Reviewer 3 (Simon Paplexiou)

This is a useful and interesting technical note on simulating stream flow time series preserving observed characteristics. Several techniques exist to approximate time series such as preserving moments, using marginal-back transformations, bootstrap, amplitude adjusted Fourier transformations methods, etc. All of them have advantages and disadvantages. This technical note is well-structured, well-written, and the real-world case is nicely demonstrated. The authors' intention to provide an easy-to-apply solution is clear, and although this is a technical note, the added value against previews works on the amplitude adjusted Fourier transformation method should be better highlighted in order to strengthen the publication.

Before providing a detailed review, I'm expressing my gratitude to the commenters referring to my 2018 work. Clarifying, I worked on this framework much earlier in 2009 for a multivariate and cyclostationary simulation of daily rainfall (13 stations in Greece) aiming to preserve marginals (the Burr type XII was used), correlations and intermittency.

The method was described in detail in a document (Papalexiou, 2010) that includes also mixed-type distributions inflated at arbitrary points and not just at zero.

The extended work was published in arXiv (Papalexiou, 2017), followed by the journal publication some months later (Papalexiou, 2018). The scheme also applied in a stationary/nonstationary disaggregation framework preserving marginals and correlations (DiPMaC) (Papalexiou et al., 2018). It was an attempt to provide a simple framework for univariate and multivariate modeling preserving continuous, discrete, binary or mixed-type marginals having positive definite autocorrelation structure (including long memory). The focus was specifically on hydroclimatic variables such as precipitation, streamflow, wind, humidity, etc.

Yet as the saying goes, most things have been already found before; indeed, the first attempts in other scientific fields to simulate time series preserving marginals and correlations using inflated correlations date back in the works of Conner and Hammond (1972), and probably much earlier. A clear presentation for continuous marginals using AR models was given by Li & Hammond in (1975). The authors may wish to check also an old paper entitled "Generation of random signals with specified probability density function and power density spectra" by Gugar and Kavanagh published in 1968.

Following Li & Hammond (1975) several papers got published in different fields (e.g., Cario & Nelson, 1997, 1998; Kugiumtzis, 2002; Macke et al., 2009; Demirtas, 2014, 2017; Emrich & Piedmonte, 1991; Macke et al., 2009 to mentioned a few) dealing with several cases. These and many other interesting works yet were not suitable for simulating intermittent processes, like precipitation or stream flows, and most of them suggested demanding iterative procedures to estimate the parent Gaussian correlations or the cross-correlation upper limits (Papalexiou, 2018). In few papers the same link between the gaussian correlation and the bivariate copula with prescribed marginals is also established (even earlier) by using the same technique, i.e., the fundamental 2-dimensional theorem of the expected value of a transformed random variable (Nataf, 1962; Liu & Der Kiureghian, 1986; H. Li et al., 2008; Lebrun & Dutfoy, 2009; Xiao, 2014). This link can also be established by using the Jacobian of the transformation (Papalexiou, 2018, Eq. 7).

The authors here focus on another method, i.e., the amplitude adjusted Fourier transformation, with the same intent and aiming to generate consistent stream flow time series. They can also see a simulation of daily stream flow preserving a heavy tailed marginal (Burr type III) and a slowly decaying autocorrelation structure in Section 4.3 in Papalexiou (2018). Specific comments that authors may find useful to improve the manuscript are:

