter file halomodel.par.

The log-likelihood function is the sum of the contribution from the angular correlation function and the galaxy number density \( n_{\text{gal}} \):
\[
\chi^2 = \sum_{i,j} \left[ w_{\text{obs}}(\theta_i) - w_{\text{model}}(\theta_i) \right] \left[ C^{-1} \right]_{ij} \left[ w_{\text{obs}}(\theta_j) - w_{\text{model}}(\theta_j) \right] + \frac{\left[ n_{\text{obs}} - n_{\text{model}} \right]^2}{\sigma_{n_{\text{gal}}}^2},
\]
(24)
where \( n_{\text{model}} \) is estimated at the mean redshift of the sample.

The number of galaxies (second term in eq. 24) can be included in the following way, with the config flag sngal_fit_type:
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- ngal_lin_fit: linear (standard; according to the above equation)
- ngal_log_fit: logarithmical
- ngal_no_fit: no inclusion, second term is omitted
- ngal_lin_fit_only: exclusive, first term is omitted

4.5.2. Deduced parameters

The following deduced parameters can be computed:

- Mean galaxy bias
  \[ b_g(z) = \int dM \frac{b_h(M, z) n(M, z) N(M)}{n_{\text{gal}}(z)}, \]  \hfill (25)

  where \( b_h \) is the halo bias, and

  \[ n_{\text{gal}}(z) = \int N(M) n(M, z) dM \]  \hfill (26)

  is the total number of galaxies.

- Mean halo mass
  \[ \langle M_{\text{halo}}(z) \rangle = \int dM \frac{M n(M, z) N(M)}{n_{\text{gal}}(z)}. \]  \hfill (27)

- Fraction of satellite galaxies
  \[ f_s(z) = 1 - f_c(z); \quad f_c(z) = \int dM \frac{N_c(M)}{n_{\text{gal}}(z)}. \]  \hfill (28)

Use the program `add_deduced_halomodel` to add those deduced parameters to a PMC sample. See the example config file `config_pmc_ded` in Demo/MC Demo/HOD/CFHTLS-T06.

4.5.3. Clustering data

The angular two-point correlation function \( w(\theta) \) is implemented, with the flag `shalodata = woftheta`. The measured (input) data \( w_{\text{mes}} \) is corrected for the integral constraint, via

\[ w(\theta) = w_{\text{mes}}(\theta) + w_C, \]  \hfill (29)

assuming that the measured correlation function can be fit by a power law

\[ w_{\text{mes}}(\theta) \approx A_w \left( \theta^{-\delta} - C \right). \]  \hfill (30)

The program `haloplot` outputs the correlation functions \( w(\theta) \) and \( \xi(r) \), the HOD function \( N(M) \), and deduced parameters for given HOD input parameters.
4.5.4. Comoving volume

The comoving volume is needed to calculate the comoving number density of galaxies, following from the halomodel and the HOD parameters. There are two possibilities to calculate the comoving volume $V_C$. First, if $z_{\text{min}}$ and $z_{\text{max}}$ are larger than zero in the HOD parameter file halomodel.par (see Table 7), $V_C$ is computed between those two redshifts. Second, if both numbers are $< 0$, $V_C$ is weighted by the redshift distribution $n(z)$, see e.g. eq. (28) in Ross & Brunner (2009). In this weighting, the maximum value of $n(z)$ is set to unity.

4.6. BAO

BAO constraints are implemented with two distance measures:

- $s_{\text{method}} = \text{distance}_A$
  The distance parameter $A$ is defined in [Eisenstein et al., 2005] as
  \[ A(z) = \frac{D_V(z) \sqrt{\Omega_m}}{c/H_0} \frac{\Omega_m}{z} \]  
  where
  \[ D_V(z) = \left[ f_K^2[w(z)] \frac{cz}{H(z)} \right]^{1/3} \]  
  is the spherically averaged distance to redshift $z$.

- $s_{\text{method}} = \text{distance}_d,z$
  The distance parameter $d$ is the ratio of sound horizon $r_s$ at drag epoch $z_d$ to spherically averaged distance (e.g. Percival et al. 2007),
  \[ d(z) = \frac{r_s(z_d)}{D_V(z)} \]  
  We use the fitting formula for the drag redshift $z_d$ from [Eisenstein & Hu, 1998] and calculate the sound horizon as the distance a sound wave can travel prior to $z_d$ by numerical integration.

4.7. Redshift distribution

Some of the cosmology modules require a redshift distribution, for example lensing and HOD. Table 3 lists the implemented redshift distributions $n(z)$, via the flag nofz.

Each redshift bin can have a different type. The syntax for a redshift bin file is described in Appendix A.1.5.
5. The configuration file

Table 3: Redshift distribution types

| nofz   | Description                  | $n(z) \propto \cdots$ | parameter list                      |
|--------|------------------------------|-----------------------|-------------------------------------|
| hist   | Histogram                    | $\sum_{i=0}^{n-1} N_i \cdot 1_{[z_i,z_{i+1}]}$ | (see text)                          |
| single | Single redshift              | $\delta_D(z - z_0)$  | $z_0, z_0$                          |
| ludo   | Fitting function             | $(z/z_0)^{\alpha} \exp\left[-{(z/z_0)}^\beta\right]$ | $z_{\text{min}}, z_{\text{max}}, \alpha, \beta, z_0$ |
| jonben | $z^a / (z^b + c)$            | $z_{\text{min}}, z_{\text{max}}, a, b, c$ |
| ymmk   | $(z^a + z^{ab}) / (z^b + c)$ | $z_{\text{min}}, z_{\text{max}}, a, b, c$ |

All redshift distributions are internally normalised as

$$\int_{z_{\text{min}}}^{z_{\text{max}}} dz n(z) = 1.$$  \hfill(34)

4.8. CMB and the power spectrum normalisation parameter

The power spectrum normalisation parameter taken as input for \texttt{camb} is $\Delta^2_R$, which is the amplitude of curvature perturbations at the pivot scale $k_0 = 0.002 \text{ Mpc}^{-1}$. For lower-redshift probes such as lensing or HOD, the normalisation is described by $\sigma_8$, the rms fluctuation of matter in spheres of 8 Mpc$/h$. To combine those probes in a PMC run, $\Delta^2_R$ has to be an input parameter, and $\sigma_8$ a deduced parameter. CMB has to come first in the list of data sets so that \texttt{camb} can calculate $\sigma_8$, which in turn is handed over to the lensing likelihood.

4.9. Parameter files

Tables 4 - 6 list the contents of the parameter files for basic cosmology, lensing, SNIa and HOD. Proto-types can be found in \texttt{COSMOPMC/par\_files}. These files specify the default values of parameters and flags. These default values are over-written if any of those parameter is used for Monte-Carlo sampling.

5. The configuration file

The programs \texttt{max\_post}, \texttt{go\_fishing}, \texttt{cosmo\_pmc}, and \texttt{cosmo\_mcmc} read a configuration file on startup. Each configuration file consist of two parts:

The first, basic part is common to all four config file types (Table 9). It consists of (1) the parameter section, (2) the data section and (3) the prior section. The data-specific entries in the
Table 4: Basic cosmology parameter file (cosmo.par)

| Parameter          | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| Omega_m            | Matter density, cold dark matter + baryons                                  |
| Omega_de           | Dark-energy density (if $w = -1$, corresponds to $\Omega_{\Lambda}$)        |
| $w_0\_de$          | Dark-energy equation-of-state parameter (constant term)                    |
| $w_1\_de$          | Dark-energy equation-of-state parameter (linear term, see sde.param)        |
| h_100              | Dimensionless Hubble parameter                                              |
| Omega_b            | Baryon density                                                              |
| Omega_nu_mass      | Massive-neutrino density (so far only for CMB)                              |
| N_eff_nu_mass      | Effective number of massive neutrinos (so far only for CMB)                 |
| normalization      | Power-spectrum normalisation at small scales (for normmode=0, see below)    |
| n_spec             | Scalar power-spectrum index                                                  |
| snonlinear         | Power spectrum prescription                                                 |
| linear             | Linear power spectrum                                                       |
| pd96               | Peacock & Dodds (1996)                                                      |
| smith03            | Smith et al. (2003)                                                         |
| smith03\_de        | Smith et al. (2003) + dark-energy correction from icosmo.org               |
| coyote10           | ‘Coyote Universe’, Heitmann et al. (2009), Heitmann et al. (2010)           |
| transfer           | Transfer function                                                           |
| bbks               | Bardeen et al. (1986)                                                       |
| eisenhu            | Eisenstein & Hu (1998) 'shape fit'                                         |
| eisenhu\_osc       | Eisenstein & Hu (1998) with BAO wiggles                                     |
| sgrowth            | Linear growth factor                                                        |
| heath              | Heath (1977) fitting formula                                                |
| growth\_de         | Numerical integration of differential equation for $\delta$ (recommended)  |
| sde\_param         | Dark-energy parameterisation                                                |
| jassal             | $w(a) = w_0 + w_1 a(1 - a)$                                                 |
| linder             | $w(a) = w_0 + w_1 (1 - a)$                                                  |
| normmode           | Normalization mode. 0: normalization=$\sigma_8$                            |
| a\_min             | Minimum scale factor                                                        |

The data section are listed in Table 11.

