

Using Machine Learning to Predict the Correlation of Spectra Using SDSS Colour Magnitudes as an Improvement to the Locus Algorithm

Tom O’Flynn^a, Eugene Hickey^{a,1}, Kevin Nolan^{a,2}, Oisin Creaner^{b,2}

^a*Department of Applied Science Dublin D24FKT9*

^b*10 Burlington Rd Dublin D04 C932 Ireland*

Abstract

The Locus Algorithm is a new technique to improve the quality of differential photometry by optimising the choices of reference stars. At the heart of this algorithm is a routine to assess how good each potential reference star is by comparing its sdss magnitude values to those of the target star. In this way, the difference in wavelength-dependent effects of the Earth’s atmospheric scattering between target and reference can be minimised. This paper sets out a new way to calculate the quality of each reference star using machine learning. A random subset of stars from sdss with spectra was chosen. For each one, a suitable reference star, also with a spectrum, was chosen. The correlation between the two spectra was taken to be the gold-standard measure of how well they match up for differential photometry. The five sdss magnitude values for each of these stars were used as predictors. A number of supervised machine learning models were constructed on a training set of the stars and were each evaluated on a testing set. The model using Support Vector Regression had the best performance of these models. It was then tested of a final, hold-out, validation set of stars to get an unbiased measure of its performance. The dataset used, the model constructions, and performance evaluation are presented here.

1. Introduction

A wealth of astrophysics information is available through the study of the brightness of celestial objects as a function of time. For example, exoplanet detection by the transit method relies critically on measurements of intrinsic variability where such variability can be a small fraction of the total stellar brightness (Giltinan et al. (2011), Everett and Howell (2001)). Ground-based observations looking for such variability are complicated by the effects of the Earth’s atmosphere which causes incoherent wavelength-dependent variations in the stellar flux detected. This can mask intrinsic variability and hamper the study of variable astrophysical phenomena (Smith et al. (2008)).

The technique of differential photometry has been developed in an attempt to mitigate the effects of the Earth’s atmosphere on studies of stellar variability. Differential photometry uses reference stars at small angular separations from the star of interest as comparators. Atmospheric effects should have similar effects on the measured flux from all of these stars causing them to vary in unison (Burdanov et al. (2014)). Because scattering in the Earth’s atmosphere is wavelength dependent, the technique is especially successful if the target star and reference stars are spectrally similar (Milone and Pel (2011), Sterken et al. (2011)).

The Locus Algorithm (Creaner et al. (2022)) has been used to create catalogues of pointings suitable for differential photometry on astronomical targets based on a novel technique of choosing appropriate reference stars (Creaner et al. (2020) and Creaner EXO’s). The algorithm no longer places the target in the centre of

*Corresponding author

Email addresses: tom.oflynn@tudublin.ie (Tom O’Flynn), eugene.hickey@tudublin.ie (Eugene Hickey), kevin.nolan@tudublin.ie (Kevin Nolan), creanero@cp.dias.ie (Oisin Creaner)

¹Corresponding Author

²Equal contribution

the field of view but, in general, repositions it so as to include the best set of reference stars. Assessment of each reference star is performed by referring to the sdss catalogue and the colour band magnitudes therein. These magnitudes can be used to infer the overall shape of the star’s spectrum. Stars that have similar spectra will be effected by scattering from the Earth’s atmosphere to a more comparable degree than stars with dissimilar spectra. The original Locus Algorithm used a rational, but ad-hoc, method to estimate the correlation of stellar spectra based on differences between their g, r, and i sdss colour magnitudes (?). This was necessary for computational efficiency. The work presented here presents a more rigorous technique to estimate the correlation of stellar spectra based on machine learning. The subset of stars in sdss that have their spectra measured are used. These stars are paired off such that each pair has similar colour magnitude differences and are thus potentially a good match for differential photometry. This corresponds to the pre-filtering step employed by ?. The correlation between each pair’s spectra is calculated. This forms the basis of a goodness-of-fit between the two spectra. The sdss magnitudes (u, g, r, i, and z for both stars in the pair) are then used to train machine learning algorithms to predict this goodness-of-fit. The models produced are then applied to other pairs of stars, the test set, to evaluate their performance. The results show a significant improvement over the original ad-hoc Locus Algorithm routine, this model will be incorporated to future generations of the Locus Algorithm.

