
maxsmooth Documentation

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INTRODUCTION

maxsmooth maximally smooth function fitting

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Homepage <https://github.com/htjb/maxsmooth>

`maxsmooth` is an open source software for fitting derivative constrained functions, DCFs such as Maximally Smooth Functions, MSFs to data sets. MSFs are functions for which there are no zero crossings in derivatives of order $m \geq 2$ within the domain of interest. They are designed to prevent the loss of signals when fitting out dominant foregrounds and in some cases can be used to highlight systematics left in the data. More generally for DCFs the minimum constrained derivative order, m can take on any value or a set of specific high order derivatives can be constrained.

You can read more about MSFs here ..

`maxsmooth` uses quadratic programming implemented with `CVXOPT` to fit data subject to a linear constraint. The constraint on an MSF can be coded like so,

$$\frac{d^m y}{d x^m} \geq 0 \text{ or } \frac{d^m y}{d x^m} \leq 0.$$

This constraint is itself not linear but `maxsmooth` is designed to test the constraint,

$$\pm \frac{d^m y}{d x^m} \leq 0$$

where a positive sign in front of the m^{th} order derivative forces the derivative to be negative for all x . For an N^{th} order polynomial `maxsmooth` can test every available sign combination but by default it implements a ‘sign-sampling’ algorithm. This is detailed in the `maxsmooth` paper (see citation) but is summarised below.

The available sign combinations act as discrete parameter spaces all with global minima and `maxsmooth` is capable of finding the minimum of these global minima by implementing a descent algorithm which is followed by a directional exploration. The descent routine typically finds an approximate to the global minimum and then the directional exploration is a complete search of the sign combinations in the neighbourhood of that minimum. The searched region is limited by factors that encapsulate enough of the neighbourhood to confidently return the global minimum.

The sign sampling method is reliant on the problem being ‘well defined’ but this is not always the case and it is in these instances possible to run the code testing every available sign combination on the constrained derivatives. For a definition of a ‘well defined’ problem and its counter part see the `maxsmooth` paper.

`maxsmooth` features a built in library of DCFs or allows the user to define their own. The addition of possible inflection points and zero crossings in higher order derivatives is also available to the user. The software has been designed with these two applications in mind and is a simple interface.

1.1 Instalation

1.2 Documentation

The documentation can be compiled from the git repository by...

1.3 Dependencies

Basic requirements:

- Python version..
- matplotlib
- numpy
- CVXOPT

1.4 Citation

MAXSMOOTH EXAMPLE CODES

This section is designed to introduce the user to the software and the form in which it is run. It provides basic examples of data fitting with a built in MSF model and a user defined model.

There are also examples of functions that can be used pre-fitting and post-fitting for various purposes including; determination of the best DCF model from the built in library for the problem being fitted, analysis of the χ^2 distribution as a function of the discrete sign spaces and analysis of the parameter space surrounding the optimum results.

2.1 Simple Example code

In order to run the `maxsmooth` software using the built in DCF models for a simple fit the user can follow the simple structure detailed here.

The user should begin by importing the `smooth` class from `maxsmooth.DCF`.

```
from maxsmooth.DCF import smooth
```

The user should then import the data they wish to fit.

```
import numpy as np

x = np.load('Data/x.npy')
y = np.load('Data/y.npy')
```

and define the polynomial orders they wish to fit.

```
N = [3, 4, 5, 6, 7, 8, 9, 10, 11]
for i in range(len(N)):
    `act on N[i]`
```

or for example,

```
N = 10
```

`smooth` can be called like so,

```
result = smooth(x, y, N, **kwargs)
```

where the `kwargs` are detailed below. It's resulting attributes can be accessed by writing `result.attribute_name`. For example printing the outputs is done like so,

```
print('Objective Funtion Evaluations:\n', result.optimum_chi)
print('RMS:\n', result.rms)
print('Parameters:\n', result.optimum_params)
print('Fitted y:\n', result.y_fit)
print('Sign Combinations:\n', result.optimum_signs)
print('Derivatives:\n', result.derivatives)
```

2.2 New Basis Example

This example code illustrates how to define your own basis function for the DCF model. It implements a modified version of the built in normalised polynomial model but the structure is the same for more elaborate models.

