maxsmooth: Derivative Constrained Function Fitting

Harry T. J. Bevins

1 Astrophysics Group, Cavendish Laboratory, J.J.Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

Summary

maxsmooth is an optimisation routine written in Python (supporting version $\geq 3.6$) for fitting Derivative Constrained Functions (DCFs) to data. DCFs are a family of functions which have derivatives that do not cross zero in the band of interest. Two special cases of DCF are Maximally Smooth Functions (MSFs) which have derivatives with order $m \geq 2$ constrained and Completely Smooth Functions (CSFs) with $m \geq 1$ constrained. Alternatively, we can constrain an arbitrary set of derivatives and we refer to these models as Partially Smooth Functions. Due to their constrained nature, DCFs can produce perfectly smooth fits to data and reveal non-smooth signals of interest in the residuals.

Statement of Need

The development of maxsmooth has been motivated by the problem of foreground modelling in Global 21-cm experiments (Bowman, Rogers, Monsalve, Mozdzen, & Mahesh, 2018; de Lera Acedo, 2019; Price et al., 2018; Singh et al., 2018). Global 21-cm cosmology is the study of the spin temperature of hydrogen gas and its relative magnitude compared to the Cosmic Microwave Background during the Cosmic Dawn (CD) and Epoch of Reionisation (EoR). During the CD and EoR the first stars formed and the properties of the hydrogen gas changed as it interacted with radiation from these stars (Barkana, 2016; Furlanetto, Oh, & Briggs, 2006; Pritchard & Loeb, 2012).

The goal of Global 21-cm experiments is to detect this structure in the sky averaged radio spectrum between $\nu = 50$ and 200 MHz. However, the signal of interest is expected to be approximately $\leq 250$ mK and masked by foregrounds $10^2 - 10^5$ times brighter (Cohen, Fialkov, Barkana, & Lotem, 2017; Cohen, Fialkov, Barkana, & Monsalve, 2019).

Modelling and removal of the foreground is essential for detection of the Global 21-cm signal. DCFs provide a powerful alternative to unconstrained polynomials for accurately modelling the smooth synchrotron/free-free emission foreground from the Galaxy and extragalactic radio sources.

To illustrate the abilities of maxsmooth we produce mock 21-cm experiment data and model and remove the foreground using an MSF. We add to a mock foreground, $\nu^{-2.5}$, a Gaussian noise with standard deviation of 0.02 K and a Gaussian signal with amplitude 0.23 K, central frequency of 100 MHz and standard deviation of 10 MHz.

The figure below shows the residuals (bottom panel, green) when fitting and removing an MSF from the data (top panel) compared to the injected signal (bottom panel, red). While the removal of the foreground does not directly recover the injected signal, rather a smooth baseline subtracted version, we see the remnant of the signal in the residuals (see Bevins et al. (2020) for more details and examples).
**maxsmooth**

DCFs can be fitted with routines such as Basin-hopping (Wales & Doye, 1997) and Nelder-Mead (Nelder & Mead, 1965) and this has been the practice for 21-cm cosmology (Sathyaranayana Rao, Subrahmanyan, Udaya Shankar, & Chluba, 2017; Singh & Subrahmanyan, 2019). However, maxsmooth employs quadratic programming via CVXOPT to rapidly and efficiently fit DCFs which are constrained such that

\[ \frac{d^m y}{dx^m} \geq 0 \text{ or } \frac{d^m y}{dx^m} \leq 0. \]

An example DCF from the maxsmooth library is given by

\[ y = \sum_{k=0}^{N} a_k x^k, \]

where \( x \) and \( y \) are the independent and dependent variables respectively and \( N \) is the order of the fit with powers from \( 0 \) to \( (N - 1) \). The library is intended be extended by future contributions from users. We find that the use of quadratic programming makes maxsmooth approximately two orders of magnitude quicker than a Basin-hopping/Nelder-Mead approach.

maxsmooth rephrases the above condition such that

\[ \pm_m \frac{d^m y}{dx^m} \leq 0, \]

where the \( \pm \) applies to a given \( m \). This produces a set of sign spaces with different combinations of constrained positive and negative derivatives. In each sign space the associated
minimum is found using quadratic programming and then \texttt{maxsmooth} identifies the optimum combination of signs, \(s\). To summarise the minimisation problem we have

\[
\min_{a; s} \frac{1}{2} a^T Q a + q^T a,
\]

s.t. \(G(s) a \leq 0,\)

where we are minimising \(\chi^2\), \(G(s)a\) is a stacked matrix of derivative evaluations and \(a\) is the matrix of parameters we are optimising for. \(Q\) and \(q\) are given by

\[
Q = \Phi^T \Phi \quad \text{and} \quad q^T = -y^T \Phi,
\]

here \(\Phi\) is a matrix of basis function evaluations and \(y\) is a column matrix of the dependent data.

The discrete spaces can be searched in their entirety quickly and efficiently or a sign navigating algorithm can be invoked using \texttt{maxsmooth} reducing the fitting time. Division of the parameter space into sign spaces allows for a more complete exploration when compared to Basin-hopping/Nelder-Mead based algorithms.