The second part is type-specific. See Table 10 for the PMC part, and Table 13 for the MCMC part. Example files can be found in subdirectories of $COSMOPMC/Demo/MC\_DEMO.$
5. The configuration file

Table 5: Weak lensing parameter file \((\text{cosmo}_\text{ lens}. \text{par})\)

| Parameter          | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| \text{cosmo\_file} | Basic cosmology file name \((\text{cosmo}. \text{par})\)                   |
| \text{nofz\_file}  | Redshift distribution master file                                           |
| \text{redshift module}\textsuperscript{a} | (see Table 8)                                                                |
| \text{stomo}       | Tomography correlations                                                     |
| \text{tomo\_all}   | All correlations                                                            |
| \text{tomo\_auto\_only} | Only auto-correlations \((ii)\)                                             |
| \text{tomo\_cross\_only} | Only cross-correlations \((i \neq j)\)                                     |
| \text{sreduced}    | Reduced-shear treatment                                                     |
| \text{none}        | No correction                                                              |
| \text{K10}         | Fitting-formulae from \cite{Kilbinger2010}                                   |
| \text{q\_mag\_size}\textsuperscript{b} | Magnification-bias coefficient, \(q = 2(\alpha + \beta - 1)\) (see \cite{Kilbinger2010}, eq. 16) |

Table 6: SNIa parameter file \((\text{cosmo\_SN}. \text{par})\)

| Parameter          | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| \text{cosmo\_file} | Basic cosmology file name \((\text{cosmo}. \text{par})\)                   |
| \text{Theta2}     | Distance modulus parameters \(-M \alpha - \beta \beta_c\)                  |

To create a config file of type \texttt{max\_post} or \texttt{go\_fishing} from a PMC config file, the script \texttt{config\_pmc\_to\_max\_and\_fish.pl} can be used.

Some flags are handled internally as integers (enumerations), but identified and set in the config file with strings. The corresponding key word carries the same name as the internal variable, preceded with an ‘s’, e.g. the integer/string pair \texttt{lensdata/slensdata}.

The prior file, indicated if desired with the flag \texttt{sprior}, is a file in \texttt{mvdens} format. It specifies a Gaussian prior with mean and covariance as given in the file. Note that the covariance and not the inverse covariance is expected in the file.
5. The configuration file

Table 7: HOD parameter file (halomodel.par)

| Parameter          | Description                                                                 |
|--------------------|-----------------------------------------------------------------------------|
| cosmo_file         | Basic cosmology file name (cosmo.par)                                       |
| nofz_file          | Redshift distribution master file                                          |
| redshift module    | (see Table 8)                                                               |
| zmin               | Minimum redshift (-1 if read from nzfile)                                   |
| zmax               | Maximum redshift (-1 if read from nzfile)                                  |
| alpha_NFW          | Halo density profile slope ($\alpha = 1$ for NFW)                           |
| c0                 | Concentration parameter at $z = 0$                                          |
| beta_NFW           | Concentration parameter slope of mass dependence                           |
| smassfct           | Halo mass function type                                                    |
| ps                 | (Press & Schechter 1974), $p = 0, q = 1$                                    |
| st                 | (Sheth & Tormen 1999), $p = 0.3, q = 0.75$                                 |
| st2                | (Sheth & Tormen 1999), $p = 0.3, q = 0.707$                                |
| j01                | (Jenkins et al. 2001)                                                       |
| M_min              | Minimal mass for central galaxies [$h^{-1} M_\odot$]                        |
| M1                 | Scale mass for satellites [$h^{-1} M_\odot$]                               |
| M0                 | Minimum mass for satellites [$h^{-1} M_\odot$]                             |
| sigma_log_M        | Logarithmic dispersion for central galaxies                                |
| alpha              | Slope for satellite mass dependence                                         |
| shod               | HOD type                                                                    |
| berwein02_hexcl    | Berlind & Weinberg (2002) with halo exclusion                              |

Table 8: Redshift module file (nofz.par)

| Parameter  | Description                                                                 |
|------------|-----------------------------------------------------------------------------|
| Nzbin      | Number of redshift bins                                                     |
| snzmode    | File mode                                                                   |
| nzfile     | File names. See Appendix A.1.5 for the file syntax.                         |

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5. The configuration file

Table 9: Basic, common part of the configuration file

| Parameter   | Type   | Description                                                                 |
|-------------|--------|-----------------------------------------------------------------------------|
| version     | double | Config file version. Upwards compatibility (config file version > CosmoPMC version) cannot be guaranteed. Downwards compatibility (config file version < CosmoPMC version) is most likely ensured. |
| npar        | integer| Number of parameters                                                        |
| n_ded       | integer| Number of deduced parameters. The deduced parameters are not sampled but deduced from the other parameters and written to the output files as well |
| spar        | string | Parameterisation type, necessary for the wrapping into the individual posterior parameters and for plotting, see Table 12 for possible parameters |
| min         | npar+n_ded doubles | Parameter minima |
| max         | npar+n_ded doubles | Parameter maxima |

Data section

| Parameter   | Type   | Description |
|-------------|--------|-------------|
| ndata       | integer| Number of data sets |
| sdata       | string | Data set 1 |
|             |        | ...         |
| sdata       | string | Data set ndata |

Prior section

| Parameter   | Type   | Description                                                                 |
|-------------|--------|-----------------------------------------------------------------------------|
| sprior      | string | Prior file name ("-" for no prior)                                         |
| [nprior     | integer| If sprior ≠ ".": Number of parameters to which prior applies               |
| [indprior   | npar × {0,1} | If sprior ≠ ".": Indicator flags for prior parameters] |
## 5. The configuration file

Table 10: PMC part of the configuration file

| Parameter   | Type   | Description                                                                 |
|-------------|--------|-----------------------------------------------------------------------------|
| nsample     | integer| Sample size per iteration                                                   |
| niter       | integer| Number of iterations                                                        |
| fsfinal     | integer| Sample size of final iteration is $\text{fsfinal} \times \text{nsample}$    |
| niter       | integer| Number of iterations (importance runs)                                      |
| nclipw      | integer| The $\text{nclipw}$ points with the largest weights are discarded           |

Proposal section

| Parameter   | Type       | Description                                                                 |
|-------------|------------|-----------------------------------------------------------------------------|
| df          | double     | Degrees of freedom ($\text{df}=-1$ is Gaussian, $\text{df}=3$ is ‘typical’ Student-t) |
| ncomp       | integer    | Number of components                                                        |
| sdead_comp  | string     | One of ‘bury’, ‘revive’                                                     |
| sinitial    | string     | Proposal type (one of $\text{fisher_rshift}$, $\text{fisher_eigen}$, file, random_position) |
| fshift$^a$  | double     | Random shift from ML point $\sim \text{U}(-r, r)$; $r = \text{fshift}/(\text{max} - \text{min})$ |
| fvar$^a$    | double     | Random multiplier of Fisher matrix                                            |
| prop_ini_name$^b$ | string | File name of initial proposal                                                |
| fmin$^c$    | double     | Components have variance $\sim \text{U}(\text{fmin},(\text{max} - \text{min})/2)$ |

Histogram section

| Parameter   | Type   | Description                                      |
|-------------|--------|--------------------------------------------------|
| nbinhist    | integer| Number of density histogram bins                 |
5. The configuration file