As always we need to import the data, define an order N and import the function fitting routine, `smooth()`.

```
import numpy as np
from maxsmooth.DCF import smooth

x = np.load('Data/x.npy')
y = np.load('Data/y.npy')

N=10
```

There are several requirements needed to define a new basis function completely for `maxsmooth` to be able to fit it. They are as summarised below and then examples of each are given in more detail,

- **args** Additional non-standard arguments needed in the definition of the basis. The standard arguments are the data (x and y), the order of the fit N the `pivot_point`, the derivative order m and the `params`. While the `pivot_point` is not strictly needed it is a required argument for the functions defining a new basis to help the user in their definition.
- **basis_functions** This function defined the basis of the DCF model ϕ where the model can be generally defined as,

$$y = \sum_{k=0}^N a_k \phi_k(x)$$

- **model** This is the function described by the equation above.
- **derivative** This function defines the m^{th} order derivative.
- **derivative_pre** This function defines the prefactors, \mathbf{G} on the derivatives where `CVXOPT`, the quadratic programming routine used, evaluates the constraints as,

$$\mathbf{Ga} \leq \mathbf{h}$$

where \mathbf{a} is the matrix of parameters and \mathbf{h} is the matrix of constraint limits. For more details on this see the `maxsmooth` paper.

We can begin defining our new basis function by defining the additional arguments needed to fit the model as a list,

```
arguments = [x[-1]*10, y[-1]*10]
```

The next step is to define the basis functions ϕ . This needs to be done in a function that has the arguments (x , y , `pivot_point`, N , `*args`). ‘args’ is optional but since we need them for this basis we are passing it in.

The basis functions, ϕ , should be an array of dimensions `len(x)` by N and consequently evaluated at each N and x data point as shown below.


```
def basis_functions(x, y, pivot_point, N, *args):

    phi = np.empty([len(x), N])
    for h in range(len(x)):
        for i in range(N):
            phi[h, i] = args[1]*(x[h]/args[0])**i

    return phi
```

We can define the model that we are fitting in a function like that shown below. This is used for evaluating χ^2 and returning the optimum fitted model once the code has finished running. It requires the arguments (*x*, *y*, *pivot_point*, *N*, *params*, **args*) in that order and again where ‘args’ is optional. ‘params’ is the parameters of the fit *a* which should have length *N*.

The function should return the fitted estimate of *y*.

```
def model(x, y, pivot_point, N, params, *args):

    y_sum = args[1]*np.sum([
        params[i]*(x/args[0])**i
        for i in range(N)], axis=0)

    return y_sum
```

Next we have to define a function for the derivatives of the model which takes arguments (*m*, *x*, *y*, *N*, *pivot_point*, *params*, **args*) where *m* is the derivative order. The function should return the m^{th} order derivative evaluation and is used for checking that the constraints have been met and returning the derivatives of the optimum fit to the user.

```
def derivative(m, x, y, N, pivot_point, params, *args):

    mth_order_derivative = []
    for i in range(N):
        if i <= m - 1:
            mth_order_derivative.append([0]*len(x))
    for i in range(N - m):
        mth_order_derivative_term = args[1]*np.math.factorial(m+i) / \
            np.math.factorial(i) * \
            params[int(m)+i]*(x)**i / \
            (args[0])** (i + 1)
        mth_order_derivative.append(
            mth_order_derivative_term)

    return mth_order_derivative
```

