

MCMC in DAOPHOT-II

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This is a guide for use of the modified version of the subroutine `NSTAR.F` which implements a Markov chain Monte Carlo (MCMC) routine for fitting blended stellar positions and fluxes. This manual assumes the user has properly installed the base version of `DAOPHOT-II`¹. Descriptions of each major section of the MCMC routine are given with example outputs. This guide includes only specific instructions for running the MCMC version of `NSTAR.F`. For instructions using any other `DAOPHOT-II` module I will refer the reader to various sections within the `DAOPHOT-II` User's Manual (DII-UM) when appropriate.

¹<http://www.star.bris.ac.uk/~mbt/daophot/>

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1 Installation

Adding this modified routine to the DAOPHOT-II workflow is quite simple:

1. Move the file `nstar-mcmc.f` into the DAOPHOT-II source code directory.
2. Open the Makefile and replace the two instances of “`nstar.o`” with “`nstar-mcmc.o`”. This will allow the user to run the command **NSTAR-MCMC** from within DAOPHOT-II.
3. Run *make daophot* (or *sudo make daophot*) in the source code directory. This should only take a few seconds as only the `nstar-mcmc.o` executable will need to be built.

Note: If the user simply adds “`nstar-mcmc.o`” to the Makefile instead of replacing “`nstar.o`” with “`nstar-mcmc.o`”, the error “`duplicate symbol in:nstar.o nstar-mcmc.o`” will likely occur.

Once again, these installation steps assume that the user has previously successfully installed the entire DAOPHOT-II software package. When using the software, the **NSTAR-MCMC** command will run the modified version, the **NSTAR** command will run the standard version without any MCMC.

2 A Typical Run of NSTAR-MCMC

Before running **NSTAR-MCMC**, the user will need to have already produced a co-added master frame and run the stock **DAOPHOT-II** pipeline on the image through the following steps:

- **ATTACH** (DII-UM pg. 12)
- **FIND** (DII-UM pg. 20)
- **PHOT** (DII-UM pg. 25)
- **PICK** (DII-UM pg. 29)
- **PSF** (DII-UM pg. 29)
- **GROUP** (DII-UM pg. 36)

The user will also need to manually remove all irrelevant groups of stars from the **.grp** file, so that only the header information and the 1, 2, or 3-star group of interest remains. Below is an example **.grp** file with one remaining group (the group of interest):

NL	NX	NY	Lowbad	Highbad	Thresh	AP1	PH/ADU	Rdnoise	Watch Progress
3	1463	1463	-71.4	9700.00	18.750	5.000	40.000	12.333	1
241	896.550	822.590	15.305	24.990					
450	890.490	823.160	15.995	25.550					
(1)	(2)	(3)	(4)	(5)					

- (1) Star ID number.
- (2) X coordinate of stellar centroid.
- (3) Y coordinate of stellar centroid.
- (4) Instrumental magnitude.
- (5) Estimated modal sky value for the star (from **PHOT**).

From inside the working directory (and inside an instance of **DAOPHOT-II** with the image “attached”), follow the steps:

- I Run **NSTAR-MCMC**. The user will first be prompted to give the **.psf** and **.grp** files (which were generated in the previous steps). The third prompt will ask the user for a filename for the output **.nst** file. This output is the default file that **NSTAR** produces using the Newton-Raphson method (see DII-UM pg. 38 and sample **.nst** output table given in DII-UM pg. 73).
- II The next prompt asks for either a 1-star, 2-star, or 3-star fit. After entering “1”, “2”, or “3” the degrees of freedom (*d.o.f*) for the fitting will be printed to the console. The

$d.o.f$ depends on the total number of pixels in the fitting box, the number of fitting parameters, and fitting constraints (if any). The fitting parameters that contribute to the overall $d.o.f$ are:

- (a) 1-star fit: x, y, total flux.
- (b) 2-star fit: x1, y1, x2, y2, separation, flux ratio, total flux.
- (c) 3-star fit: x1, y1, x2, y2, x3, y3, lens-source (star 1-2) separation, blend-source (star 1-3) separation, lens-source (star 1-2) flux ratio, blend-source (star 1-3) flux ratio, total flux.