Table 11: Data-specific entries in the configuration file’s data section

| Weak gravitational lensing | Lensing |
|---------------------------|---------|
| slensdata                 | string  |
|                          | Data type, one of xipm, xip, xim, map2poly, map2gauss, gsqr, decompEb, pkappa, map3gauss, map3gauss_diag, map2gauss_map3gauss, map2gauss_map3gauss_diag, decompEb_map3gauss, decompEb_map3gauss_diag |
| sdecomp Eb filter         | string  |
|                          | One of FK10_SN, FK10_FoM_eta10, FK10_FoM_eta50, COSEBI_log |
| th_min                   | double  |
|                          | Minimum angular scale |
| th_max                   | double  |
|                          | Maximum angular scale |
| path                     | double  |
|                          | Path to COSEBI files |
| sformat                  | string  |
|                          | Data format of angular scales, one of angle_center, angle_mean, angle_wlinear, angle_wquadr |
| a1                       | double  |
|                          | Linear weight |
| a2                       | double  |
|                          | Quadratic weight, \( w = a1 \cdot \theta/\text{arcmin} + a2 \cdot (\theta/\text{arcmin})^2 \) |
| datname                  | string  |
|                          | Data file name |
| scov_scaling             | string  |
|                          | One of cov_const, cov_ESH09 |
| covname                  | string  |
|                          | Covariance file name |
| covname M                | string  |
|                          | Covariance mixed term file name |
| covname D                | string  |
|                          | Covariance shot-noise term file name |
| corr_invcov              | double  |
|                          | Correction factor for inverse covariance ML estimate, see [Hartlap et al. (2007)](https://example.com) |
| Nexclude                 | integer |
|                          | Number of redshift bin pairs to be excluded from analysis |
| exclude                  | Nexclude integers |
|                          | Indices of redshift pairs to be excluded |
| model_file               | string  |
|                          | Parameter file name, e.g. cosmo_lens |
| sspecial                 | string  |
|                          | Additional prior, one of none (recommended), unity, de_conservative |
5. The configuration file

| Supernovae type Ia  | SNIa                      |
|---------------------|---------------------------|
| **datname**         | string Data file name     |
| **datformat**       | string Data format, SNLS_firstyear |
| **schi2mode**       | string \(\chi^2\) and distance modulus estimator type (one of chi2_simple, chi2_Theta2_denom_fixed, chi2_betaz, chi2_dust, chi2_residual) |
| **Theta2_denom**    | 2 doubles Fixed \(\alpha, \beta\) in \(\chi^2\)-denominator |
| **zAV_name**        | string File with \(A_V(z)\) table |
| **datname_beta**    | string Prior file (mvdens format) on \(\beta_d\) ("-" if none) |
| **add_logdetCov**   | integer 1 if 0.5 log det Cov is to be added to log-likelihood, 0 if not (recommended; see Sect. 4.3) |
| **model_file**      | string Parameter file name, e.g. cosmo_SN |
| **sspecial**        | string Additional prior, one of none (recommended), unity, de_conservative |

Table 11: Data-specific entries in the configuration file's data section (continued).

| CMB anisotropies | CMB                                      |
|------------------|------------------------------------------|
| **scamb_path**   | string /path/to/scamb                   |
| **data_path**    | string /path/to/wmap-data. This path should contain the directory data with subdirectories healpix_data, highl, lowlP, lowlP |
| C1_SZ_file       | string File with SZ correction angular power spectrum ("-" if none) |
| lmax             | integer Maximum \(\ell\) for angular power spectrum |
| **accurate**     | 0|1 Accurate reionisation and polarisation calculations in camb |
| **model_file**   | string Parameter file name, e.g. cosmoDP.par |
| **sspecial**     | string Additional prior, one of none (recommended), unity, de_conservative |

| WMAP distance priors | CMBDistPrior                  |
|----------------------|--------------------------------|
| **datname**          | string Data (ML point and inverse covariance) file |
| **model_file**       | string Parameter file name, e.g. cosmo_lens.par |
| **sspecial**         | string Additional prior, one of none (recommended), unity, de_conservative |
5. The configuration file

| Galaxy clustering (HOD) | GalCorr |
|-------------------------|---------|
| shalodata               | string  |
| shalomode               | string  |
| dataname                | string  |
| covname$^a$             | string  |
| corr_invcov             | double  |
| dataname                | string  |
| model_file              | string  |

| Table 11: Data-specific entries in the configuration file’s data section (continued). |
|-------------------------|---------|
| Baryonic acoustic oscillations | BAO |
| smethod                 | string  |
| dataname                | string  |
| model_file              | string  |
| ssppecial               | string  |

Table 12 contains a list of input parameters, which can be given as strings to the `spar` key in the config file.

| Galaxy clustering (HOD) | Baryonic acoustic oscillations |
|-------------------------|--------------------------------|
| shalodata               | smethod                        |
| shalomode               | dataname                       |
| dataname                | model_file                     |
| covname$^a$             | sspacial                       |

| Baryonic acoustic oscillations | BA0 |
|-------------------------------|-----|
| smethod                      | string  |
| dataname                     | string  |
| model_file                   | string  |
| sspacial                     | string  |

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5. The configuration file

Table 12: Input parameters

| Name                  | Symbol    | Description                                                                 |
|-----------------------|-----------|-----------------------------------------------------------------------------|
| Basic cosmology       | (some of them given in `cosmo.par`) |                                                                             |
| Omega_m               | $\Omega_m$ | Matter density, cold dark matter + baryons                                  |
| omega_m               | $\omega_m$ |                                                                             |
| Omega_b               | $\Omega_b$ | Baryon density                                                              |
| omega_b               | $\omega_b$ |                                                                             |
| 100_omega_b           | $100 \times \omega_b$ |                                                                      |
| Omega_de              | $\Omega_{de}$ | Dark-energy density (if $w = -1$, corresponds to $\Omega_\Lambda$)          |
| omega_de              | $\omega_{de}$ |                                                                            |
| Omega_nu_mass         | $\Omega_{\nu,\text{mass}}$ | Massive-neutrino density (so far only for CMB)                             |
| omega_nu_mass         | $\omega_{\nu,\text{mass}}$ |                                                                            |
| Omega_c               | $\Omega_c$ | Cold dark matter                                                            |
| omega_c               | $\omega_c$ |                                                                            |
| Omega_K               | $\Omega_K$ | Curvature density parameter                                                 |
| omega_K               | $\omega_K$ |                                                                            |
| w0_de                 | $w_0$ | Dark-energy equation-of-state parameter (constant term)                     |
| w1_de                 | $w_1$ | Dark-energy equation-of-state parameter (linear term, see sde.param)       |
| h_100                 | $h$ | Dimensionless Hubble parameter                                              |
| N_eff_nu_mass         | $N_{\text{eff},\text{nu, mass}}$ | Effective number of massive neutrinos (so far only for CMB)                   |
| sigma_8               | $\sigma_8$ | Power-spectrum normalisation at small scales                                |
| Delta2_R              | $\Delta_2^R$ | Power-spectrum normalization at large scales (CMB)                         |
| n_spec                | $n_s$ | Scalar power-spectrum index                                                 |
| alpha_s               | $\alpha_s$ | Running spectral index (so far only for CMB)                                |
| n_t                   | $n_t$ | Tensor power-spectrum index                                                 |
| r                     | $r$ | Tensor to scalar ratio                                                      |
| ln_r                  | $\ln r$ |                                                                            |
| tau                   | $\tau$ | Optical depth for reionisation                                              |
| A_SZ                  | $A_{SZ}$ | SZ-power spectrum amplitude                                                 |
### 6. Post-processing and auxiliary programs

All scripts described in this section are located in $\text{COSMOPMC}/\text{bin}$.

#### Table 12: Input parameters (continued)

| Parameter       | Description                                              |
|-----------------|----------------------------------------------------------|
| $M$             | $M - \log_{10} h_{70}$ Universal SNIa magnitude          |
| $\alpha$        | Linear response factor to stretch                        |
| $\beta$         | Linear response factor to color                          |
| $\beta_z$       | Redshift-dependent linear response to color              |
| $\beta_d$       | Linear response to the color component due to intergalactic dust |
| $M_{\text{min}}$ | Minimum halo mass for central galaxies [$M_{\odot} h^{-1}$] |
| $M_1$           | Scale mass for satellite galaxies [$M_{\odot} h^{-1}$]    |
| $M_0$           | Minimum halo mass for satellite galaxies [$M_{\odot} h^{-1}$] |
| $\sigma_{\log M}$ | Dispersion for central galaxies                          |
| $\alpha_{\text{halo}}$ | Slope of satellite occupation distribution               |
| $M_{\text{halo av}}$ | Average halo mass [$M_{\odot} h^{-1}$]                  |
| $\langle M_h \rangle$ | Average halo bias                                      |
| $\langle N_g \rangle$ | Average galaxy number per halo                          |
| $f_s$           | Fraction of satellite galaxies to total                  |
| $n_g$           | Comoving galaxy number density [$\text{Mpc}^{-3} h^3$]  |