2. Data

This work uses 3556 stellar spectra from the SDSS SEGUE and BOSS observations and their physical parameters from the 13th SDSS data release (Aguado et al. (2018)). The spectra are clipped to just the wavelengths contained in the sdss r band (between 550nm and 700nm). Stars are paired off based on their sdss colour magnitudes so that both stars in a pair are of similar colour. Specifically, both $(g_1 - r_1) - (g_2 - r_2)$ and $(r_1 - i_1) - (r_2 - i_2)$ will be between 0 and 0.3. This ensures that these stars would be realistic matches for differential photometry. In addition, stars were chosen that had r colour magnitude values between 15 and 20. The SQL queries used to download physical parameters and the spectra are given in the supplementary materials for this paper. Correlations between spectra are calculated using the usual Pearson Correlation formula, equation (1).

$$r_{xy} = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n \sum x_i^2 - (\sum x_i)^2} \sqrt{n \sum y_i^2 - (\sum y_i)^2}}. \quad (1)$$

where x_i refer to the flux from the first star at a given wavelength, i , in units of $erg/cm^2/s\text{\AA}$, y_i refer to the flux from the second star at the same wavelength. Figure 1 shows some pairs of stars along with their correlations. The first pair, A and B, are representative of the sample. The second pair, C and D, were chosen to have an unusually low correlation for this sample set.

Correlation is usually bounded by -1 and 1. And because these are spectra from stars and they have similar colour magnitudes, the correlations tend to be clustered near this higher end, see the histogram in figure 2A below. Machine learning algorithms work better with normally distributed values (need reference) and this is especially true when it comes to analysing model performance (another reference), so the correlation values were transformed. First of all by a logit transformation (2):

$$\text{logit}(x) = \ln \left(\frac{1+x}{1-x} \right) \quad (2)$$

And then by scaling and normalising the values to have a mean of 0 and a standard deviation of 1. The resulting transformed values are shown in figure 2B.

The data is split into test and training sets, with 70% of the data (2668 samples) in the training set and the remainder (888 samples) in the test set. Each set has a representative sample of correlation values, to do this the original sample of 3556 pairs is split into five groups based on percentiles of the correlation and both testing and training sets get a commensurate proportion of each group. A additional, completely independent set of 526 pairs of stars are used for final validation of the chosen model.

