

ShOpt.jl: A Julia Package for Empirical Point Spread Function Characterization of JWST NIRCам Data

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Summary

Introduction

When astronomers capture images of the night sky, several factors – ranging from diffraction and optical aberrations to atmospheric turbulence and telescope jitter – affect the incoming light. The resulting distortion and blurring are summarized in the image's point spread function (PSF), the response of an optical system to an idealized point source. The PSF can obscure or even mimic the astronomical signal of interest, making its accurate characterization essential. By effectively modeling the PSF, we can predict image distortions at any location and proceed to deconvolve the PSF, ultimately reconstructing distortion-free images.

The PSF characterization methods used by astronomers fall into two main classes: forward-modeling approaches, which use physical optics propagation based on models of the optics, and empirical approaches, which use stars as fixed points to model and interpolate the PSF across the rest of the image. (Stars are essentially point sources before their light passes through the atmosphere and telescope, so the shape and size of their surface brightness profiles define the PSF at that location.) Empirical PSF characterization proceeds by first cataloging the observed stars, separating the catalog into validation and training samples, and interpolating the training stars across the field of view of the camera. After training, the PSF model can be validated by comparing the reserved stars to the PSF model's prediction.

Shear Optimization with ShOpt.jl introduces modern techniques, tailored to James Webb Space Telescope (JWST) imaging, for empirical PSF characterization across the field of view. ShOpt has two modes of operation: approximating stars with analytic profiles, and a more realistic pixel-level representation. Both modes take as input a catalog with image cutouts – or “vignettes” – of the stars targeted for analysis.

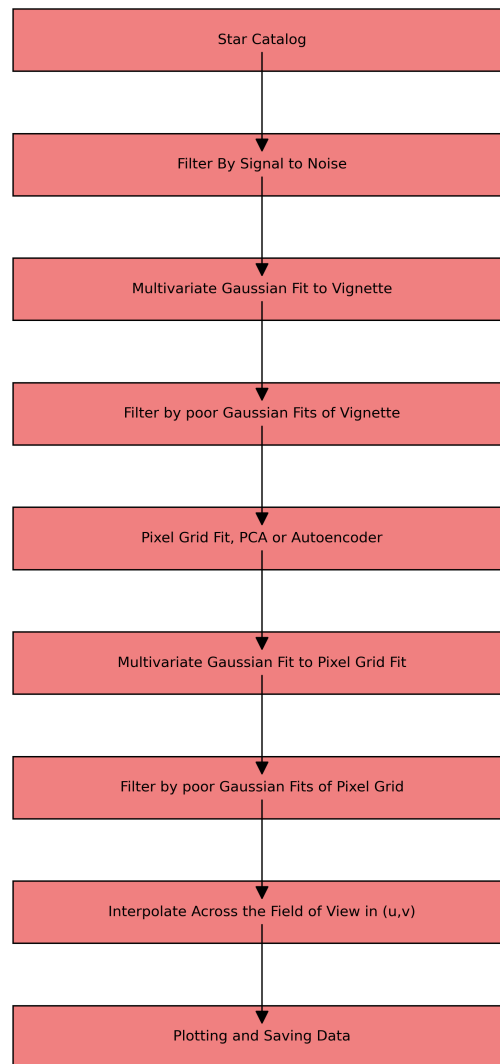


Figure 1: ShOpt Workflow

Statement of need

Empirical PSF characterization tools like PSFEx (Bertin, 2011) and PIFF (Jarvis et al., 2020) are widely popular in astrophysics. However, the quality of PIFF and PSFEx models tends to be quite sensitive to the parameter values used to run the software, with optimization sometimes relying on brute-force guess-and-check runs. PIFF is also notably inefficient for large, well-sampled images, taking hours in the worst cases. The James Webb Space Telescope's (JWST) Near Infrared Camera (NIRCam) offers vast scientific opportunities (Casey, Kartaltepe, et al., 2023); at the same time, this unprecedented data brings new challenges for PSF modeling:

- (1) Analytic functions like Gaussians are incomplete descriptions of the NIRCam PSF, as evident from Figure 2. This calls for well-thought-out, non-parametric modeling and

diagnostic tools that can capture the full dynamic range of the NIRCам PSF. Sh0pt provides these models and diagnostics out of the box.