#### Galaxy-clustering-specific (some of them given in halomodel.par)

| Parameter       | Description                                              |
|-----------------|----------------------------------------------------------|
| $\log_{10} M_{\text{min}}$ | $\log_{10} M_{\text{min}}/(M_{\odot} h^{-1})$             |
| $M_1$           | $M_1/(M_{\odot} h^{-1})$                                 |
| $\log_{10} M_0$ | $\log_{10} M_0/(M_{\odot} h^{-1})$                       |
| $\sigma_{\log M}$ | $\sigma_{\log M}$                                        |
| $\alpha_{\text{halo}}$ | $\alpha_{\text{halo}}$                                   |
| $M_{\text{halo av}}$ | $\langle M_h \rangle$                                   |
| $\log_{10} M_{\text{halo av}}$ | $\log_{10} M_{\text{halo av}}/(M_{\odot} h^{-1})$        |
| $\langle b_h \rangle$ | $\langle b_h \rangle$                                   |
| $\langle N_g \rangle$ | $\langle N_g \rangle$                                   |
| $f_s$           | $f_s$                                                     |
| $n_g$           | $n_g$                                                     |
6. Post-processing and auxiliary programs

6.1. Plotting and nice printing

6.1.1. Posterior marginal plots

Marginals in 1d and 2d can be plotted in two ways, using (1) `plot_contour2d.pl` or (2) `plot_confidence.R`. The first is a perl script calling yorick for plotting, the second is an R script. The second option produces nicer plots in general, in particular, smoothing works better without producing over-smoothed contours. Further, filled contours with more than one data set are only possible with the R option, yorick can only combine several plots with empty contours. The computation time of the R script is however much longer.

1. `plot_contour2d.pl` creates 1d and 2d marginals of the posterior, from the histogram files `chi2_j` and `chi2_j_k`.

   To smooth 1d and 2d posteriors with a Gaussian, use `plot_contour2d.pl -n -g FACTOR`. The width of the Gaussian is equal to the box size divided by FACTOR. It is recommended to test the smoothing width FACTOR by setting it to a negative number which causes both smoothed and unsmoothed curves being plotted. This can reveal cases of over-smoothing. If contours have very different width in different dimension, the addition option `-C` uses the PMC sample covariance (from the file `covar+ded.fin`) as the covariance for the Gaussian. For the final plot, replace `-FACTOR` with FACTOR to remove the unsmoothed curves. Remove the option `-n` to add color shades to the 2d contours.

   The file `log_plot` contains the last plot command with all options. This can be used to reproduce and modify a plot which has been generated automatically by other scripts, e.g. `cosmo_pmc.pl`.

2. `plot_confidence.R` creates 1d and 2d marginals of the posterior, from the re-sample file `sample`.

   Smoothing is done with a kernel density estimation using the R function `kde2d`. The kernel width can be set with the option `-g`. The number of grid points, relevant both for smoothing and filled contours, is set with `-N`. Use both `-i` and `-j` options to only plot the 2D marginals of parameters `i` and `j` to save computation time.

6.2. Mean and confidence intervals

From a “mean” output file, containing parameter means and confidence levels, one can create a ps/pdf file using the command `mean2eps.pl`.

This is equivalent to the following steps (see also `essential_cosmo_pmc_run.pl`):

- `meanvar2tab.pl` creates a table with parameter names and values formatted in \TeX-format.
- `tab2tex.pl` wraps a LaTeX table header around the table.
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- txt2tex.pl wraps a \LaTeX\ header around the file.

Example:

```bash
> meanvar2tab.pl -s 1 -p 2 -e iter_9/mean > mean.tab
> tab2tex.pl -s 1.25 mean.tab > mean_in.tex
> txt2tex.pl mean_in.tex > mean.tex
```

6.2.1. PMC proposal

`proposal_mean.pl` and `proposal_var.pl` creates plots of the proposal component’s means (variances) as function of the iteration.

6.3. Importance sampling

A PMC simulation file (`pmcsim`) from an earlier PMC run, corresponding to a sample from posterior $p_1$, can be used to do importance sampling with another posterior $p_2$. For that, simply replace the data section of the earlier config file with the corresponding data section of posterior $p_2$. The command `importance_sample` creates a new PMC simulation which corresponds to a sample under the posterior product $p_1 \cdot p_2$.

6.4. Bayesian evidence, Bayes’ factor

`evidence.pl` calculates and prints the evidence from a PMC simulation file. The same information is printed to the file `evidence` during a PMC run.

`bayes_factor.pl` prints Bayes’ factor between two PMC runs together with the Jeffrey scale.

`evidence_list.pl` prints a list of evidences for a number of PMC runs.

6.5. Reparameterisation

`remap.sh` swaps and removes parameters from a MCMC or PMC run. The histogram files, mean and covariances are remapped. This is useful if different runs are to be reduced to a common parameter set for comparison or joint plotting. The removal of parameters is equivalent to marginalisation over the corresponding parameter subspace.

For example, suppose there is a SNIa run in directory `Sn`, and a lensing run in `Lensing`. SNIa has the following parameters:

Omegam OmegaDE w0DE M alpha beta
6. Post-processing and auxiliary programs

Lensing has the parameters:

\texttt{Omega_m \; \sigma_8 \; \omega_de \; \Omega_m \; \omega_de \; h100}

In \texttt{Sn}, create the file \texttt{remap.dat} with the line

0 1 2

In \texttt{Lensing}, create the file \texttt{remap.dat} with the line

0 3 2

In both directories run the command

\texttt{> remap.sh -i iter\_<niter-1>}

which creates sub-directories \texttt{remap} containing symbolic links and/or copies of histogram files to/from \texttt{iter\_[niter-1]}, mean, covariance files and updated configuration files.

To create joint marginal plots, simply run

\texttt{> plot_contours2d.pl -c /path/to/Sn/remap/config.pmc -n /path/to/Sn/remap /path/to/Lensing/remap}

New parameters, sampled from a flat or Gaussian distribution, can be added using \texttt{add\_par\_from\_prior.pl}

6.6. Analysis

6.6.1. \texttt{mvdens/mix\_mvdens} format utilities

See Sect.\texttt{A.3} for a description of the \texttt{mvdens} and \texttt{mix\_mvdens} formats.

\texttt{fisher\_to\_meanvar.pl} reads a \texttt{mvdens} file, inverts the covariance matrix and prints the mean and variance.

\texttt{corr\_coeff.sh} reads a \texttt{mvdens} or block matrix file and prints the correlation matrix of the covariance.

\texttt{diag\_mvdens.pl} replaces the covariance by its diagonal.

\texttt{add\_par\_to\_mvdens.pl} adds parameters to a \texttt{mvdens} file. Useful, if CosmoPMC is run with additional parameters, and the initial proposal is chosen from a previous run with the reduced parameter set.
7. Using and modifying the code

6.6.2. PMC simulation/MCM chain utilities

`sample2fixpar.pl` reads a sample file and fixes a parameter by cutting off all points outside a given (narrow) range.

6.6.3. PMC proposal diagnostics

`neff_proposal.pl` calculates the effective number of components (eq. [5]). It is the same quantity which is printed to the file `enc`.

7. Using and modifying the code

7.1. Modifying the existing code

Note: Code to be used with MPI should not contain global variables and static variables.

7.2. Creating a new module

In this section, the steps required to add a new cosmology module to CosmoPMC are described.

1. Create the directory `newmodule` and create (or copy) files with the necessary code to deal with the data and likelihood. Include files (`*.h`) should be in `newmodule/include`, source files (`*.c`) in `newmodule/src`. Edit the (or create a new) Makefile (in `newmodule`) and add the rules `libnewmodule.so`, `libnewmodule.dylib` and `libnewmodule.a` as well as the rule `clean`.

2. In `wrappers/include/types.h`:
   Define a new data type by extending the enumeration `data_t`. Add the corresponding string (for identification of the module in the configuration file) in the macro `sdata_t(i)`, and increase `Ndata_t` by one.

3. In `wrappers/include/all_wrappers.h`:
   Add the line
   ```
   #include "newmodule.h"
   ```

4. In `tools/include/par.h`:
   If necessary, add new parameter types (p_newparameter) to enumeration `par_t`, add the corresponding identifier strings to the macro `spar_t`, and increase `Npar_t` by one.

Optional: Add the parameter name and syntax for different programs (e.g. `gnuplot`, `yorick`, `\LaTeX`) to `bin/spar.txt`. 
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5. In wrappers/src/wrappers.c:
   Add the corresponding case to the ‘switch’ instruction in the function init_func.t. This function sets the data type.

6. Create the files wrappers/include/newmodule.h and wrappers/src/newmodule.c. (Those files need to have different names than the files in newmodule/{src,include}.)
   Write the following functions:
   a) init_function_newmodule
   b) read_from_config_newmodule
   c) init_newmodule
   d) likeli_newmodule (returning log \( L \))
   e) special_newmodule (optional)
   f) print_newmodule (optional)
   To see what these functions are supposed to do, have a look at already existing modules, e.g. in bao.c.