The sign navigating approach uses a cascading algorithm to identify a candidate optimum \(s\) and \(a\). The algorithm starts with a randomly generated \(s\). Each individual sign is then flipped, from the lowest order derivative first, until the objective function decreases in value. The signs associated with the lower \(\chi^2\) value become the optimum set and the process is repeated until \(\chi^2\) stops decreasing. This is followed by a limited exploration of the neighbouring sign spaces to identify the true global minimum.

**Figure 2:** The time taken to fit polynomial data following an approximate \(x^n\) power law using both \texttt{maxsmooth} quadratic programming methods and for comparison a method based in Basin-hopping and Nelder-Mead routines. We show the results using the later method up to \(N = 7\) after which the method begins to fail without adjustments to the routine parameters. For \(N = 3 - 7\) we find a maximum difference of 0.04\% between the optimum \texttt{maxsmooth} \(\chi^2\) values and the Basin-hopping results. Figure taken from Bevins et al. (2020).

Documentation for \texttt{maxsmooth} is available at ReadTheDocs and the code can be found on Github. The code is also pip installable (PyPI). Continuous integration is performed with Travis and CircleCi. The associated code coverage can be found at CodeCov.
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References

Barkana, R. (2016). The rise of the first stars: Supersonic streaming, radiative feedback, and 21-cm cosmology. *Physics Reports*, 645, 1–59. doi:10.1016/j.physrep.2016.06.006

Bevins, H. T. J., Handley, W. J., Fialkov, A., Lera de Acedo, E., Greenhill, L. J., & Price, D. C. (2020). maxsmooth: Rapid maximally smooth function fitting with applications in Global 21-cm cosmology. *arXiv e-prints*, arXiv:2007.14970. Retrieved from http://arxiv.org/abs/2007.14970

Bowman, J. D., Rogers, A. E. E., Monsalve, R. A., Mozdzen, T. J., & Mahesh, N. (2018). An absorption profile centered at 78 megahertz in the sky-averaged spectrum. *Nature*, 555(7694), 67–70. doi:10.1038/nature25792

Cohen, A., Fialkov, A., Barkana, R., & Lotem, M. (2017). Charting the parameter space of the global 21-cm signal. *Monthly Notices of the Royal Astronomical Society*, 472(2), 1915–1931. doi:10.1093/mnras/stx2065

Cohen, A., Fialkov, A., Barkana, R., & Monsalve, R. (2019). Emulating the Global 21-cm Signal from Cosmic Dawn and Reionization. *arXiv e-prints*, arXiv:1910.06274. Retrieved from http://arxiv.org/abs/1910.06274

de Lera Acedo, E. (2019). REACH: Radio experiment for the analysis of cosmic hydrogen. 2019 *International Conference on Electromagnetics in Advanced Applications* (ICEAA), 0626–0629. doi:10.1109/ICEAA.2019.8879199

Furlanetto, S. R., Oh, S. P., & Briggs, F. H. (2006). Cosmology at low frequencies: The 21 cm transition and the high-redshift Universe. *Physics Reports*, 433(4-6), 181–301. doi:10.1016/j.physrep.2006.08.002

Nelder, J. A., & Mead, R. (1965). A Simplex Method for Function Minimization. *The Computer Journal*, 7(4), 308–313. doi:10.1093/comjnl/7.4.308

Price, D. C., Greenhill, L. J., Fialkov, A., Bernardi, G., Garsden, H., Barsdell, B. R., Kocz, J., et al. (2018). Design and characterization of the Large-aperture Experiment to Detect the Dark Age (LEDA) radiometer systems. *Monthly Notices of the Royal Astronomical Society*, 478(3), 4193–4213. doi:10.1093/mnras/sty1244

Pritchard, J. R., & Loeb, A. (2012). 21 cm cosmology in the 21st century. *Reports on Progress in Physics*, 75(8), 086901. doi:10.1088/0034-4885/75/8/086901

Sathyanarayana Rao, M., Subrahmanyan, R., Udaya Shankar, N., & Chluba, J. (2017). Modeling the radio foreground for detection of cmb spectral distortions from the cosmic dawn and the epoch of reionization. *The Astrophysical Journal*, 840(1), 33. doi:10.3847/1538-4357/aa69bd

Singh, S., & Subrahmanyan, R. (2019). The Redshifted 21 cm Signal in the EDGES Low-band Spectrum. *The Astrophysical Journal*, 880(1), 26. doi:10.3847/1538-4357/ab2879

Singh, S., Subrahmanyan, R., Udaya Shankar, N., Sathyanarayana Rao, M., Girish, B. S., Raghunathan, A., Somashekara, R., et al. (2018). SARAS 2: a spectral radiometer for probing cosmic dawn and the epoch of reionization through detection of the global 21-cm signal. *Experimental Astronomy*, 45(2), 269–314. doi:10.1007/s10686-018-9584-3
Wales, D. J., & Doye, J. P. K. (1997). Global optimization by basin-hopping and the lowest energy structures of lennard-jones clusters containing up to 110 atoms. The Journal of Physical Chemistry A, 101(28), 5111–5116. doi:10.1021/jp970984n