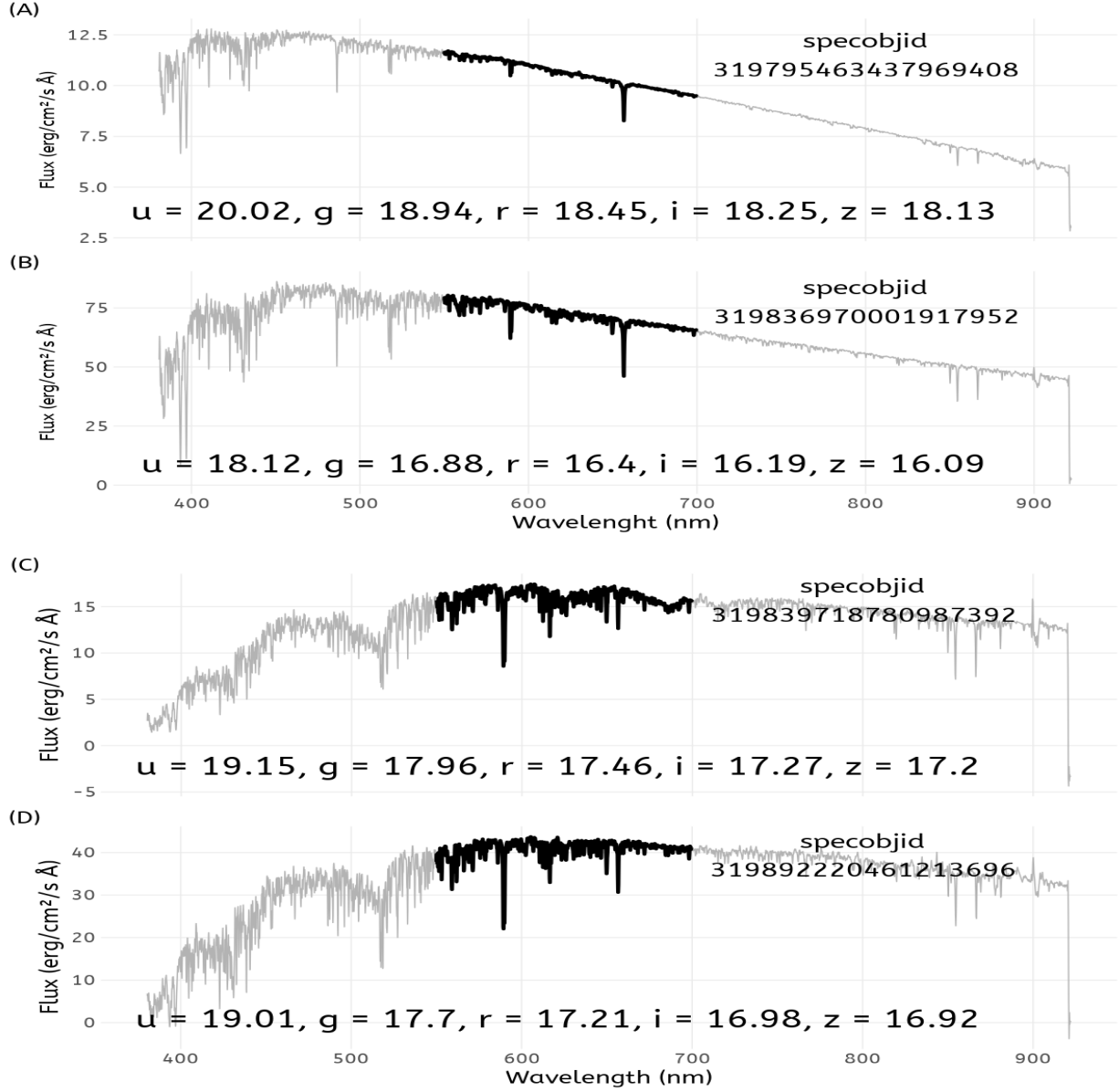


Figure 1: Two pairs of spectra downloaded from SDSS. The ugriz colour magnitudes for each star is given below its spectrum. The darkened area of the spectral line corresponds to the r-band wavelengths. The correlation between spectra A and C is 0.96. That between spectra B and D is 0.75.

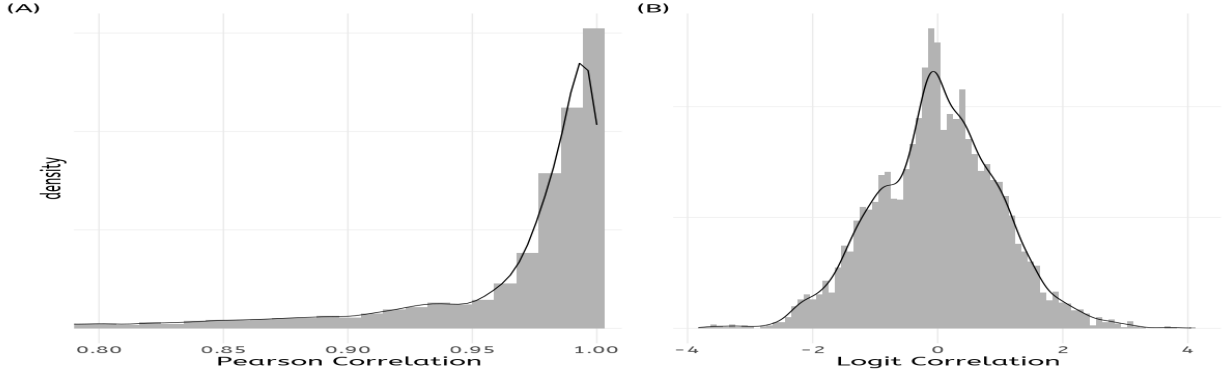


Figure 2: (A) Histogram of Pearson correlation values between r-band spectra between pairs of matched stars. (B) Values in (A) transformed by a logit function.

3. Models

Four types of machine learning algorithms were used: support vector regression (SVR), random forest (RF), extreme gradient boosting (XGB), and a linear model (LM). In each of the four cases, a model was built on the training set, using 10 predictors, namely the ugriz values for both stars in each pair. The target value was the $\text{logit}(\text{correlation})$ value. Cross validation, 20-fold repeated 10 times, was used to minimise model bias. Hyperparameters for each model were tuned. The results for RMSE, MAE, and R^2 for all models are given in ?? .The details are given below:

- *Support Vector Regression* This used a radial basis kernel function (Karatzoglou2004). A grid search on the hyperparameters Cost (C) and sigma (σ) was undertaken for values $8 < C < 25$ and $0.08 < \sigma < 0.20$. The model was optimised based on the RMSE of the training set. The best tune was obtained for $C = 20$ and $\sigma = 0.12$.
- *Stochastic Gradient Boosting* This used Friedman’s gradient boosting algorithm (Boehmke and Greenwell (2019)). A grid search on the hyperparameters Number of Boosting Iterations (n.trees), Maximum Tree Depth (interaction.depth), Shrinkage (shrinkage), and Minimum Terminal Node Size (n.minobsinnode) was undertaken. The model was optimised based on the RMSE of the training set. The best tune was obtained for n.trees = 100, interaction.depth = 10, shrinkage = 0.1 and n.minobsinnode = 10.
- *Random Forrest* This used the *ranger* fast implementation of random forrests (Wright and Ziegler (2017)). The Minimum Node Size was set to be 5, the splitting rule was chosen to be *variance*. The number of variables to possibly split at each node (mtry) was tuned to be 6.
- *Linear Model* The final model was a linear model from the MASS R package (Venables and Ripley (2002)). There were no tunable parameters.

A regression model was built on the training set. An eXtreme Gradient Boosting model (Friedman et al. (2000), Chen and Guestrin (2021)) was used. This was chosen because of its performance and reliability (Bentéjac et al. (2020)). Cross validation was performed using a bootstrap method (Efron (1983)). The model was fit with the maximum number of boosting iterations set to 150, the learning rate set to 0.3, the maximum tree depth set to 3. It was set to minimise the RMSE on the training set. The final model fit was produced after 106 iterations.

4. Model Evaluation

The table below gives the values for RMSE, MAE, and R^2 for each of the four values as they applied to the test set.

Table 1: A stunning table

	RMSE	R^2	MAE
SVR	0.554	0.693	0.394
GBM	0.584	0.655	0.423
RF	0.590	0.648	0.427
LM	0.639	0.587	0.480

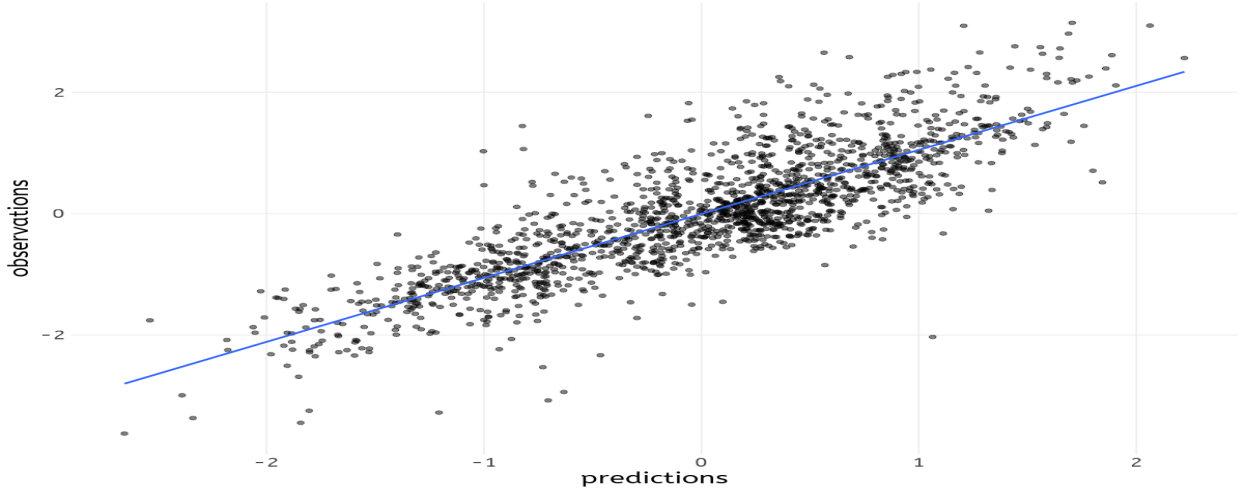


Figure 3: Observed versus predicted logit correlation values

The model was then used to predict the logit correlation values from the 1676 star pairs from the test set. Figure 3 shows the resulting values of observed logit correlation values against predicted logit correlation values. Figure 4 shows the resulting values of the residuals, the observations minus the predicted values, against predicted logit correlation values. Figure 5 shows a histogram of the residual values, figure 6 shows a quantile-quantile (QQ) plot of the residuals. The shape of this last plot shows the residuals to be somewhat platykurtic which is acceptable for a machine learning fit (ref??).

The R^2 value of predicted logit correlation on the test set was found to be 71%. The RMSE on the test set was found to be 0.55. The performance of the original function used in Creaner et al. (2022) was worse, with an R^2 of 13%.