(2) The NIRCам detectors have pixel scales of 0.03 (short wavelength channel) and 0.06 (long wavelength channel) arcseconds per pixel (Beichman et al., 2012a; Rieke et al., 2003, 2005). At these pixel scales, star vignettes need to be at least 131 by 131 pixels across to fully capture the wings of the PSFs (4-5 arcseconds). These vignette sizes are 3-5 times larger than the ones used in surveys such as DES (Jarvis et al., 2020) and SuperBIT (McCleary et al., 2023) and force us to evaluate how well existing PSF fitters scale to this size. Sh0pt has been designed for computational efficiency and aims to meet the requirements of detectors like NIRCам.

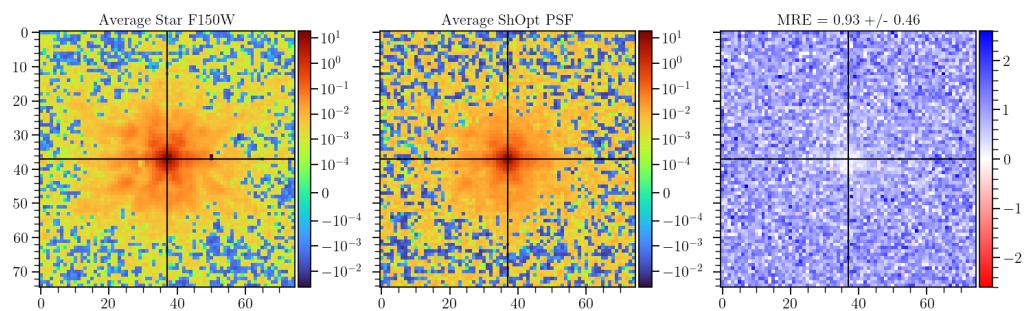


Figure 2: The plot on the left shows the average cutout of all stars in a supplied catalog. The plot in the middle shows the average point spread function model for each star. The plot on the right shows the average normalized error between the observed star cutouts and the point spread function model.

Sh0pt bridges the speed of PSFex with the features of PIFF using fewer configurable hyperparameters. Sh0pt employs a myriad of techniques to optimize the speed of the program. First and foremost, Sh0pt is equipped with support for multithreading. Polynomial interpolation is used for handling PSF variations across the field of view. The polynomials given to each basis element of the PSF are independent of one another and therefore can be distributed to different CPU threads to be run in parallel. Sh0pt also introduces new methods for fitting both analytic profiles and pixel based profiles. If an analytic profile is used to model the PSF, then there are 3 basis elements parameterizing the model. We choose 2D elliptical Gaussians for these analytic profiles because they are cheap to compute. Moreover, we use the Limited Memory Broyden–Fletcher–Goldfarb–Shanno algorithm (LBFGS) to find these parameters. This is faster but more memory intensive than Conjugate Gradient, the algorithm used in PIFF. Moreover, the 3 basis elements are constrained to the manifold $B_2(r) \times \mathbb{R}_+$. We constructed a function that maps any point in \mathbb{R}^3 into $B_2(r) \times \mathbb{R}_+$. The LBFGS algorithm uses successive iterations to converge to a solution for the 3 basis elements, and so we use this function to ensure that our update steps in LBFGS do not leave the constraint. For the pixel basis, both PIFF and PSFex approximate the PSF by minimizing the reduced χ^2 between a grid of pixels and a star vignette. PCA can quickly achieve the same purpose of approximating the input vignette without overfitting to background noise. We also provide an autoencoder mode, which uses deep learning to reconstruct the image. The weights and biases are not reset between stars, so the knowledge of how to reconstruct one star is transferred to the next. This in turn leads to less training iterations. Finally, Sh0pt is written in Julia. Julia uses a just in time compiler which makes it faster than interpreted languages such as Python and has shown to be a good choice for performance critical code (Stanitzki & Strube, 2021).

72 State of the Field

73 The JWST captures images at high resolution and at wavelengths of light that have been
74 previously unexplored (Gardner et al., 2006). With these images we are seeing farther into the
75 early universe than we ever have before. The difficulties of producing good PSF models for
76 the JWST are emblematic of a larger problem: Our data sets are getting bigger and existing
77 software was not built to scale. That is to say, the advancements in software are falling
78 behind the advances in instrumentation. Not only does ShOpt produces PSF models for JWST
79 NIRCam images, it also sets the precedent for designing software that scales.