1. The authors write: "We hereafter refer to such methods, which are also known as amplitude-adjusted Fourier transformations (Lancaster et al., 2018), as phase randomization simulations. In hydrology, phase randomization simulation has rarely been applied for purposes other than hypothesis testing (Fleming et al., 2002), even though it has desirable properties which make it suitable for a wider range of applications. (. . .) However, its application is limited to Gaussian data. We here propose the use of phase randomization simulation for the stochastic generation of streamflow time series at individual and multiple sites. To allow for non-Gaussian distributions, as commonly observed for daily streamflow values, we combine the data simulated by phase randomization with the Kappa distribution," Probably missing something here, but amplitude-adjusted Fourier transformations can account for non-Gaussian amplitude distributions. The method proposed by Prichard and Theiler (1994) (authors cite indeed this paper) accounts for non-Gaussian marginal distributions as stated by the authors at page 953 "We account for non-Gaussian amplitude distribution by using the amplitude adjusting algorithm described in in Ref. [8] for each component". Prichard and Theiler (1994) use the algorithm described in Sec 2.4.3 of Theiler et al (1992), which reads as follows "The idea is to first rescale the values in the original time series so they are gaussian. Then the FF or WFT algorithm can be used to make surrogate time series which have the same Fourier spectrum as the rescaled data. Finally, the gaussian surrogate is then rescaled back to have the amplitude distribution as the original time series.". These techniques (Amplitude adjusted Fourier transformations) are known to preserve the linear correlations of the parent Gaussian process rather than those of the target. Indeed, they were further refined as Iterative Amplitude adjusted Fourier transformations in order to match ACF and marginal distributions of the target variables as closely as possible (Kugiumtzis, 1999; Schreiber & Schmitz, 1996; e.g., Serinaldi & Lombardo, 2017; Venema et al., 2006). So, if not missing something here I see that the methodology proposed in this technical note is related to the procedure applied by Prichard and Theiler (1994) in their second example with a difference spotted in the rescaling of the marginal distribution, where empirical CDF is replaced by a parametric Kappa distribution. Thus, maybe the statement that AAFT cannot deal with non-Gaussian marginals should be revised as my understanding is that AAFT it was devised to deal exactly with this. Of course, replacing empirical CDF with Kappa is more appropriate for stream flow simulations.

Reply: *We agree that the amplitude-adjusted Fourier transformation procedure proposed by Prichard and Theiler (1994) can deal with non-Gaussian data. However, it does usually not allow for the use of parametric distributions in the back-transformation process. We adjusted the text accordingly by acknowledging that amplitude-adjusted Fourier transform allows for the generation of non-Gaussian data. We specified that our approach differs from amplitude-adjusted Fourier transformation by that it allows for the generation of values beyond the values in the empirical distribution.*

2. An important point regards the underestimation of cross-correlation reported by the authors (it could be also observed also in the autocorrelation). It was proven mathematically long time ago (Kendall & Stuart, 1979, p. 600) (Embrechts et al., 2002) that any nonlinear transformation of a gaussian time series reduces the strength of the linear correlations as expressed by the Pearson correlation coefficient. Obviously, this does not affect the rank correlations. Since the authors are not calculating the inflated autocorrelations (or inflated spectrum) it is expected the generated time series to have lower correlations. However, in practice this depends on the transformation used. If the target marginal is bell-shaped then typically it has a small effect in reducing the autocorrelation, yet the effect can be very large for j-shaped target marginals with heavy tails and zero inflated (see Fig. 1 and Fig. 2 and the simulation examples in Fig4-Fig7 in Papalexiou (2018) and the discussion therein). Therefore, the fact that the authors don't observe large differences in the autocorrelation of the simulated time series is case specific and not generally true. This point is important and should be mentioned as there are streamflow series highly inflated at zero and highly skewed; without using inflated correlations for the parent gaussian process it is certain that the transformed series will not match the target process.

Reply: *We agree that the autocorrelation of a stochastically generated time series might not in all cases well reproduced the autocorrelation of observed time series. We add a section to the discussion section, that discusses this issue: "While the reproduction of the temporal dependence was well reproduced here, this is not necessarily the case under all conditions. Embrechts et al., 2010 have shown that any nonlinear transformation of a Gaussian time series, which is done during backtransformation, reduces the strength of the linear correlations in the time series as expressed by Pearson's correlation coefficient. If one is working with heavy-tailed and zero inflated marginals, it can happen that autocorrelations are reduced during backtransformation (Papalexiou, 2018)."*

3. As previously mentioned early approaches in simulating nongaussian timeseries preserving marginals and correlations date back long time ago (e.g. S. T. Li & Hammond, 1975), yet this framework as it was formulated didn't include the modeling of mixed-type marginals (see Papalexiou 2018) which allows easy simulation of intermittent processes such as precipitation or stemflows of ephemeral streams. To increase the novelty of the paper the authors can easily include mixed-type quantiles (see Eq. 17 in Papalexiou 2018) with the kappa distribution. As far as I know this approach has not been implemented in amplitude adjusted Fourier transformations.

