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/

Contents

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, both the **NSTAR** and **NSTAR-MCMC** commands will run the modified version.

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 (pre-determined) 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 The next prompt asks the user for a "renormalization factor". This is used for re-normalizing the χ^2 per degree of freedom ($\chi^2 \simeq 1$) in order to obtain more reasonable error bars on the MCMC chains. If running the MCMC for the first time, this value should always equal '1'. After calculating the renormalization factor (i.e. best-fit χ^2 divided by degrees of freedom) and running the MCMC a second time with the proper renormalization factor, the routine will usually take longer to run and possibly have a lower acceptance rate, as expected.

IV 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. During the first run of NSTAR-MCMC, the user should type "1" for this value. To read more about this parameter, refer to section 4.5.1.

V 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.

VI 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 the 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 VI, the routine begins. A counter will print the current step at every 50,000 iterations. 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
 Renormalization Factor (type '1' if first time run):
1
 Number of MCMC Iterations:
150000
 Star 1 x,y:
896,822
 Star 2 x,y:
890,824
 Star 1 Flux Contribution (0.0 - 1.0):
0.8
 50000
100000
150000
       X1              Y1              X2              Y2             SEP           F_RATIO         F_TOTAL          CHI2
   896.654541      822.602112      890.186646      824.326843      66.5508118     0.848842144     0.955875576      163.875229

    Done.
```

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.

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 ∼1.5x 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 flux contamination, this value will usually deviate 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 ∼1.5x FWHM, as well as an initial guess for the flux ratio of the stars. 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 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.

3.3 Triple Star MCMC

The third major function in DAOPHOT-MCMC is simultaneous fitting of three stars. The fitting will work on three blended stars, two blended stars and a nearby neighbor, or three nearby (non-blended) stars. Of course, factors like the star separations and flux ratios will influence the properties of the MCMC runs. Similar to the dual-star fitting scenario, if the stars have very small separations and similar fluxes (or large separation and very different fluxes), some difficulty may arise when attempting to accurately fit their positions.

Just like before, the iteration begins at a user-defined pixel location (for all three stars) and initial guess for the flux ratios. The routine takes random steps in any direction and flux ratios (star1-2 and star1-3 flux ratios). The measurement of the total flux distribution at each step is:

$$f_T = f_1\psi(i - x_1, j - y_1) + (1 - f_1 - f_3)\psi(i - x_2, j - y_2) + f_3\psi(i - x_3, j - y_3),$$

where f_1 is the flux contribution from star 1, $(1 - f_1 - f_3)$ is the flux contribution from star 2, f_3 is the flux contribution from star 3, and x_3, y_3 are initial guess central pixel values for star 3. Similar to the previous major routines, a χ^2 minimization routine is performed (i.e. section 4.5) and the best-fit parameters are printed to the screen when the process has finished.

The total flux for the three-star fitting is calculated as follows:

$$\frac{\sum_{i,j}^{n} P_{i,j} - s_{i,j}}{\sum_{i,j}^{n} f_1\psi(i - x_1, j - y_1) + (1 - f_1 - f_3)\psi(i - x_2, j - y_2) + f_3\psi(i - x_3, j - y_3)},$$

where the new factor in the denominator comes from the flux distribution of the third star. The new parameters that are calculated for three star fitting are: star 3's x,y position and flux contribution, and star 1-3 separation. The separation given again by the simple equation:

$$\Omega\sqrt{(x_1 - x_3)^2 + (y_1 - y_3)^2},$$

where Ω is the pixel scale in mas/pixel.

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

4.5.1 Renormalization

A Fitting Constraints

B Data Files and Sample Outputs

5 Change Log

- **2020 July 16**: Added separation constraint (commented out by default).
- **2020 July 7**: χ^2 renormalization implemented (`v1.2` release).
- **2020 July 2**: Fix dimension size to match pre-determined 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