80 There are several existing empirical PSF fitters, in addition to a forward model of the JWST
81 PSFs developed by STScI (Jarvis et al., 2020 ; Bertin, 2011; Perrin et al., 2014 ; Perrin et
82 al., 2012). We describe them here and draw attention to their strengths and weaknesses to
83 further motivate the development of ShOpt.jl. As described in the statement of need, PSFex
84 was one of the first precise and general purpose tools used for empirical PSF fitting. However,
85 the Dark Energy Survey collaboration reported small but noticeable discrepancies between the
86 sizes of PSFex models and the sizes of observed stars. They also reported ripple-like patterns
87 in the spatial variation of star-PSF residuals across the field of view (Jarvis et al., 2020), which
88 they attributed to the astrometric distortion solutions for the Dark Energy Camera.

89 These findings motivated the Dark Energy Survey's development of PIFF (Point Spread
90 Functions in the Full Field of View). PIFF works in sky coordinates on the focal plane, as
91 opposed to image pixel coordinates used in PSFex, which minimized the ripple patterns in
92 the star-PSF residuals and the PSF model size bias. (Based on the DES findings, ShOpt
93 also works directly in sky coordinates.) PIFF is written in Python, a language with a large
94 infrastructure for astronomical data analysis, for example Astropy (Astropy Collaboration et
95 al., 2022) and Galsim (Rowe et al., 2015). The choice of language makes PIFF software more
96 accessible to programmers in the astrophysics community than PSFex, which was first written in
97 C twenty-five years ago and much less approachable for a community of open source developers.
98 One of the motivations of ShOpt was to write astrophysics specific software in Julia, because
99 Julia provides a good balance of readability and speed with its high-level functional paradigm
100 and just-in-time compiler (Stanitzki & Strube, 2021). Julia ranks behind Python, IDL, Matlab,
101 and Fortran in full-text mentions in astronomical literature (Collaboration et al., 2022). We
102 are optimistic that ShOpt will demonstrate that Julia is an appealing choice for programming
103 in astronomy despite its low adoption to date.

104 While WebbPSF provides highly precise forward models of the JWST PSF, these models
105 are defined for single-epoch exposures (Perrin et al., 2014, 2012). Much of the NIRCam
106 science is accomplished with image mosaics – essentially, the combination of single exposure
107 detector images into a larger, deeper image. The rotation of the camera between exposures,
108 the astrometric transformations and resampling of images before their combination into a
109 mosaic, and the mosaic's large area all make the application of WebbPSF models to mosaics a
110 non-trivial procedure. This has been done quite effectively (Ji et al., 2023), however, it is not
111 as easy to reproduce compared to running an empirical characterization tool like ShOpt.

112 As outlined in the state of the field, ShOpt is a tool built with the user experience in mind
113 that attempts to bridge the strengths of existing PSF fitters. ShOpt's combination of speed,
114 user friendliness, and accuracy enable the science goals of the COSMOS-Web survey, detailed
115 below.

116 The COMOS-Web survey is the largest cycle 1 JWST extragalactic survey according to area
117 and prime time allocation (Casey, Kartaltepe, et al., 2023), and takes up 0.54 deg^2 (Beichman
118 et al., 2012b; Rieke et al., 2023). Among other science goals, the COMOS-Web survey will
119 use the JWST to detect thousands of galaxies in the Epoch of Reionization ($6 \sim z \sim 11$) to
120 create one of the highest resolution large scale structure maps of the early universe (Casey,
121 Kartaltepe, et al., 2023). JWST data has also been used to pick out active galactic nuclei from
122 host galaxies (Zhuang & Shen, 2023) and identify 15 candidate galaxies whose luminosities

push the limits of our Λ CDM galaxy formation models (Casey, Akins, et al., 2023). These science cases all rely upon good PSF modeling and underscore the importance of ShOpt.