Reply: *We agree that the use of mixed-type marginals can be beneficial in certain cases, where the process to simulate from is intermittent. We therefore made PRSim even more flexible by introducing user-defined distributions to be used in the backtransformation process. The software illustrates the functionality with GEV and GB2 distributions. This user-defined distribution can potentially be a mixture distribution. We did not include an example of a mixture distribution in our technical note because the time series chosen for the analysis were not characterized by intermittency. Furthermore, the use of mixtures of a discrete and a continuous part is delicate as we cannot resort on classical/standard definitions of likelihood tests or confidence intervals.*

Minor points (p = page, L = Line)

p2L33-p3L4: We can easily use large order AR models to simulate time series having long memory or any other strong autocorrelation structure. Especially AR models have an analytical solution (Yule-Walker system) and the fit and the application e.g., of an AR of order 10000 is a matter of less than a second. This means that we can reproduce exactly the autocorrelation structure up to order p. It should be clear that fitting an AR of any large order to a long memory autocorrelation structure is parsimonious and efficient as all the AR parameters are analytically and without uncertainty estimated by the autocorrelation structure, e.g., if an AR of order 10000 is fitted to an fGn correlation then it is an one-parameter model and not a 10000 parameter model. More details can be found in Papalexiou (2018), where the authors can also see examples of long memory process simulations using AR models and preserving marginals. Also long memory can be approximated by the sum of independent AR(1) processes as suggested by Mandelbrot (1971). So, it is a matter of how these models are applied and definitely they can reproduce long memory or any other autocorrelation structure.

Reply: *We agree that it is possible to approximate an arbitrary spectrum with either a large order AR or many AR(1) processes. However, this approach remains an approximation. A long-memory process can be characterized with a polynomial decay of the spectrum. AR processes have an exponential decay. Hence, it will not be possible to generate a «truly» long range process. It is possible to approximate arbitrarily precisely an empirical spectrum. If one observes a spectrum of length n, n AR(1) processes will allow for the approximation of an empirical spectrum. We specified in the introduction that AR models can be used to generate seemingly long-memory processes if a parametric autocorrelation structure is used to fit the data.*

p4L6-p4L9: The Kappa distribution is a well-established distribution in hydrology and since Hosking (1994) introduced the four-parameter version it has been applied countless times (e.g., Hanson & Vogel, ; Kjeldsen et al., 2017; Park et al., 2009)). Its importance and flexibility stems for the fact that generalizes important distribution such as the GP, GEV, GLO etc, but it can also be seen as a special case and generalization at the same time of the Burr type XII. Maybe the great disadvantage of the four-parameter version is the location parameter which can end up in supporting a range of values which is inconsistent with the variable under study. For stream flows expected to range in the positive axis this can be problematic. If distributions like the Generalized Gamma or the Burr type XII didn't work, maybe the authors should try with the Burr type III (1 scale, 2 shape pars) (Burr, 1942) or the Generalized beta of the second kind (Mielke & Johnson, 1974) (1 scale, 3 shapes) which has great flexibility and is defined in (0, Infinity). This would solve the issue of negative values or of a lower positive limit but of course the authors may neglect this suggestion.

Reply: *Thank you for this suggestion. We tested the Generalized beta distribution of the second kind. It seems to be rather flexible and works fine for certain catchments. In other catchments, however, it produces very extreme, and rather implausible high-flow values. As the distribution is defined in the interval [0,Infinity], it solves the problem with the zero values, but introduces a problem with infinity values. While this and other distributions tested (GEV, Burr type XII, generalized Gamma, Wakeby) were not found to be suitable in our application example, they might be appropriate in other cases. We therefore adjusted the PRSim R-package (version > 1.0) to allow for any type of distribution specified by the user in the back-transformation process.*

p5L19 and P6L9-11: To clarify regarding the normal transformation. The authors have fitted the Kappa in each day and then use the Kappa cdf to transform to uniform and then apply the gaussian quantile? Even if they did so the final time series might have normal marginal but the autocorrelation may be different in each week/month or season.