7. In Makefile.main:
   a) In the section “Additional directories”, define the path to the new module’s directory as
      \[ \text{NEWMODULE} = $(COSMOPMC)/newmodule \]
   b) In the section “Libraries”, define the library of the new module as
      \[ \text{LIBNEWMODULE} = libnewmodule.$(EXT) \]
   c) In the section “Combined cosmo include and linker flags”, add the following flags:
      - \[ -I$(NEWMODULE)/include \] to the variable IINCDIRS
      - \[ -L$(NEWMODULE) \] to LLIBDIRS
      - \[ -lnewmodule \] to LLIBS.

8. In exec/Makefile:
   Define the new rule:
   \[ $(LIBNEWMODULE): \]
   \[ \text{cd} \ $(NEWMODULE) \ & \ $(MAKE) \ @ \]
   (The second line has to start with a <TAB> and not with spaces.)

9. Optional: Extend newdir_pmc.sh
7. Using and modifying the code

7.3. Error passing system

Most of the situations where an error occurs are intercepted by the program. In such a case, a variable *err of type error* is set via the macros

*err = addError(error_type, "message", *err, __LINE__);

or

*err = addErrorVA(error_type, "formatted message", *err, __LINE__, VA_LIST);

printing the current line and function in the code, a message and the error type (negative integer). With

testErrorRet(test, error_type, "message", *err, __LINE__, return_value);

or

testErrorRetVA(test, error_type, "formatted message", *err, __LINE__, return_value, VA_LIST);

a conditional error is produced if the (Boolean) expression test is true. The error is transported up the stack to the calling function with the macro

forwardError(*err, __LINE__, return_value);

Omit return_value in case of a void function. This can be used as diagnostics even for errors deep in the hierarchy of functions.

During the calculation of the importance weights, any error is intercepted and the corresponding point does not contribute to the final sample. See Sect. for more details. Therefore, in the routines which calculate the importance weights, the following is used:

forwardErrorNoReturn(*err, __LINE__, return_value);

ParameterErrorVerb(*err, param, quiet, ndim);

In case of an error, the first line forwards the error but does not return from the current routine. The second line prints the ndim-dimensional parameter param to stderr (if quiet! =1) and purges the error.

To exit on an error, use

40
quitOnError(*err, __LINE__, FILE)

This is usually done only from the main program.

More macros and functions regarding error communication and handling can be found in the files `errorlist.h`, `errorlist.c` which are part of `pmclib`.

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\(^7\) [http://www.roe.ac.uk/~jap/haloes](http://www.roe.ac.uk/~jap/haloes)

\(^8\) [http://www.lanl.gov/projects/cosmology/CosmicEmu](http://www.lanl.gov/projects/cosmology/CosmicEmu)
7. Using and modifying the code

**PMC references**

Introductory papers on PMC

| Author(s)               | Year | Title |
|-------------------------|------|-------|
| Cappé et al.            | 2004 | Population Monte Carlo |
| Cappé et al.            | 2008 | Adaptive importance sampling in general mixture classes |

Comparison of sampling methods including PMC

| Author(s)               | Year | Title |
|-------------------------|------|-------|
| Robert & Wraith         | 2009 | Computational methods for Bayesian model choice |

Main papers on CosmoPMC

| Author(s)               | Year | Title |
|-------------------------|------|-------|
| Wraith et al.           | 2009 | Estimation of cosmological parameters using adaptive importance sampling |
| Kilbinger et al.        | 2010 | Bayesian model comparison in cosmology with Population Monte Carlo |

PMC applied to cosmological data

| Author(s)               | Year | Title |
|-------------------------|------|-------|
| Schrabback et al.       | 2010 | Evidence of the accelerated expansion of the Universe from weak lensing tomography with COSMOS |
| Ménard et al.           | 2010 | On the impact of intergalactic dust on cosmology with Type Ia supernovae |
| Benabed et al.          | 2009 | TEASING: a fast and accurate approximation for the low multipole likelihood of the cosmic microwave background temperature |
| Coupon et al.           | 2012 | Galaxy clustering in the CFHTLS-Wide: the changing relationship between galaxies and haloes since \( z \sim 1.2 \star \) |
| Kilbinger et al.        | 2012 | CFHTLenS: Combined probe cosmological model comparison using 2D weak gravitational lensing |
| Benjamin et al.         | 2012 | CFHTLenS tomographic weak lensing: Quantifying accurate redshift distributions |
| Simpson et al.          | 2012 | CFHTLenS: Testing the Laws of Gravity with Tomographic Weak Lensing and Redshift Space Distortions |

Other publications which use PMC

| Author(s)               | Year | Title |
|-------------------------|------|-------|
| Joachimi & Taylor       | 2011 | Forecasts of non-Gaussian parameter spaces using Box-Cox transformations |
| Beaujean et al.         | 2012 | Bayesian fit of exclusive \( b \rightarrow s \ell \ell \) decays: the standard model operator basis |
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A. File formats

A.1. Data files

A.1.1. Lensing

For all $\text{lensdata}_t$ types, the data format is the same. Each line contains the data for a given angular scale and (arbitrary many) redshift bin pair combinations.

The angular scales are defined as follows. For $\text{lensformat} = \text{angle}_\text{center}$, the first column contains the angular bin center in arc minutes. For the cases $\text{lensformat} = \text{angle}_\text{mean}$,
angle\_wlinear and angle\_wquad\_r, first two columns specify the lower and upper end of the angular bin.

Following the angular information are the data. For $N_z$ redshift bins, $N_z(N_z + 1)/2$ columns specify all pair combinations $(i,j)_{i\leq j}$ in lexical order, that is (11)(12)(13)…($N_z$)(22)(23)…($N_z$)$N_z$). Note that for lensdata = xipm the first $N_\theta$ lines of the data file contain $\xi_+$ for $N_\theta$ angular scales, the last $N_\theta$ lines contain $\xi_-$, where the angular scales (first or first two columns) are identical in both halves.

The covariance matrix is in block format: It consists of $N$ lines and $N$ columns, where $N = N_sN_z(N_z + 1)/2$ is the length of the data. Usually, $N_s$ is the number of measured angular scales, $N_\theta$, unless there is more than one data point per scale (e.g. for lensdata = xipm, $N_s = 2N_\theta$).

A matrix element $C_{ij}$ equals $\langle d_i d_j \rangle - \langle d_i \rangle \langle d_j \rangle$, where $d_i$ is the $i^{th}$ data point. In the counting over angular scale and redshift, the former varies faster than the latter\[9\]. For example, with two redshift bins and three angular scales, the element $C_{77}$ is the data variance for the redshift pair (11) and angular scale $\theta_1$ (starting counting at zero). Or, in other words, the covariance matrix consists of $N_z(N_z + 1)/2$ block sub-matrices, each of size $N_s \times N_s$. Each sub-matrix corresponds to one redshift bin combination. It is therefore easy to exclude some redshift bins, by (1) setting the diagonal of a sub-matrix to a very high value, and (2) setting the off-diagonal to zero (see the $\text{Nexclude}$ parameter in the config file, Table [?]).

\[A.1.2. SNIa\]

The SNIa data file in SNI\_SALT format starts with the following two lines:

@INTRINSIC\_DISPERSION double
@PECULIAR\_VELOCITY double

The peculiar velocity value is in units of km/s. This is followed by a list of supernovae, one object on each line as follows:

name z m s c $< m^2 >$ $< s^2 >$ $< c^2 >$ $< ms >$ $< mc >$ $< sc >$

\[A.1.3. BAO\]

The BAO distance measures are modeled as Gaussian variables, the data files are in mvdens format (see Sect. [A.3]). In the same file, following the mvdens data, there is a list of redshifts, corresponding to where the distances are measured.

\[\text{\footnotesize*This was wrongly stated here until version 1.01.}\]
A. File formats

A.1.4. CMB

The CMB data for WMAP are the ones released by the WMAP team. They are not included in CosmoPMC and can be obtained e.g. from the LAMBDA site\[10\].

The SZ correction power spectrum file has two columns in each row containing $\ell$ and $C_\ell$, respectively. The first line has to start with $\ell = 2$.

The CMB distance priors (Komatsu et al. 2009) are given in mvdens format.