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References

- Astropy Collaboration, Price-Whelan, A. M., Lim, P. L., Earl, N., Starkman, N., Bradley, L., Shupe, D. L., Patil, A. A., Corrales, L., Brasseur, C. E., Nöthe, M., Donath, A., Tollerud, E., Morris, B. M., Ginsburg, A., Vaher, E., Weaver, B. A., Tocknell, J., Jamieson, W., ... Astropy Project Contributors. (2022). The Astropy Project: Sustaining and Growing a Community-oriented Open-source Project and the Latest Major Release (v5.0) of the Core Package. 935(2), 167. <https://doi.org/10.3847/1538-4357/ac7c74>
- Beichman, C. A., Rieke, M., Eisenstein, D., Greene, T. P., Krist, J., McCarthy, D., Meyer, M., & Stansberry, J. (2012b). Science opportunities with the near-IR camera (NIRCam) on the James Webb Space Telescope (JWST). In M. C. Clampin, G. G. Fazio, H. A. MacEwen, & J. M. O. Jr. (Eds.), *Space telescopes and instrumentation 2012: Optical, infrared, and millimeter wave* (Vol. 8442, p. 84422N). International Society for Optics; Photonics; SPIE. <https://doi.org/10.1117/12.925447>
- Beichman, C. A., Rieke, M., Eisenstein, D., Greene, T. P., Krist, J., McCarthy, D., Meyer, M., & Stansberry, J. (2012a). Science opportunities with the near-IR camera (NIRCam) on the James Webb Space Telescope (JWST). In M. C. Clampin, G. G. Fazio, H. A. MacEwen, & J. Oschmann Jacobus M. (Eds.), *Space telescopes and instrumentation 2012: Optical, infrared, and millimeter wave* (Vol. 8442, p. 84422N). <https://doi.org/10.1117/12.925447>
- Bertin, E. (2011). Automated Morphometry with SExtractor and PSFEx. In I. N. Evans, A. Accomazzi, D. J. Mink, & A. H. Rots (Eds.), *Astronomical data analysis software and systems XX* (Vol. 442, p. 435).
- Casey, C. M., Akins, H. B., Shuntov, M., Ilbert, O., Paquereau, L., Franco, M., Hayward, C. C., Finkelstein, S. L., Boylan-Kolchin, M., Robertson, B. E., Allen, N., Brinch, M., Cooper, O. R., Ding, X., Drakos, N. E., Faisst, A. L., Fujimoto, S., Gillman, S., Harish, S., ... Zavala, J. A. (2023). *COSMOS-web: Intrinsically luminous $z \gtrsim 10$ galaxy candidates test early stellar mass assembly*. <https://arxiv.org/abs/2308.10932>
- Casey, C. M., Kartaltepe, J. S., Drakos, N. E., Franco, M., Harish, S., Paquereau, L., Ilbert, O., Rose, C., Cox, I. G., Nightingale, J. W., Robertson, B. E., Silverman, J. D., Koekemoer, A. M., Massey, R., McCracken, H. J., Rhodes, J., Akins, H. B., Amvrosiadis, A., Arango-Toro, R. C., ... Zavala, J. A. (2023). *COSMOS-web: An overview of the JWST cosmic origins survey*. <https://arxiv.org/abs/2211.07865>