5. Conclusions

The last numbered section should briefly summarise what has been done, and describe the final conclusions which the authors draw from their work.

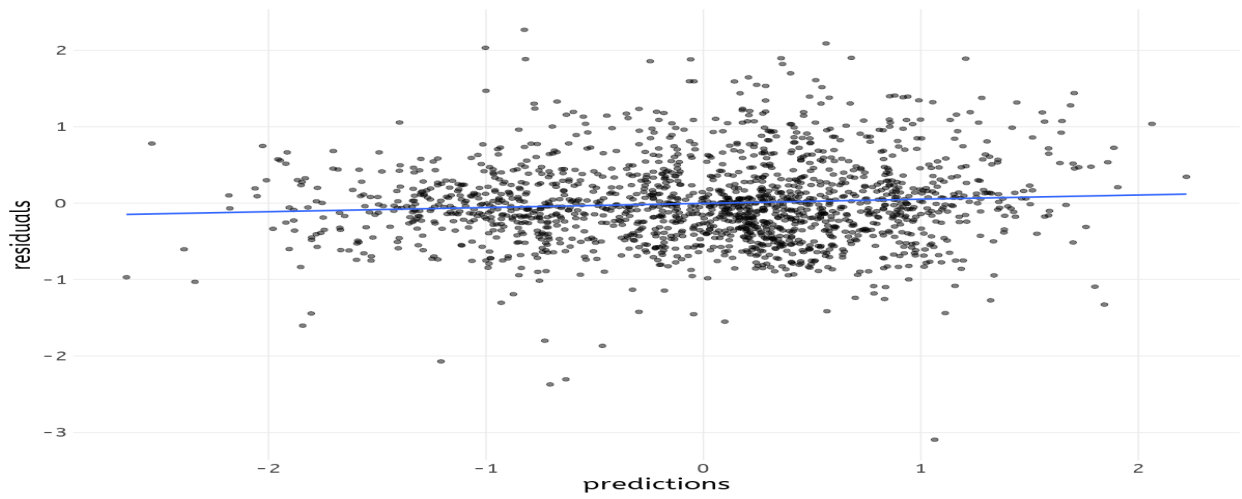


Figure 4: Residuals versus predicted logit correlation values

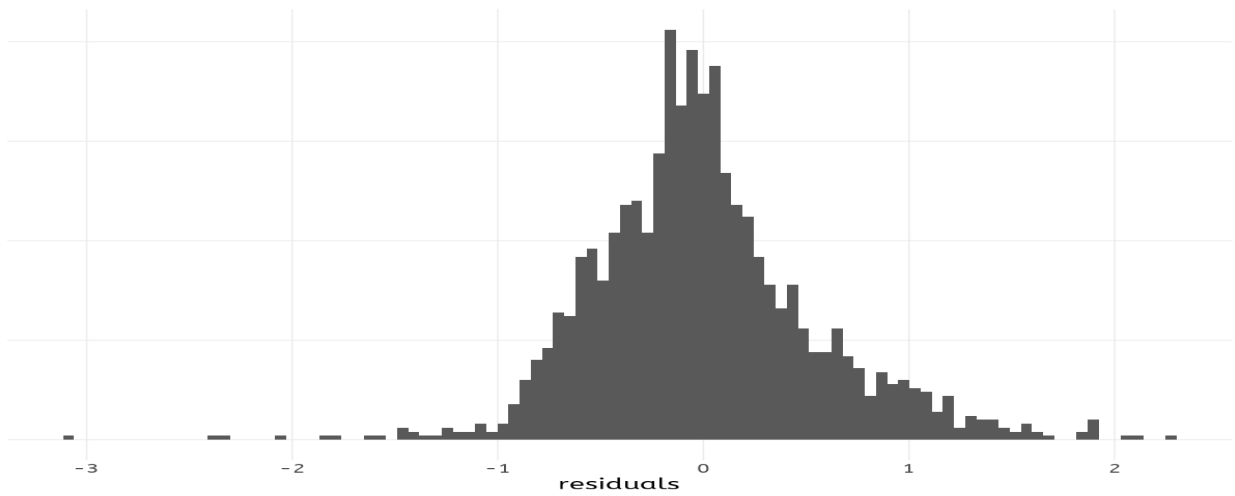


Figure 5: Observed versus predicted logit correlation values

Table 2: This is an example table. Captions appear above each table. Remember to define the quantities, symbols and units used.