Finally we have to define **G** which is used by CVXOPT to build the derivatives and constrain the functions. It takes arguments (*m*, *x*, *y*, *pivot_point*, **args*) and should return the prefactor on the m^{th} order derivative. For a more thorough definition of the prefactor on the derivative and an explanation of how the problem is constrained in quadratic programming see the maxsmooth paper.

```
def derivative_pre(m, x, y, pivot_point, *args):

    mth_order_derivative = []
    for i in range(N):
        if i <= m - 1:
            mth_order_derivative.append([0]*len(x))
    for i in range(N - m):
        mth_order_derivative_term = args[1]*np.math.factorial(m+i) / \
```

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```
        np.math.factorial(i) * \
        (x)**i / \
        (args[0])** (i + 1)
    mth_order_derivative.append(
        mth_order_derivative_term)

    return mth_order_derivative
```

With our functions and additional arguments defined we can pass these to the `maxsmooth smooth()` function as is shown below. This overwrites the built in DCF model but you are still able to modify the fit type i.e. testing all available sign combinations or sampling them.

```
result = smooth(x, y, N,
               basis_functions=basis_functions, model=model,
               derivatives=derivative, der_pres=derivative_pre, args=arguments)
```

The output of the fit can be accessed as before,

```
print('Objective Funtion Evaluations:\n', result.optimum_chi)
print('RMS:\n', result.rms)
print('Parameters:\n', result.optimum_params)
print('Fitted y:\n', result.y_fit)
print('Sign Combinations:\n', result.optimum_signs)
print('Derivatives:\n', result.derivatives)
```

2.3 Best Basis Example

This function can be used to identify which of the built in DCFs fits the data best before running joint fits.

To use it we begin by loading in the data,

```
import numpy as np

x = np.load('Data/x.npy')
y = np.load('Data/y.npy')
```

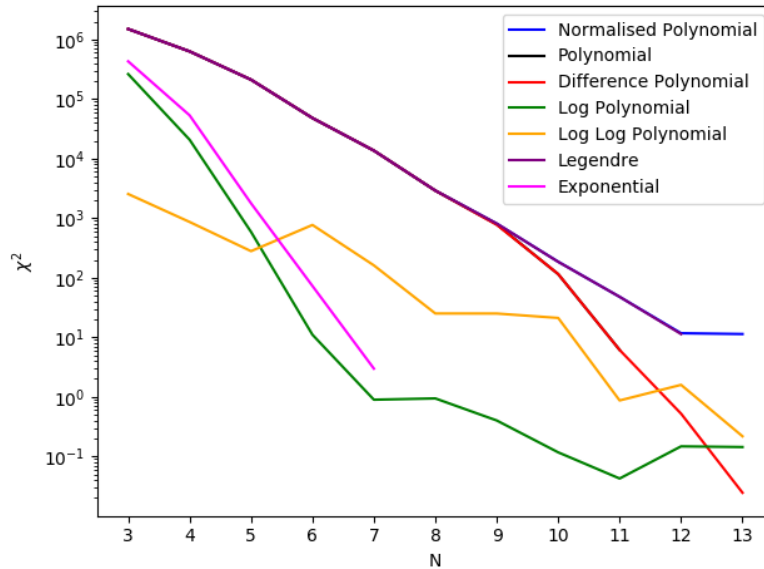
and then importing the `basis_test()` function.

```
from maxsmooth.best_basis import basis_test
```

To call the function we use,

```
basis_test(x, y, base_dir='examples/')
```

The function only requires the data but we can provide it with a base directory, fit type and range of DCF orders to test. By default it uses the sign sampling algorithm and tests $N = 3 - 13$. The resultant graph is saved in the base directory and the example generated here is shown below.



2.4 χ^2 Distribution Example

This example will show you how to generate a plot of the χ^2 distribution as a function of the discrete sign combinations on the constrained derivatives.

First you will need to import your data and fit this using `maxsmooth` as was done in the simple example code.