A.1.5. Redshift distribution

The first line of a file describing the redshift distribution for a redshift bin contains the type, see Sect. 4.7:

```plaintext
# nofz
```

This is followed by the list of parameter values, in the order given in Table [3]. Each parameter value has to be in a new line, with the exception of the histogram, nofz = single. In that case, the parameter lines are as follows:

```
z_0 \quad N_0 
z_1 \quad N_1 
... 
z_{n-1} \quad N_{n-1} 
z_n \quad 0
```

$N_i$ is the number of galaxies in the bin $[z_i; z_{i+1}]$. The last line denotes the upper limit of the last histogram bin $z_n = z_{\text{max}}$, followed by a zero. For nofz = single, the file has to contain two identical lines with the value of $z_0$ in each line.

A.2. Output file names

The default names of all output files are defined in stdnames.h. Edit this file and to make clean; make to set user-defined file names. Note however that some of the pre-processing scripts expect the default names.

A.3. Multi-variate Gaussian/Student-t (mvdens), mixture models (mix_mvdens)

The mvdens file format is as follows. The first (header) line contains four integers:

\[10\]http://lambda.gsfc.nasa.gov
A. File formats

$p \nu B \ c.$

Here, $p$ is the number of dimensions, $\nu$ the degrees of freedom. For a multi-variate Gaussian, choose $\nu = -1$, and $\nu > 0$ for Student-t. $B$ indicates the number of secondary diagonal of the covariance matrix which are updated during the PMC iterations. For most purposes, $B$ can be set equal to $p$, which corresponds to the whole matrix being updated. Finally, $c$ is 1 if the matrix is Cholesky-decomposed and 0 otherwise.

This is followed by $p$ doubles indicating the mean, followed by $p$ lines with $p$ doubles each, giving the (symmetric) covariance matrix.

Here is an example of a 5-dimensional multi-variate Gaussian (not Cholesky-decomposed):

5 -1 5 0
0.38559 -1.5238 19.338 1.3692 -2.4358
0.0053677 -0.0011893 0.00087517
-0.025608 0.16837 -0.0079163 0.0027364 -0.0035709
0.0006748 -0.0079163 0.0011077 0.0010986 -0.00067815
-0.0011893 0.0027364 0.0010986 0.016716 0.0026266
0.00087517 -0.0035709 -0.00067815 0.0026266 0.014881

The mix_mvdens format has two doubles as the header:

$D \ p$

where $D$ is the number of components of the mixture and $\text{ndim}$ the dimension. This is followed by $D$ blocks specifying the weights $w_d$ (doubles) and data $m_d$ (in mvdens format) of the $D$ multi-variate densities of the mixtures.

$$w_1 \ m_1 \ w_2 \ m_2 \ \ldots \ w_D \ m_D.$$  

The weights should be normalised, $\sum_{d=1}^{D} w_d = 1$.

In many cases, an mvdens file indicates a parameter covariance matrix, for example to be used as Gaussian prior using the config file flag $\text{sprior}$. In some cases, the inverse covariance matrix is expected, as in the case of the Fisher matrix.
B. Syntax of all commands

All following scripts are located in `$COSMOPMC/bin`. All programs (executables) are located in `$COSMOPMC/exec` and linked from `$COSMOPMC/bin` after running `make` in `$COSMOPMC`.

- **add_deduced_halomodel**
  
  Usage: `add_deduced_halomodel [OPTIONS] PSIM [PAR_1 [PAR_2 [...]]]

  OPTIONS:
  - `-c CONFIG` Configuration file (default: config_pmc)
  - `-o OUTNAME` Output pmcsim name (default: psim+ded)
  - `PSIM` pmc simulation file (pmcsim_iter)
  - `PAR_i` String for deduced parameter #i. If not given, deduced parameters are read from the config file (default)

- **add_par_from_prior.pl**
  
  Usage: `add_par_from_prior.pl [OPTIONS] sample`

  Adds a new random parameter to a PMC sample file, drawn under a distribution

  OPTIONS:
  - `-o OUT` Output sample file OUT (default: '<sample>.out')
  - `-p DIST` Prior distribution, DIST one of 'Flat' (default), 'Gauss'
  - `-P ARG` Prior arguments (white-spaced list if more than one). For DIST = Flat: ARG = 'min max' (default '-1 1')
    Gauss: ARG = 'mean sigma'
  - `-C COL` Column COL of new parameter (default: last)
  - `-s STR` Name string STR of new parameter
  - `-h` This message

- **add_par_to_mvdens.pl**
  
  Usage: `add_par_to_mvdens.pl [OPTIONS] FILE`

  Adds a parameter to a (mix)mvdens file (e.g. Fisher matrix, PMC proposal)

  OPTIONS:
  - `-c COL` Adds parameter in column and row COL (default: last column)
  - `-m VAL` Parameter mean VAL (default 0)
  - `-v VAL` Parameter variance VAL (default 1)
  - `-x` File is in 'mixmvdens' format
  - `-h` This message

- **bayes_factor.pl**
  
  Usage: `bayes_factor.pl [OPTIONS] DIR1 DIR2`

  Calculates the Bayes factor between models. The corresponding evidence files (from PMC) have to be in the directories DIR1 and DIR2

  OPTIONS:
  - `-i 'ITER1 [ITER2]'` Use iteration ITER1 for DIR1 and ITER2 for DIR2 (default: all iterations)
  - `-f 'EVI1 [EVI2]` Use files DIR1/EVI1 and DIR2/EVI2 (default: 'evidence')
  - `-s` Short output, last iteration only
  - `-l` Laplace approx. from Fisher matrix (denoted with iter=-1)
  - `-h` This message

- **cl_one_sided**
B. Syntax of all commands

Usage: cl_one_sided [OPTIONS] sample
OPTIONS:
- c CONFIG Configuration file (default: config_pmc)
- i INDEX Parameter index
- d DIR Direction (DIR=+1,-1)
- v VALUE Starting value
- w WHICH WHICH=0: 68%,95%,99.7% c.l. (default)
     WHICH=1: 68%,90%,95% c.l.
sample
The options -i INDEX, -d DIR and -v VALUE are required

• config_pmc_to_max_and_fish.pl

Usage: config_pmc_to_max_and_fish.pl [OPTIONS]
OPTIONS:
- M Create config file for maximum search (max_post)
- F Create config file for Fisher matrix (go_fishing)
- c CONFIG Input PMC config file CONFIG (default: 'config_pmc')
- r Random starting point (for maximum search)
- f FID Fiducial starting point FID. FID is a white-space
     separated list in quotes, e.g. '0.25 0.75'
- p FILE Fiducial parameter from FILE (e.g. 'maxlogP')
- t TOLERANCE Tolerance for maximum-search (default: 0.01)
- d Calculate only diagonal of Fisher matrix (go_fishing)
- h This message
One of '-M' or '-F' is obligatory
The default starting point for maximum search is (max-min)/2
For Fisher matrix ('-F'), a fiducial parameter has to be indicated with '-f FID'
     or '-p FILE'

• corr_coeff.sh

Usage: corr_coeff filename [mvdens|block]

• cosmo_mcmc

Usage: cosmo_mcmc [OPTIONS]
OPTIONS:
- c CONFIG Configuration file (default: config_mcmc)
- s SEED Use SEED for random number generator. If SEED=-1 (default)
     the current time is used as seed.
- h This message

• cosmo_pmc

Usage: cosmo_pmc [OPTIONS]
OPTIONS:
- c CONFIG Configuration file (default: 'config_pmc')
- s SEED Use SEED for random number generator. If SEED=-1 (default)
     the current time is used as seed.
- q Quiet mode
- h This message

• cosmo_pmc.pl

Usage: cosmo_pmc.pl [OPTIONS]
B. Syntax of all commands

OPTIONS:
- \( n \) NCPU Run PMC in parallel on NPCU cpus using 'mpirun' (default: 1)
- \( c \) CONFIG Configuration file for PMC (default: config_pmc)
- \( f \) FID Fiducial starting point FID. FID is a white-space separated list in quotes, e.g. '0.25 0.75'
- \( r \) Random starting point for maximum search (default: (max-min)/2)
- \( m \) Maximum-search method: 'c' (cg), 'a' (amoeba)
- \( d \) Calculate only diagonal of Fisher matrix
- \( D \) Do not force Fisher matrix \( F \) to be positiv. If \( F \) is negative, script exits with an error
- \( a \) Adaptive numerical differentiation for Fisher matrix
- \( s \) SEED Use SEED for random number generator. If SEED=-1 (default) the current time is used as seed.
- \( S \) Stops after maximum search ('M') or Fisher matrix ('F')
- \( A \) Default answer to all questions on stdin
- \( P \) PATH Use PATH as CosmoPMC directory (default: environment variable $COSMOPMC)
- \( e \) Create 'essential' plots
- \( p \) PRO Plotting scripts: 'y' (yorick; default), 'R' (R) or 'n' (none) Combinations of letters are possible, e.g. 'yR'
- \( M \) Output sample MULT times input (default 1) Valid if plotting script is 'R'
- \( O \) Pass options OPT to 'plot_contour2d.pl'
- \( q \) Quiet mode
- \( h \) This message

• diag_mvdens.pl
Usage: diag_mvdens.pl IN
Prints the mvdens file 'IN' with the covariance replaced by its diagonal.