A	B	C	D
1	2	3	4
2	4	6	8
3	5	7	9

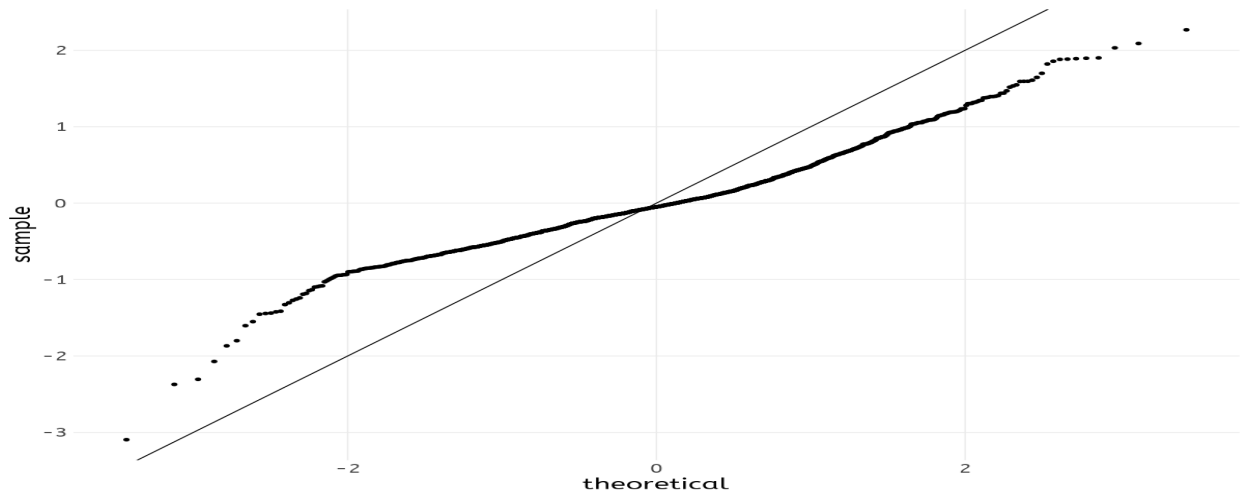


Figure 6: Observed versus predicted logit correlation values

References

- D. S. Aguado, Romina Ahumada, Andres Almeida, Scott F. Anderson, Brett H. Andrews, Borja Anguiano, Erik Aquino Ortiz, Alfonso Aragon-Salamanca, Maria Argudo-Fernandez, Marie Aubert, Vladimir Avila-Reese, Carles Badenes, Sandro Barboza Rembold, Kat Barger, Jorge Barrera-Ballesteros, Dominic Bates, Julian Bautista, Rachael L. Beaton, Timothy C. Beers, Francesco Belfiore, Mariangela Bernardi, Matthew Bershad, Florian Beutler, Jonathan Bird, Dmitry Bizyaev, Guillermo A. Blanc, Michael R. Blanton, Michael Blomqvist, Adam S. Bolton, Mederic Boquien, Jura Borissova, Jo Bovy, William Nielsen Brandt, Jonathan Brinkmann, Joel R. Brownstein, Kevin Bundy, Adam Burgasser, Nell Byler, Mariana Cano Diaz, Michele Cappellari, Ricardo Carrera, Bernardo Cervantes Sodi, Yanping Chen, Brian Cherinka, Peter Doohyun Choi, Haeun Chung, Damien Coffey, Julia M. Comerford, Johan Comparat, Kevin Covey, Gabriele da Silva Ilha, Luiz da Costa, Yu Sophia Dai, Guillermo Damke, Jeremy Darling, Roger Davies, Kyle Dawson, Victoria de Sainte Agathe, Alice Deconto Machado, Agnese Del Moro, Nathan De Lee, Aleksandar M. Diamond-Stanic, Helena Dominguez Sanchez, John Donor, Niv Drory, Helion du Mas des Bourboux, Chris Duckworth, Tom Dwelly, Garrett Ebelke, Eric Emsellem, Stephanie Escoffier, Jose G. Fernandez-Trincado, Diane Feuillet, Johanna-Laina Fischer, Scott W. Fleming, Amelia Fraser-McKelvie, Gordon Freischlad, Peter M. Frinchaboy, Hai Fu, Lluís Galbany, Rafael Garcia-Dias, D. A. Garcia-Hernandez, Luis Alberto Garma Oehmichen, Marcio Antonio Geimba Maia, Hector Gil-Marin, Kathleen Grabowski, Meng Gu, Hong Guo, Jaewon Ha, Emily Harrington, Sten Hasselquist, Christian R. Hayes, Fred Hearty, Hector Hernandez Toledo, Harry Hicks, David W. Hogg, Kelly Holley-Bockelmann, Jon A. Holtzman, Bau-Ching Hsieh, Jason A. S. Hunt, Ho Seong Hwang, Hector J. Ibarra-Medel, Camilo Eduardo Jimenez Angel, Jennifer Johnson, Amy Jones, Henrik Jonsson, Karen Kinemuchi, Juna Kollmeier, Coleman Krawczyk, Kathryn Kreckel, Sandor Kruk, Ivan Lacerna, Ting-Wen Lan, Richard R. Lane, David R. Law, Young-Bae Lee, Cheng Li, Jianhui Lian, Lihwai Lin, Yen-Ting Lin, Chris Lintott, Dan Long, Penelope