```
import numpy as np

x = np.load('Data/x.npy')
y = np.load('Data/y.npy')

from maxsmooth.DCF import smooth

N = 10
result = smooth(x, y, N, base_dir='examples/',
               data_save=True, fit_type='qp')
```

Here we have used some additional keyword arguments for the ‘smooth’ fitting function. ‘data_save’ ensures that the files containing the tested sign combinations and the corresponding objective function evaluations exist in the base directory which we have changed to ‘base_dir=’examples/’. These files are essential for the plotting the χ^2 distribution and are not saved by `maxsmooth` without ‘data_save=True’. We have also set the ‘fit_type’ to ‘qp’ rather than the default ‘qp-sign_flipping’. This ensures that all of the available sign combinations are tested rather than a sampled set giving us a full picture of the distribution when we plot it. We have used the default DCF model to fit this data.

We can import the ‘chi_plotter’ like so,

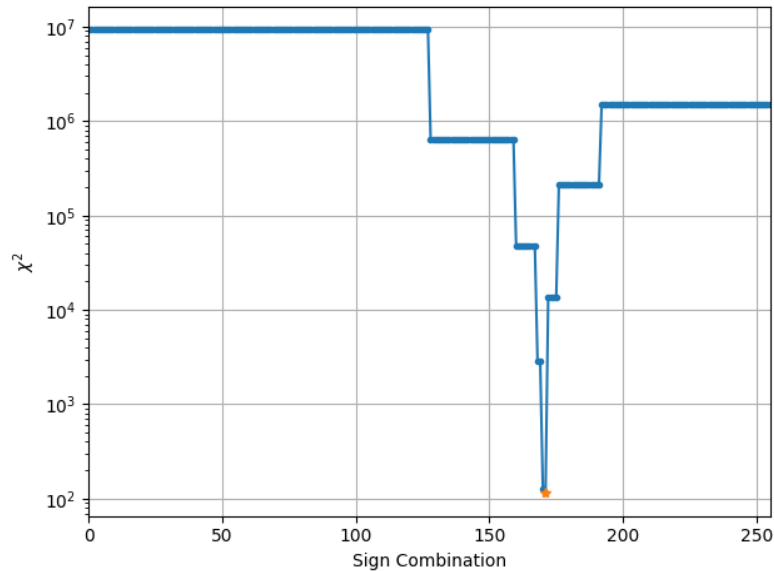
```
from maxsmooth.chidist_plotter import chi_plotter
```

and produce the fit which gets placed in the base directory with the following code,

```
chi_plotter(N, base_dir='examples/', fit_type='qp')
```

We pass the same ‘base_dir’ as before so that the plotter can find the correct output files. We also give the function the same ‘fit_type’ used for the fitting which ensures that the files can be read.

The resultant plot is shown below and the yellow star shows the global minimum. This can be used to determine how well the sign sampling approach using a descent and directional exploration can find the global minimum. If the distribution looks like noise then it is unlikely the sign sampling algorithm will consistently find the global minimum. Rather it will likely repeatedly return the local minima found after the descent algorithm and you should use the 'qp' method testing all available sign combinations in any future fits to the data with this DCF model.



2.5 Parameter Plotter Example

We can assess the parameter space around the optimum solution found using `maxsmooth` with the `param_plotter()` function. This can help us identify how well a problem can be solved using the sign sampling approach employed by `maxsmooth` or simply be used to identify correlations between the foreground parameters. For more details on this see the `maxsmooth` paper.

We begin by importing and fitting the data as with the `chi_plotter()` function illustrated above.

```
import numpy as np

x = np.load('Data/x.npy')
y = np.load('Data/y.npy')