So for a 2-star MCMC run over a fitting box of 700 total pixels, the total $d.o.f = 700 + 7 = 707$. Note that including constraints on any of the fitting parameters will reduce the total $d.o.f$ by the number of parameters being constrained. The fitting box and degrees of freedom are discussed further in Section 4.1, and fitting constraints are discussed in Appendix A.

- III Next, the user is prompted for “Number of MCMC iterations”. This is straight forward. The larger the iteration size, the longer the routine will take to run.
- IV The next prompt asks for initial guesses for the stellar positions of star 1, 2, and/or 3. The number of times this prompt repeats will of course depend on how many stars the user is attempting to fit. The initial guess needs to be within the fitting box or an error will be thrown. It is recommended that the user chooses star-1 to be the brightest, star-2 the second brightest, and star-3 the faintest. This is not a strict requirement, however the routine was originally written with the expectation that star-1 is always the brightest so there may be weird bugs that appear if this condition is altered.
- V After the initial position guesses, the user is prompted to enter an initial guess for the source (star-1) flux contribution to the total flux. For the trivial case of 1-star fitting, a good initial guess for this parameter is 1.0. For 2 and 3-star fitting, one can obtain an initial guess for this parameter by converting the instrumental magnitudes in the `.grp` file to fluxes and finding their individual contributions to their overall total flux. For example:

$$\frac{10^{(-0.4*m_1)}}{10^{(-0.4*m_1)} + 10^{(-0.4*m_2)}}$$

where m_1 and m_2 are the instrumental magnitudes of star-1 and star-2 respectively. If performing a 3-star fit, this prompt will be repeated for the 3rd star (also referred to as ‘blend’ star in the routine).

After the prompt in step V, the routine begins. Once completed, the best fit parameters are printed to the console, which includes the χ^2 value for the best fit. The following screenshot shows the terminal after a successful (2-star) run has completed:

```

Command: NSTAR-MCMC

    File with the psf (default image.psf):
    File with stellar groups (default image.grp):
    File for results (default image.nst):

1, 2, or 3 star fit:
2
Degrees of Freedom =      787
Number of MCMC Iterations:
100000
Initial Source x,y:
894,820
Initial Lens x,y:
889,825
Initial Source Flux Contribution (0.0 - 1.0):
0.75

```

X1	Y1	X2	Y2	SEP	F_RATIO	F_TOTAL	CHI2
896.640991	822.620483	890.141113	824.270630	66.6717682	0.850586116	0.955864966	163.899826

```

Done.

Command: █

```

In addition to the best fit parameters that are printed to the terminal, an output file is generated titled “mcmc_fit.dat”. This file includes all of the (accepted) MCMC steps in the chain. The header columns in this file are identical to the headers for the best-fit values printed to the terminal. One can use this raw output for various calculations like; using the MCMC chains as a probability distribution to estimate errors for the best-fit values, producing contour plots with confidence intervals for the best-fit parameters, etc.

If one intends to normalize the errors by the $\chi^2/d.o.f$, then manually commenting or adjusting several lines in the source code is required at present. A future update to the code will include a user-friendly method to normalize the best-fit errors that does not require hard coding from the user (no later than v1.3 release).

3 Description of Major Routines

3.1 Single Star MCMC

DAOPHOT-MCMC has functionality for fitting the position and flux for the trivial case of a single star. The star, of course, could actually be a binary or have a very close companion such that the separation is significantly smaller than some fraction of the FWHM, which would show no significant signal detected in the residual. For the purposes of this section, we will assume the star is indeed a single stellar object.