• essential_cosmo_pmc_run.pl
Usage: essential_cosmo_pmc_run.pl [OPTIONS]
OPTIONS:
- \( c \) CONFIG Uses config file CONFIG (default: 'config_pmc')
- \( P \) PATH Use PATH as CosmoPMC directory (default: environment variable $COSMOPMC)
- \( k \) Keep temporary files
- \( v \) Verbose
- \( h \) This message

• evidence.pl
Usage: evidence.pl [OPTIONS] SAMPLE
OPTIONS:
- \( h \) This message
SAMPLE PMC sample file

• evidence_list.pl
Usage: evidence_list.pl [OPTIONS] DIR1 [DIR2 [...]]
OPTIONS:
- \( r \) N Subtract log(E) from DIRN (default: no subtraction)
B. Syntax of all commands

For $N=-1$ subtract $\log(E_{\min})$

- $k$ KEY Use KEY (string list) instead of directory names (default)
- $s$ SEP Use SEP as input separator for KEY list
- $S$ SEP Use SEP as output separator (default for both: white-space)
- $n$ Write number of model parameters
- $L$ Use Laplace approximation (reading file 'evidence_fisher')
- $h$ This message

**fisher_to_meanvar.pl**

fisher_to_meanvar.pl [OPTIONS] file

OPTIONS:

- $n$ No inverse
- $m$ Marginal errors (don't invert matrix)
- $x$ mixmvdens format (default: mvdens format)
- $k$ Keep temporary file 'fishtmp.i'
- $h$ This message

Options '-m' and '-n' exclude each other

**get_spar.pl**

Usage: get_spar.pl [OPTIONS] LANG [PAR1 [PAR2 [...]]]

OPTIONS:

- $c$ CONFIG Configuration file ONFIG (default 'config_pmc')
- $i$ INDEX Returns only par[INDEX]
- $P$ PATH Use PATH as CosmoPMC directory (default: environment variable $COSMOPMC)
- $p$ Print 'p<i>' for unknown parameters instead of input string
- LANG One of 'yorick', 'gnuplot', 'TeX', 'R'. More languages can be defined in spar.txt
- PAR1 ... Parameter strings

**go_fishing**

Usage: go_fishing [OPTIONS]

OPTIONS:

- $c$ CONFIG Configuration file (default: config_fish)
- $a$ Adaptive numerical differentiation (default: fixed difference)
- $f$ Force positive Fisher matrix
- $q$ Quiet mode
- $h$ This message

Run in parallel on NP cpu's: 'mpirun -np NP go_fishing [OPTIONS]

**haloplot**

Usage: haloplot log10(M_min) log10(M1) log10(M0) sigma_log_M alpha_halo halomodel.par [OPTIONS]

Outputs HOD-derived quantities

OPTIONS:

- $o$ OUT Output file name
- $t$ TYPE Output type, TYPE in [wtheta, wp, xi, xi halo, deltaSig, nofm, halo, pk], default: wtheta
- $nbins$ Number of bins
B. Syntax of all commands

- **-range** Range (linear scale): min,max
- **-z Z** Used fixed redshift Z (no w(theta) output)
- **-Mhalo log10M** log10(Halo mass) for deltaSig and xihalo (in M_{sol}/h)
- **-c CONFIG** PMC config file, to calculate chi^2
- **-h** This message

M_min, M1 and M0 are in units of M_{sol}/h.

• **histograms_sample**

Usage: histograms_sample [OPTIONS] sample

OPTIONS:
- **-c CONFIG** Configuration file (default: config_pmc)
- **-1** Only 1d histograms
- **-2** Only 2d histograms
- **sample** PMC sample file
- **-h** This message

• **importance_sample**

Usage: importance_sample [OPTIONS] INSAMPLE

Performs an importance run on a PMC sample. Run in parallel with MPI (use mpirun)

OPTIONS:
- **-c CONFIG** Configuration file (default: config_pmc)
- **-o OUTSAMPLE** Output sample name (default: 'insample.out')
- **-q** Quiet mode
- **-h** This message
- **INSAMPLE** Input sample name

• **max_post**

Usage: max_post [OPTIONS]

OPTIONS:
- **-c CONFIG** Configuration file (default: config_max)
- **-m [c|a|n]** Maximum-search method: 'a' (amoeba, default), 'c' (cg), 'n' (none; print posterior for fiducial parameter and exit)
- **-t** Test maximum at the end
- **-s SEED** Use SEED for random number generator. If SEED=-1 (default) the current time is used as seed.
- **-p** Prints the maximum-posterior model to the file 'model_maxlog'
- **-q** Quiet mode
- **-h** This message

• **mean2eps.pl**

Usage: mean2eps.pl [OPTIONS] MEAN

OPTIONS:
- **MEAN** File containing mean and confidence levels (output of 'cosmo_pmc' or 'histograms_sample')
- **-c CONFIG** Uses config file CONFIG (default: 'config_pmc')
- **-P PATH** Use PATH as CosmoPMC directory (default: environment variable $COSMOPMC)
- **-o BASE** Outname BASE (default: <MEAN>)
- **-v** Verbose

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B. Syntax of all commands

- meanvar2tab.pl

Usage: meanvar2tab.pl [OPTIONS] file [file2 [...]]

Options:
- -h This message
- -s [123] 68% (1), 95% (2) or 99.7% (3) errors (default = 1)
- -p PREC Output with PREC digits ('%PREC' format string)
- -e Error(s) written to PREC significant digits (use -p PREC)
- -c CONFIG Uses config file CONFIG (default: 'config_pmc')
- -t TITLE Title (table heading) TITLE is string list with entries according to the number of input files
- -S SEP Use SEP as input separator for TITLE list (default: white space)
- -P PATH Use PATH as CosmoPMC directory (default: environment variable $COSMOPMC)
- -h This message

- meanvar_sample

Usage: meanvar_sample [OPTIONS] sample

OPTIONS:
- -c CONFIG Configuration file (default: config_pmc)
- -w Ignore weights (default: weights=first column of sample file)
- -C Write covariance and inverse covariance to files
- -E Output evidence
- -h This message

- neff_proposal.pl

Usage: neff_proposal.pl PROP

Calculates the effective number of components for the mix_mvdens file 'PROP'

- newdir_pmc.sh

Usage: newdir_pmc.sh [DIR]

Directory DIR (default: read on input) is created.
Links are set to data files in \$COSMOPMC/data.
Parameter files are copied on request from \$COSMOPMC/par_files.

- plot_confidence.R

Usage: plot_confidence.R [options]

Options:
- -h, --help
  Show this help message and exit
- -N NGRID, --Ngrid=NGRID
  Number of grid points for smoothing (kde2d) (default 100). Use <=30 for fast-but-dirty plots
- -g GSMOOTH, --gsmooth=GSMOOTH
  Smoothing kernel width, with respect to box size (default 30). In case of more
B. Syntax of all commands

than one sample, use list separated with '_' for more than value

-S, --solid
All contours with solid lines

-w WIDTH, --width=WIDTH
Line width (default 1)

-k, --with_keys
Add key to plots

-K KEYSTRING, --keystring=KEYSTRING
Key strings (separate items with '_')

-L, --no_key_line
Do not add a line to the keys in the legend

-c CONFIG, --config=CONFIG
Config file (default 'config_pmc')

-t TITLE, --title=TITLE
Title string for each panel (default empty)

-i INDEX_I, --index_i=INDEX_I
Only create plots with i-th parameter on x-axis

-j INDEX_J, --index_j=INDEX_J
Only create plots with j-th parameter on y-axis

-s SIGMA, --sigma=SIGMA
Plot SIGMA confidence levels (default 3)

-F COLOR_SCHEME, --color_scheme=COLOR_SCHEME
Color scheme (0, 1; default 0)

• plot_contour2d.pl

Usage: plot_contour2d.pl [OPTIONS] [DIR1 [DIR2 [...]]]