from maxsmooth.DCF import smooth

N = 5
result = smooth(x, y, N, base_dir='examples/', fit_type='qp')
```

We have changed the order of the fit to 5 to illustrate that for order $N \leq 5$ and fits with derivatives $m \geq 2$ constrained the function will plot each region of the graph corresponding to different sign functions in a different colourmap. If the constraints are different or the order is greater than 5 then the viable regions will have a single colourmap. Invalid regions are plotted as black shaded colourmaps and the contour lines are contours of χ^2 .

We can import the function like so,

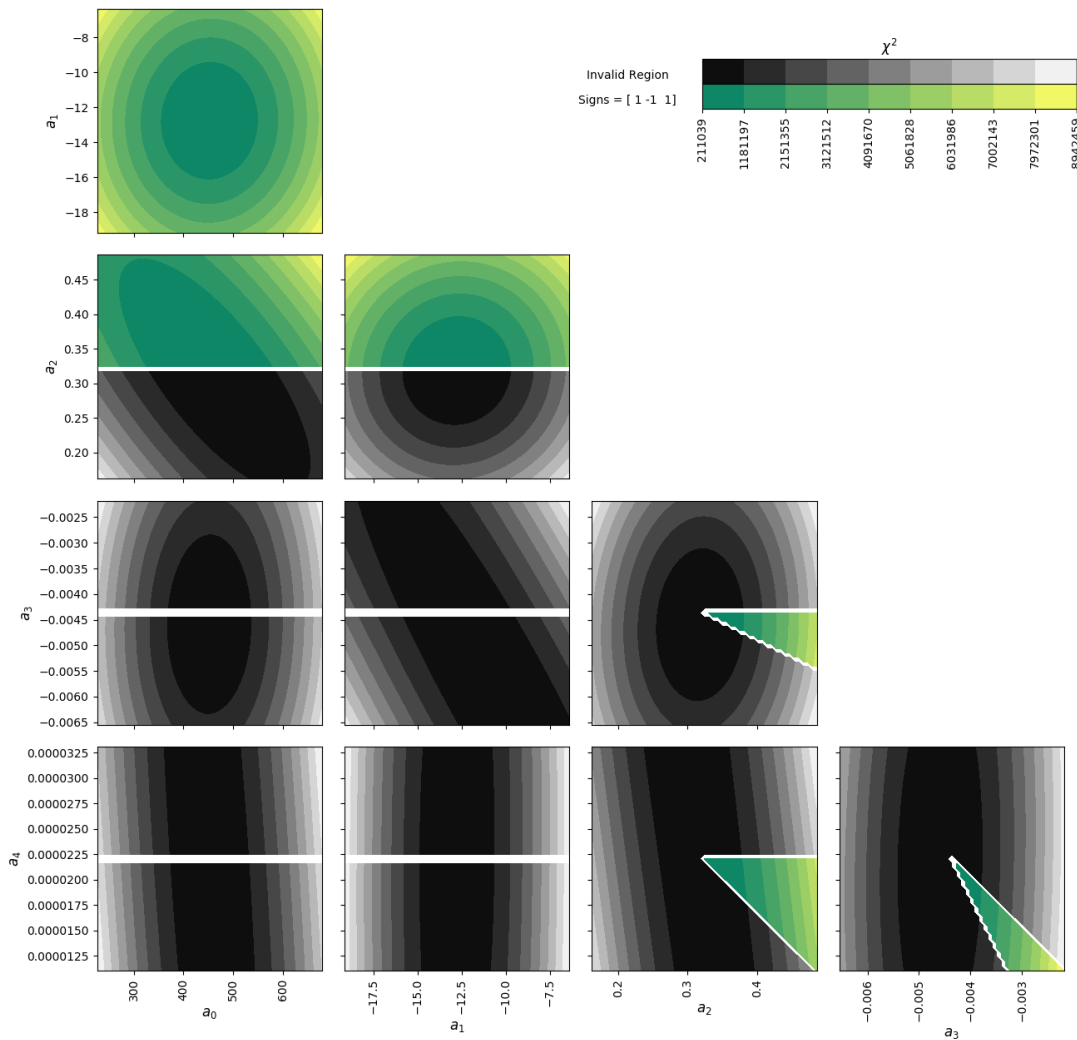
```
from maxsmooth.parameter_plotter import param_plotter
```

and access it using,