- 168 Collaboration, T. A., Price-Whelan, A. M., Lim, P. L., Earl, N., Starkman, N., Bradley, L.,
169 Shupe, D. L., Patil, A. A., Corrales, L., Brasseur, C. E., Nöthe, M., Donath, A., Tollerud,
170 E., Morris, B. M., Ginsburg, A., Vaher, E., Weaver, B. A., Tocknell, J., Jamieson, W., ...
171 Contributors, A. P. (2022). The astropy project: Sustaining and growing a community-
172 oriented open-source project and the latest major release (v5.0) of the core package*. *The*
173 *Astrophysical Journal*, 935(2), 167. <https://doi.org/10.3847/1538-4357/ac7c74>
- 174 Gardner, J. P., Mather, J. C., Clampin, M., Doyon, R., Greenhouse, M. A., Hammel, H. B.,
175 Hutchings, J. B., Jakobsen, P., Lilly, S. J., Long, K. S., Lunine, J. I., Mccaughrean, M. J.,
176 Mountain, M., Nella, J., Rieke, G. H., Rieke, M. J., Rix, H.-W., Smith, E. P., Sonneborn,
177 G., ... Wright, G. S. (2006). The james webb space telescope. *Space Science Reviews*,
178 123(4), 485–606. <https://doi.org/10.1007/s11214-006-8315-7>
- 179 Jarvis, M., Bernstein, G. M., Amon, A., Davis, C., Lé get, P. F., Bechtol, K., Harrison, I., Gatti,
180 M., Roodman, A., Chang, C., Chen, R., Choi, A., Desai, S., Drlica-Wagner, A., Gruen, D.,
181 Gruendl, R. A., Hernandez, A., MacCrann, N., Meyers, J., ... and, R. D. W. (2020). Dark
182 energy survey year 3 results: Point spread function modelling. *Monthly Notices of the*
183 *Royal Astronomical Society*, 501(1), 1282–1299. <https://doi.org/10.1093/mnras/staa3679>
- 184 Ji, Z., Williams, C. C., Tacchella, S., Suess, K. A., Baker, W. M., Alberts, S., Bunker,
185 A. J., Johnson, B. D., Robertson, B., Sun, F., Eisenstein, D. J., Rieke, M., Maseda,
186 M. V., Hainline, K., Hausen, R., Rieke, G., Willmer, C. N. A., Egami, E., Shivaiei,
187 I., ... Sandles, L. (2023). *JADES + JEMS: A detailed look at the buildup of central*
188 *stellar cores and suppression of star formation in galaxies at redshifts $3 < z < 4.5$* .
189 <https://arxiv.org/abs/2305.18518>
- 190 McCleary, J. E., Everett, S. W., Shaaban, M. M., Gill, A. S., Vassilakis, G. N., Huff, E. M.,
191 Massey, R. J., Benton, S. J., Brown, A. M., Clark, P., & others. (2023). Lensing in the
192 blue II: Estimating the sensitivity of stratospheric balloons to weak gravitational lensing.
193 *arXiv Preprint arXiv:2307.03295*.
- 194 Perrin, M. D., Sivaramakrishnan, A., Lajoie, C.-P., Elliott, E., Pueyo, L., Ravindranath, S., &
195 Albert, Loic. (2014). Updated point spread function simulations for JWST with WebbPSF.
196 In Jr. Oschmann Jacobus M., M. Clampin, G. G. Fazio, & H. A. MacEwen (Eds.), *Space*
197 *telescopes and instrumentation 2014: Optical, infrared, and millimeter wave* (Vol. 9143, p.
198 91433X). <https://doi.org/10.1117/12.2056689>
- 199 Perrin, M. D., Soummer, R., Elliott, E. M., Lallo, M. D., & Sivaramakrishnan, A. (2012).
200 Simulating point spread functions for the James Webb Space Telescope with WebbPSF. In
201 M. C. Clampin, G. G. Fazio, H. A. MacEwen, & Jr. Oschmann Jacobus M. (Eds.), *Space*
202 *telescopes and instrumentation 2012: Optical, infrared, and millimeter wave* (Vol. 8442, p.
203 84423D). <https://doi.org/10.1117/12.925230>
- 204 Rieke, M. J., Baum, S. A., Beichman, C. A., Crampton, D., Doyon, R., Eisenstein, D., Greene,
205 T. P., Hodapp, K.-W., Horner, S. D., Johnstone, D., Lesyna, L., Lilly, S., Meyer, M.,
206 Martin, P., Jr., D. W. M., Rieke, G. H., Roellig, T. L., Stauffer, J., Trauger, J. T., & Young,
207 E. T. (2003). NGST NIRCам scientific program and design concept. In J. C. Mather (Ed.),
208 *IR space telescopes and instruments* (Vol. 4850, pp. 478–485). International Society for
209 Optics; Photonics; SPIE. <https://doi.org/10.1117/12.489103>
- 210 Rieke, M. J., Kelly, D. M., Misselt, K., Stansberry, J., Boyer, M., Beatty, T., Egami, E., Florian,
211 M., Greene, T. P., Hainline, K., Leisenring, J., Roellig, T., Schlawin, E., Sun, F., Tinnin,
212 L., Williams, C. C., Willmer, C. N. A., Wilson, D., Clark, C. R., ... Young, E. T. (2023).
213 Performance of NIRCам on JWST in flight. *Publications of the Astronomical Society of*
214 *the Pacific*, 135(1044), 028001. <https://doi.org/10.1088/1538-3873/acac53>
- 215 Rieke, M. J., Kelly, D., & Horner, S. (2005). Overview of James Webb Space Telescope and
216 NIRCам's Role. In J. B. Heaney & L. G. Burriesci (Eds.), *Cryogenic optical systems and*
217 *instruments XI* (Vol. 5904, pp. 1–8). <https://doi.org/10.1117/12.615554>

- 218 Rowe, B., Jarvis, M., Mandelbaum, R., Bernstein, G. M., Bosch, J., Simet, M., Meyers, J.
219 E., Kacprzak, T., Nakajima, R., Zuntz, J., Miyatake, H., Dietrich, J. P., Armstrong, R.,
220 Melchior, P., & Gill, M. S. S. (2015). *GalSim: The modular galaxy image simulation*
221 *toolkit*. <https://arxiv.org/abs/1407.7676>
- 222 Stanitzki, M., & Strube, J. (2021). Performance of julia for high energy physics analyses. *Com-*
223 *puting and Software for Big Science*, 5(1). <https://doi.org/10.1007/s41781-021-00053-3>
- 224 Zhuang, M.-Y., & Shen, Y. (2023). *Characterization of JWST NIRCам PSFs and implications*
225 *for AGN+host image decomposition*. <https://arxiv.org/abs/2304.13776>

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