OPTIONS:
-i NITER Number of iterations (needed if do_proposal=2)
-c CONFIG_FILE Configuration file (default: in order config_mcmc, config_pmc)
-t TITLE Title string for each panel (default empty)
-T TITLE Title string for all_contour2d.{eps|pdf} (default empty)
-n No shade
-w WIDTH Line width WIDTH (default 4)
-1 OPT Add 1d posterior plots. OPT can contain the following letters:
  m Plot line at mean position
  123 Plot line at 68%, 95%, 99.7 density
B. Syntax of all commands

- Write mean and 68% confidence intervals as text
  (use with ‘m’ and ‘l’)
- All contours with solid lines
- Outermost level is N sigma
-Aspect ratio=1, changes plot limits such that dx=dy
- Gaussian smoothing of 2d-histograms with variance
  box-width/|FACTOR|. If FACTOR is negative, plots
  unsmoothed histogram in addition (use with ‘-n’).
  Note: For multiple contours, use a list of values “g1 g2 ...”
- Gaussian smoothing of 1d-histograms (default: 2d factor)
- Use covariance (file covar.fin) for Gaussian smoothing
- Normalisation of 1d posterior
  ‘m’ Maximum = 1 (default)
  ‘i’ Integral over posterior = 1
- Color scheme, NUM=0,1,2
- Add key to plots
- “KEY1 [KEY2 [...]” Key strings (default: directory names)
- Font size FS (default 24)
- Output file format, FORMAT=eps|pdf (default: eps)
- Writes the chi2 files in block format
- Plots a mark at position PAR (e.g. best-fit). PAR is white-space
  separated list (use quotes or ‘\’, e.g. ‘0.3 0.8’)
- Use PATH as CosmoPMC root directory (default: environment
  variable $COSMOPMC)
- Run quietly, no verbose
- This message

• proposal_mean.pl

Usage: proposal_mean.pl [OPTIONS]
OPTIONS:
- Directory DIR containing the sub-directories ‘iter_*’
  with the proposal files (default ‘.’)
- Configuration file CONFIG (default ‘DIR/config_pmc’)
- No plotting, only creates ‘.gnu’ file
- x- and y-axes inverted
- x- and y-labels on top/right
- Use PATH as CosmoPMC root directory (default: environment
  variable $COSMOPMC)
- This message

• proposal_var.pl

Usage: proposal_var.pl [OPTIONS]
OPTIONS:
- Directory DIR containing the sub-directories ‘iter_*’
  with the proposal files (default ‘.’)
- Configuration file CONFIG (default ‘DIR/config_pmc’)
- Use PATH as CosmoPMC root directory (default: environment
B. Syntax of all commands

variable $COSMOPMC

-h  This message

-remap.sh

Usage: remap.sh [OPTIONS]

OPTIONS:
  -c CONFIG Input PMC configuration file (default './config_pmc')
  -i INPUT Input directory INPUT (default '.')
  -s PMCSIM Sample/PMC simulation file PMCSIM
  -o OUTPUT Output directory OUTPUT (default './remap')
  -r REMAP Remap file REMAP (default './remap.dat')
  -n NPAR Number of parameters NPAR (default: read from remap file)
  -d NDED Number of deduced parameters NDED (default: 0)
  -h  This message

-sample2fixpar.pl

Usage: sample2fixpar.pl SAMPLE_IN COL MIN MAX

SAMPLE_IN Input sample (PMC simulation or MCM chain)
COL Column number of fixed parameter 
  (Note that par #i is in column i+2)
MIN, MAX Minimum and maximum values for fixed parameter

-tab2tex.pl

Usage: tab2tex.pl [OPTIONS] file

OPTIONS:
  -a Produce tex array, not tex table
  -b Bare output, no table/array header
  -s STRETCH Set arraystretch to STRETCH
  -m Add '$' around entries (tex inline math mode)
  -l MODE Print vertical lines between rows according to MODE;
  a  all lines (default)
  n  no lines
  h  header lines
  -L MODE Print horizontal lines between columns according to Mode:
  a  all lines (default)
  n  no lines
  -h  This message

-test_suite_cosmo_pmc.pl

Usage: test_suite_cosmo_pmc.pl [OPTIONS]

OPTIONS:
  -r Do PMC test runs
  -R Only do PMC test runs
  -n NCPUS Run PMC in parallel on NCPUS cpus (default: 1)
  -c Include CMB tests
  -P PATH Use PATH as CosmoPMC root directory (default: environment variable $COSMOPMC)
  -s Short, without time-taking PMC runs (e.g. Lensing/COSMOS-S10)
  -k Keep temporary files
  -x Clean previous run and exit
We provide a Metropolis-Hastings Monte-Carlo Markov Chain sampler, which is included in the CosmoPMC package. This MCMC implementation has been used in Wraith et al. (2009) in the comparison with PMC. In the following, we briefly describe our MCMC program.
Table 13: MCMC section of the configuration file

| Parameter | Type    | Description                                                                 |
|-----------|---------|-----------------------------------------------------------------------------|
| nchain    | integer | Chain Length                                                                |
| ncov      | integer | Interval between updates of the proposal covariance                          |
| fburnin   | double  | Burn-in phase are the first $n_{cov} \times n_{cor}$ points                 |
| ndecorr   | double  | De-correlation (thinning-out): one in $n_{dec}$ points is kept in the final chain |
| fudge     | double  | Proposal covariance is multiplied by $fudge^2/n_{par}$                      |
| sinitial  | string  | Initial proposal type, one of Fisher, Fisher, Fisher, previous, Hessian, Hessian_diag, diag. |
| boxdiv    | double  | Diagonal of proposal covariance is $(\text{max-min})/\text{boxdiv}$         |
| sstart    | string  | Starting point type, one of ran, fid, min, max, nul                        |
| fid       | double  | Starting parameter                                                          |
| nbinhist  | integer | Number of density histogram bins                                            |

*only if sinitial = diag
*only if sstart = fid

C.1. MCMC configuration file

C.2. Proposal and starting point

The proposal for the Metropolis-Hastings algorithm is a multi-variate Gaussian distribution. After choosing an initial proposal, a new proposal can optionally be re-calculated after a number of ncov (accepted) steps. The covariance of this new proposal is the chain covariance from steps up to this point. This proposal is then updated after each ncov accepted steps using all previous accepted points.

There are several options for the initial proposal:

1. **sinitial = diag** A diagonal covariance with width being a fraction of the box size.
2. **sinitial = Fisher** The Hessian at a given point in parameter space. If this point is the maximum-likelihood point, the Hessian corresponds to the Fisher matrix.
3. **sinitial = Fisher_inv** The inverse Hessian/Fisher matrix, e.g. the covariance from a previous chain. This can be useful for ill-conditioned matrices which are difficult to invert numerically.
4. **sinitial = previous** A proposal read from a file, e.g. from a previous MCMC run.

The starting point is either chosen randomly or specified in the config file. The second case might be convenient if the prior volume is very large and a very long burn-in phase is to be
avoided. For example, the ML-point or best-fit value from a previous experiment can be chosen [Dunkley et al. (2009)]

C.3. Output files

The MCMC output files have the same format as their PMC counterparts (see Sect. 3.3.2). A complete run of cosmo_mcmc produces three files containing the points of the Markov chain:

1. chain.all containing all, accepted and rejected, sample points. This is the only chain file will not be read or used in subsequent calls of cosmo_mcmc.
2. chain.acc containing the accepted points.
3. chain.fin containing the accepted points after removal of the burn-in phase and after de-correlating (thinning-out) the chain. The results produced by cosmo_mcmc (mean, errors, histograms, covariance) are based on this file.

The chains are ASCII-files, in the same format as the PMC sample files. All weights are 1, and the second column contains the log-likelihood (only in chain.all).

The parameter mean and confidence intervals are printed to the file mean. The names of files containing the histograms and parameter covariances are the same as for PMC.

C.4. Diagnostics

In general it is not straight-forward to diagnose an MCM chain. There exists tests but no formal proofs for convergence (e.g. Gellman-Rubin), which in addition require very long or multiple chains. We have not implemented such tests in the code. However, there are a few (rather hand-waving) diagnostic tools to check the reliability of an MCMC run.

Firstly, the acceptance rate $\eta$ should be in the range between 15% and 25%. A larger $\eta$ most probably corresponds to a chain which stayed mainly in the high-density region and strongly under-sampled the lower-density posterior regions. In that case the error bars will be underestimated. A very small $\eta$ means probably an under-sampling of the posterior since only few points are accepted. However, this need not cause a bias for the parameters and errors if the chain has been run long enough.

C.5. Resuming an interrupted run

Sometimes a MCMC run is interrupted before finishing, or one wishes a previous run to be extended, for example because its convergence is doubted. The MCMC program allows to read in and extend a previous chain. To that end, rename the file chain.acc into chain.pre. The proposal for the resumed run can but need not be calculated from the previous chain (to be
controlled in the config file, see Sect. C.2. In the config file, the number of desired sample points has to be larger than the previous chain.