```
param_plotter(result.optimum_params, result.optimum_signs,
              x, y, N, base_dir='examples/')

```

The function takes in the optimum parameters and signs found after the fit as well as the data and order of the fit. There are a number of keyword arguments detailed in the following section and the resultant fit is shown below. The function by default samples the parameter ranges 50% either side of the optimum and calculates 50 samples for each parameter. In each panel the two labelled parameters are varied while the others are maintained at their optimum values.



MAXSMOOTH FUNCTIONS

This section details the specifics of the built in functions in `maxsmooth` including the relevant key word arguments and default parameters for all.

3.1 `smooth()`

smooth, as demonstrated in the examples section, is used to call the fitting routine. There are a number of `**kwargs` that can be assigned to the function which change how the fit is performed, the model that is fit and various other attributes. These are detailed below.

```
class maxsmooth.DCF.smooth (x, y, N, **kwargs)
```

Parameters:

x: numpy.array

The x data points for the set being fitted.

y: numpy.array

The y data points for fitting.

N: int

The number of terms in the DCF.

Kwargs:

fit_type: Default = 'qp-sign_flipping'

This kwarg allows the user to switch between sampling the available discrete sign spaces (default) or testing all sign combinations on the derivatives which can be accessed by setting to 'qp'.

model_type: Default = 'difference_polynomials'

Allows the user to access default Derivative Constrained Functions built into the software. Available options include the default, 'polynomial', 'normalised_polynomial', 'legendre', 'log_polynomial', 'loglog_polynomial' and 'exponential'. For more details on the functional form of the built in basis see the `maxsmooth` paper.

pivot_point: Default = len(x)//2 else integer

Some of the built in models rely on pivot points in the data sets which by default is set as the middle index. This can be altered via this kwarg which can occasionally lead to a better quality fit.

base_dir: Default = 'Fitted_Output/'

The location of the outputted data from `maxsmooth`. This must be a string and end in `'/'`. If the file does not exist then `maxsmooth` will create it. By default the only outputted data is a summary of the best fit but additional data can be recorded by setting the keyword argument `'data_save = True'`.

data_save: Default = False

By setting this to True the algorithm will save every tested set of parameters, signs and objective function evaluations into files in `base_dir`. These files will be over written on repeated runs but they are needed to run the `'chidist_plotter'`.

all_output: Default = False

If set to True this outputs to the terminal every fit performed by the algorithm. By default the only output is the optimal solution once the code is finished.

cvxopt_maxiter: Default = 10000 else integer

This shouldn't need changing for most problems however if `CVXOPT` fails with a `'maxiters reached'` error message this can be increased. Doing so arbitrarily will however increase the run time of `maxsmooth`.

initial_params: Default = None else list of length N

Allows the user to overwrite the default initial parameters used by `CVXOPT`.

constraints: Default = 2 else an integer less than or equal to N - 1

The minimum constrained derivative order which is set by default to 2 for a Maximally Smooth Function.

ifp_list: Default = None else list of integers

Allows you to specify if the conditions should be relaxed on any of the derivatives between constraints and the highest order derivative. e.g. a 6th order fit with just a constrained 2nd and 3rd order derivative would have an `ifp_list = [4, 5]`.

cap: Default = (len(available_signs))/N + N else an integer

Determines the maximum number of signs explored either side of the minimum χ^2 value found after the decent algorithm has terminated.

chi_squared_limit: Default = 2*min(chi_squared) else float or int

The maximum allowed increase in χ^2 during the directional exploration. If this value is exceeded then the exploration in one direction is terminated and started in the other. For more details on this and `'cap'` see the `maxsmooth` paper.

The following Kwarg can be used by the user to define thier own basis function and will overwrite the `'model_type'` kwarg.

basis_function: Default = None else function with parameters (x, y, pivot_point, N)

This is a function of basis functions for the quadratic programming. The variable `pivot_point` is the index at the middle of the datasets `x` and `y` by default but can be adjusted.

model: Default = None else function with parameters (x, y, pivot_point, N, params)

This is a user defined function describing the model to be fitted to the data.

der_pres: Default = None else function with parameters (m, i, x, y, pivot_point)

This function describes the prefactors on the `i`th term of the `m`th order derivative used in defining the constraint.

derivatives: Default = None else function with parameters (m, i, x, y, pivot_point, params)

User defined function describing the i th term of the m th order derivative used to check that conditions are being met.

args: Default = None else list

Extra arguments for *smooth* to pass to the functions detailed above.

Output