Longa-Pena, J. Ted Mackereth, Axel de la Macorra, Steven R. Majewski, Olena Malanushenko, Arturo Manchado, Claudia Maraston, Vivek Mariappan, Mariarosa Marinelli, Rui Marques-Chaves, Thomas Masseron, Karen L. Masters, Richard M. McDermid, Nicolas Medina Pena, Sofia Meneses-Goytia, Andrea Merloni, Michael Merrifield, Szabolcs Meszaros, Dante Minniti, Rebecca Minsley, Dimitri Muna, Adam D. Myers, Preethi Nair, Janaina Correa do Nascimento, Jeffrey A. Newman, Christian Nitschelm, Matthew D. Olmstead, Audrey Oravetz, Daniel Oravetz, Rene A. Ortega Minakata, Zach Pace, Nelson Padilla, Pedro A. Palicio, Kaike Pan, Hsi-An Pan, Taniya Parikh, James Parker, Sebastien Peirani, Samantha Penny, Will J. Percival, Ismael Perez-Fournon, Thomas Peterken, Marc Pinsonneault, Abhishek Prakash, Jordan Raddick, Anand Raichoor, Rogemar A. Riffel, Rogerio Riffel, Hans-Walter Rix, Annie C. Robin, Alexandre Roman-Lopes, Benjamin Rose, Ashley J. Ross, Graziano Rossi, Kate Rowlands, Kate H. R. Rubin, Sebastian F. Sanchez, Jose R. Sanchez-Gallego, Conor Sayres, Adam Schaefer, Ricardo P. Schiavon, Jaderson S. Schimoia, Edward Schlafly, David Schlegel, Donald Schneider, Mathias Schultheis, Hee-Jong Seo, Shoaib J. Shamsi, Zhengyi Shao, Shiyin Shen, Shravan Shetty, Gregory Simonian, Rebecca Smethurst, Jennifer Sobeck, Barbara J. Souter, Ashley Spindler, David V. Stark, Keivan G. Stassun, Matthias Steinmetz, Thaisa Storchi-Bergmann, Guy S. Stringfellow, Genaro Suarez, Jing Sun, Manuchehr Taghizadeh-Popp, Michael S. Talbot, Jamie Tayar, Aniruddha R. Thakar, Daniel Thomas, Patricia Tissera, Rita Tojeiro, Nicholas W. Troup, Eduardo Unda-Sanzana, Octavio Valenzuela, Mariana Vargas-Maga Na, Jose Antonio Vazquez Mata, David Wake, Benjamin Alan Weaver, Anne-Marie Weijmans, Kyle B. Westfall, Vivienne Wild, John Wilson, Emily Woods, Renbin Yan, Meng Yang, Olga Zamora, Gail Zasowski, Kai Zhang, Zheng Zheng, Guangtun Zhu, Joel C. Zinn, and Hu Zou. The Fifteenth Data Release of the Sloan Digital Sky Surveys: First Release of MaNGA Derived Quantities, Data Visualization Tools and Stellar Library. dec 2018. doi: 10.3847/1538-4365/aaf651. URL <http://arxiv.org/abs/1812.02759><http://dx.doi.org/10.3847/1538-4365/aaf651>.
- Candice Bentéjac, Anna Csörgő, and Gonzalo Martínez-Muñoz. A comparative analysis of gradient boosting algorithms.