The MCMC routine begins at a pixel location chosen by the user. The size of the fitting box is ~ 1.5 x the FWHM of the PSF in both directions and is pre-determined by DAOPHOT-II before the iteration begins. The iteration proceeds by taking random steps in any direction and measuring the total flux (f_T) distribution:

$$f_T = f_1 \psi(i - x_1, j - y_1),$$

where f_1 is the fractional flux contribution from the single star (presumably 1.0 for a single-star fit), ψ is the two-dimensional ePSF, x_1 and y_1 are the initial pixel coordinates. A χ^2 value is also computed at each step in the chain. Once the routine is finished, the best-fit parameters are printed to the terminal screen (i.e. X1, Y1, Total Flux, χ^2). For the ideal case of 100% of the flux in the fitting box coming from the star (minus background), the best-fit total flux value would be 1.00. However, due to photon noise, imperfect PSF shape, and other subtle sources of error, this value will usually deviate a few percent from unity. The total flux calculation is rather simple; it is just the ratio of the total sum of each raw pixel value (minus background) and the total sum of the measured flux distribution at each pixel across the grid:

$$\frac{\sum_{i,j}^n P_{i,j} - s_{i,j}}{\sum_{i,j}^n f_1 \psi(i - x_1, j - y_1)},$$

where P is the raw pixel value and s is the background. Finally, the χ^2 minimization routine used for the single-star fitting, as well as the other main routines, is given in section 4.5.

3.2 Dual Star MCMC

DAOPHOT-MCMC can simultaneously fit the positions, separations, and fluxes for a two-star blend. Similar to the single-star routine, the iteration begins at a user-defined pixel location (for both stars) inside the fitting box of ~ 1.5 x FWHM. The iteration proceeds by taking random steps in any direction and any flux ratio. This flux ratio is an additional parameter to consider for the two stellar objects. The routine measures the total flux distribution at each step in the chain:

$$f_T = f_1\psi(i - x_1, j - y_1) + (1 - f_1)\psi(i - x_2, j - y_2),$$

with the additional parameters as follows; $(1 - f_1)$ is the flux contribution from the second (fainter) star, x_2 and y_2 are the central pixel positions for the second (fainter) star. Similar to the single-star fit, a χ^2 value is calculated at each step, and the best-fit parameters are printed to the screen once the routine has finished (i.e. X1, Y1, X2, Y2, Separation, Flux Ratio, Total Flux, χ^2). As mentioned in the previous section, the best-fit total flux may deviate a few percent from unity. Theoretically, one could perform many MCMC simulations and attempt to characterize this “excess” (an unresolved companion for example) or “deficit” of total flux in a statistical sense. The total flux is calculated similarly to the previous section:

$$\frac{\sum_{i,j}^n P_{i,j} - s_{i,j}}{\sum_{i,j}^n f_1\psi(i - x_1, j - y_1) + (1 - f_1)\psi(i - x_2, j - y_2)},$$

where the additional parameters from the second (fainter) star are now included.

The separation between star-1 and star-2 is measured at each step in the chain, the calculation is very straightforward:

$$\Omega\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2},$$

where Ω is the pixel scale. For the NIRC2 instrument using adaptive optics (AO) on-board the Keck-II 10m telescope, $\Omega = 9.942$ mas/pixel. Currently, the only way to adjust Ω is by hard-coding. However, there are plans to make this value user-defined before the MCMC routine begins.

3.3 Triple Star MCMC

4 Description of Internal Functions

4.1 Degrees of Freedom

4.2 Separation

4.3 Flux Ratio

4.4 Total Flux

4.5 χ^2 Minimization

A Fitting Constraints

B Data Files and Sample Outputs

5 Change Log

- **2020 July 2:** Fix dimension size to match computed gridsize via `ALLOCATABLE`.
- **2020 June 30:** Added column headers to raw MCMC output file.
- **2020 June 26:** Fix bug printing `star(1-2)` separation and `star(1-3)` separation for triple-star MCMC.
- **2020 June 10:** Cleaner printing of best-fit parameters to the terminal, minor bug fix in degree of freedom (*d.o.f*) calculation (**v1.1** release).
- **2020 May 30:** Added functionality for 3-star fitting, minor bug fixes.
- **2020 May 15:** **v1.0** release