If N is a list with length greater than 1 then the outputs from *smooth* are lists and arrays with dimension 0 equal to $\text{len}(N)$.

.y_fit: numpy.array

The fitted arrays of y data from *smooth*.

.optimum_chi: float

The optimum chi squared values for the fit calculated by,

$$X^2 = \sum (y - y_{fit})^2.$$

.optimum_params: numpy.array

The set of parameters corresponding to the optimum fits.

.rms: float

The rms value of the residuals $y_{res} = y - y_{fit}$ calculated by,

$$rms = \sqrt{\frac{\sum (y - y_{fit})^2}{n}}$$

where n is the number of data points.

.derivatives: numpy.array

The m^{th} order derivatives.

.optimum_signs: numpy.array

The sign combinations corresponding to the optimal results.

3.2 best_basis()

This function allows you to test the built in basis and their ability to fit the data. It produces a plot that shows χ^2 as a function of N for the 7 built in models and saves the figure to the base directory.

class maxsmooth.best_basis.basis_test ($x, y, **kwargs$)

Parameters:

x: numpy.array

The x data points for the set being fitted.

y: numpy.array

The y data points for fitting.

Kwargs:

fit_type: Default = 'qp-sign_flipping'

This kwarg allows the user to switch between sampling the available discrete sign spaces (default) or testing all sign combinations on the derivatives which can be accessed by setting to 'qp'.

base_dir: Default = 'Fitted_Output/'

The location of the outputted graph from function. This must be a string and end in '/'. If the file does not exist then the function will create it.

N: Default = [3, ..., 13] in steps of 1 else list or numpy array of integers

The DCF orders to test each basis function with. In some instances the basis function may fail for a given N and higher orders due to overflow/underflow errors or CVXOPT errors.

3.3 chidist_plotter()

This function allows the user to produce plots of the χ^2 distribution as a function of the available discrete sign spaces for the constrained derivatives. This can be used to identify whether or not the problem is *ill defined*, see the maxsmooth paper for a definition, and if it can be solved using the sign sampling approach.

It can also be used to determine whether or not the 'cap' and maximum allowed increase on the value of χ^2 during the directional exploration are sufficient to identify the global minimum for the problem.

The function is reliant on the output of the maxsmooth smooth() function. The required outputs can be saved when running smooth() using the 'data_save = True' kwarg.

class maxsmooth.chidist_plotter.chi_plotter(N , ****kwargs**)

Parameters:

N: int

The number of terms in the DCF.

Kwargs:

fit_type: Default = 'qp-sign_flipping'

This kwarg is the same as before. Here it allows the files to be read from the base directory.

base_dir: Default = 'Fitted_Output/'

The location of the outputted data from maxsmooth. This must be a string and end in '/' and must contain the files 'Output_Evaluations/' and 'Output_Signs/' which can be obtained by running smooth() with data_save=True.

chi: Default = None else list or numpy array

A list of χ^2 evaluations. If provided then this is used over outputted data in the base directory. It must have the same length as the outputted signs in the file 'Output_Signs/' in the base directory. It must also be ordered correctly otherwise the returned graph will not be correct. A correct ordering is one for which each entry in the array corresponds to the correct sign combination in 'Output_Signs/'. Typically this will not be needed but if the χ^2 evaluation in 'Output_Evaluations/' in the base directory is not in the desired parameter space this can be useful. For example the built in logarithmic model calculates χ^2 in logarithmic space. To plot the distribution in linear space we can calculate χ^2 in linear space using a function for the model and the tested parameters which are found in 'Output_Parameters/' in the base directory.

constraints: Default = 2 else an integer less than or equal to N - 1

The minimum constrained derivative order which is set by default to 2 for a Maximally Smooth Function. Used here to determine the number of possible sign combinations available.

ifp_list: Default = None else list of integers

Allows you to specify if the conditions should be relaxed on any of the derivatives between constraints and the highest order derivative. e.g. a 6th order fit with just a constrained 2nd and 3rd order derivative would have an `ifp_list = [4, 5]`. Again this is used in determining the possible sign combinations available.

plot_limits: Default = False

Determines whether the limits on the directional exploration are plotted on top of the χ^2 distribution.

cap: Default = (len(available_signs)/N) + N else an integer

Determines the maximum number of signs explored either side of the minimum χ^2 value found after the decent algorithm has terminated.

chi_squared_limit: Default = 2*min(chi_squared) else float or int

The maximum allowed increase in χ^2 during the directional exploration. If this value is exceeded then the exploration in one direction is terminated and started in the other. For more details on this and 'cap' see the `maxsmooth` paper.

3.4 parameter_plotter()

This function allows you to plot the parameter space around the optimum solution found when running `maxsmooth` and visualise the constraints with contour lines given by χ^2 .