- Artificial Intelligence Review* 2020 54:3, 54(3):1937–1967, aug 2020. ISSN 1573-7462. doi: 10.1007/S10462-020-09896-5. URL <https://link.springer.com/article/10.1007/s10462-020-09896-5>.
- Brad Boehmke and Brandon Greenwell. Hands-On Machine Learning with R. *Hands-On Machine Learning with R*, nov 2019. doi: 10.1201/9780367816377. URL <https://www.taylorfrancis.com/books/mono/10.1201/9780367816377/hands-machine-learning-brad-boehmke-brandon-greenwell>.
- Artem Y Burdanov, Vadim V Krushinsky, and Alexander A Popov. Astrokit-an Efficient Program for High-Precision Differential CCD Photometry and Search for Variable Stars. *Translated from Astrofizicheskij Byulleten*, 69(3), 2014.
- Tianqi Chen and Carlos Guestrin. Extreme Gradient Boosting [R package xgboost version 1.5.0.2]. *Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 13-17-Aug:785–794, nov 2021. doi: 10.1145/2939672.2939785. URL <https://cran.r-project.org/package=xgboost>.
- Oisín Creaner, Kevin Nolan, Niall Smith, David Grennan, and Eugene Hickey. A catalogue of Locus Algorithm pointings for optimal differential photometry for 23 779 quasars. *Monthly Notices of the Royal Astronomical Society*, 498(3):3720–3729, nov 2020. ISSN 13652966. doi: 10.1093/MNRAS/STAA2494.
- Oisín Creaner, Kevin Nolan, Eugene Hickey, and Niall Smith. The Locus Algorithm: A novel technique for identifying optimised pointings for differential photometry. *Astronomy and Computing*, 38:100537, jan 2022. ISSN 2213-1337. doi: 10.1016/J.ASCOM.2021.100537. URL <http://arxiv.org/abs/2003.04582>.
- Bradley Efron. Estimating the error rate of a prediction rule: Improvement on cross-validation. *Journal of the American Statistical Association*, 78(382):316–331, 1983. ISSN 1537274X. doi: 10.1080/01621459.1983.10477973.
- Mark E. Everett and Steve B. Howell. A Technique for Ultrahigh-Precision CCD Photometry. *Publications of the Astronomical Society of the Pacific*, 113(789):1428–1435, nov 2001. ISSN 0004-6280. doi: 10.1086/323387/0.
- Jerome Friedman, Trevor Hastie, and Robert Tibshirani. Additive logistic regression: A statistical view of boosting. *Annals of Statistics*, 28(2):337–407, 2000. ISSN 00905364. doi: 10.1214/AOS/1016218223.
- Alan Giltinan, Dylan Loughnan, Adrian Collins, and Niall Smith. Using EMCCD’s to improve the photometric precision of ground-based astronomical observations. *Journal of Physics: Conference Series*, 307(1), 2011. ISSN 17426596. doi: 10.1088/1742-6596/307/1/012010.
- E. F. Milone and Jan Willem Pel. The High Road to Astronomical Photometric Precision: Differential Photometry. pages 33–68, 2011. doi: 10.1007/978-1-4419-8050-2_2. URL https://link.springer.com/chapter/10.1007/978-1-4419-8050-2_2.
- Niall Smith, Alan Giltinan, Aidan O’Connor, Stephen O’Driscoll, Adrian Collins, Dylan Loughnan, Andreas Papageorgiou, Niall Smith, Alan Giltinan, Aidan O’Connor, Stephen O’Driscoll, Adrian Collins, Dylan Loughnan, and Andreas Papageorgiou. EMCCD Technology in High Precision Photometry on Short Timescales. *ASSL*, 351:257, oct 2008. doi: 10.1007/978-1-4020-6518-7_13. URL <https://ui.adsabs.harvard.edu/abs/2008ASSL..351..257S/abstract>.
- Christiaan Sterken, E. F. Milone, and Andrew T. Young. Photometric Precision and Accuracy. pages 1–32, 2011. doi: 10.1007/978-1-4419-8050-2_1. URL https://link.springer.com/chapter/10.1007/978-1-4419-8050-2_1.
- W. N. Venables and B. D. Ripley. Modern Applied Statistics with S. 2002. doi: 10.1007/978-0-387-21706-2. URL <http://link.springer.com/10.1007/978-0-387-21706-2>.
- Marvin N. Wright and Andreas Ziegler. ranger: A Fast Implementation of Random Forests for High Dimensional Data in C++ and R. *Journal of Statistical Software*, 77(1):1–17, mar 2017. ISSN 1548-7660. doi: 10.18637/JSS.V077.I01. URL <https://www.jstatsoft.org/index.php/jss/article/view/v077i01>.