```
class maxsmooth.parameter_plotter.param_plotter(best_params, optimum_signs, x, y, N,
                                                **kwargs)
```

Parameters:**best_params: numpy.array**

The optimum parameters found when running a DCF fit to the data.

optimum_signs: numpy.array

The optimum signs for the DCF fit which are used when the derivatives are equal to 0 across the band.

x: numpy.array

The x data points.

y: numpy.array

The y data points.

N: int

The number of terms in the DCF.

Kwargs:**model_type: Default = 'difference_polynomial'**

The functional form of the model being plotted. If a the user has defined their own basis they can supply this with the Kwargs below and this will be overwritten.

base_dir: Default = 'Fitted_Output/'

The location in which the parameter plot is saved.

constraints: Default = 2 else an integer less than or equal to N - 1

The minimum constrained derivative order which is set by default to 2 for a Maximally Smooth Function. Used here to determine the number of possible sign combinations available.

ifp_list: Default = None else list of integers

Allows you to specify if the conditions should be relaxed on any of the derivatives between constraints and the highest order derivative. e.g. a 6th order fit with just a constrained 2nd and 3rd order derivative would have an ifp_list = [4, 5]. Again this is used in determining the possible sign combinations available.

samples: Default = 50

The sampling rate across the parameter ranges defined with the optimum solution and width.

width: Default = 0.5

The range of each parameter to explore. The default value of 0.5 means that the χ^2 values for parameters ranging 50% either side of the optimum result are tested.

warnings: Default = True

Used to highlight when a derivative is 0 across the band and that in these instances the optimum signs are assumed for the colourmap if $N \leq 5$, constraints=2 and the ifp_list is empty.

gridlines: Default = False

Plots gridlines showing the central value for each parameter in each panel of the plot.

The following Kwargs are used to plot the parameter space for a user defined basis function and will overwrite the 'model_type' kwarg.

basis_function: Default = None else function with parameters (x, y, pivot_point, N)

This is a function of basis functions for the quadratic programming. The variable pivot_point is the index at the middle of the datasets x and y by default but can be adjusted.

model: Default = None else function with parameters (x, y, pivot_point, N, params)

This is a user defined function describing the model to be fitted to the data.

der_pres: Default = None else function with parameters (m, i, x, y, pivot_point)

This function describes the prefactors on the ith term of the mth order derivative used in defining the constraint.

derivatives: Default = None else function with parameters (m, i, x, y, pivot_point, params)

User defined function describing the ith term of the mth order derivative used to check that conditions are being met.

args: Default = None else list

Extra arguments for *smooth* to pass to the functions detailed above.

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