Reply: *It is correct that the kappa distribution was fitted to each day individually and that the autocorrelation shows monthly variations.*

p6L3: The KS-test is not a very robust test. It will not change anything to the analysis, but maybe more robust tests should be used and promoted, e.g., the Anderson-Darling. If it's not much of a trouble the authors could test the fit based on the AD test.

Reply: *We agree that the KS-test is not very robust and added the AD test as a goodness-of-fit test. The PRSim package now allows for choosing one of the two tests.*

p6L20: I might be missing something here but why is 0 the lower bound of the four parameter Kappa?

Reply: *It is correct that the kappa distribution does not have a lower bound. The sentence was rephrased to "Negative simulated values are replaced by 0, because the kappa distribution does not allow for setting a lower bound".*

Summarizing, this is well-written and useful technical note that deserves publication after some amendments and literature updates.

References

1. Burr, I. W. (1942). Cumulative Frequency Functions. The Annals of Mathematical Statistics, 13(2), 215–232.

2. Cario, M. C., & Nelson, B. L. (1997). Modeling and generating random vectors with arbitrary marginal distributions and correlation matrix. Technical Report, Department of Industrial Engineering and Management Sciences, Northwestern University, Evanston, Illinois.

3. Cario, M. C., & Nelson, B. L. (1998). Numerical methods for fitting and simulating autoregressive-to-anything processes. INFORMS Journal on Computing, 10(1), 72– 81.

4. Demirtas, H. (2014). Joint generation of binary and nonnormal continuous data. Journal of Biometrics & Biostatistics, (S12), 1.

5. Demirtas, H. (2017). Concurrent generation of binary and nonnormal continuous data through fifth-order power polynomials. Communications in Statistics-Simulation and Computation, 46(1), 344–357.

6. Embrechts, P., McNeil, A., & Straumann, D. (2002). Correlation and dependence in risk management: properties and pitfalls. Risk Management: Value at Risk and Beyond, 176223.

7. Emrich, L. J., & Piedmonte, M. R. (1991). A method for generating high-dimensional multivariate binary variates. The American Statistician, 45(4), 302–304.

8. Hanson Lars S., & Vogel Richard. (n.d.). The Probability Distribution of Daily Rainfall in the United States. World Environmental and Water Resources Congress 2008, 1– 10. https://doi.org/10.1061/40976(316)585

9. Hosking, J. R. M. (1994). The four-parameter kappa distribution. IBM Journal of Research and Development, 38(3), 251–258. https://doi.org/10.1147/rd.383.0251 10. Kendall, M., & Stuart, A. (1979). Handbook of Statistics. Griffin & Company, London.

11. Kjeldsen, T. R., Ahn, H., & Prosdocimi, I. (2017). On the use of a four-parameter kappa distribution in regional frequency analysis. Hydrological Sciences Journal, 62(9), 1354–1363. https://doi.org/10.1080/02626667.2017.1335400 12. Kugiumtzis, D. (1999). Test your surrogate data before you test for nonlinearity. Physical Review. E, Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics, 60(3), 2808–2816.

13. Kugiumtzis, D. (2002). Statically transformed autoregressive process and surrogate data test for nonlinearity. Physical Review E, 66(2), 025201.

14. Lebrun, R., & Dutfoy, A. (2009). An innovating analysis of the Nataf transformation from the copula viewpoint. Probabilistic Engineering Mechanics, 24(3), 312–320. https://doi.org/10.1016/j.probengmech.2008.08.001

15. Li, H., Lü, Z., & Yuan, X. (2008). Nataf transformation based point estimate method. Chinese Science Bulletin, 53(17), 2586. https://doi.org/10.1007/s11434-008-0351-0 16. Li, S. T., & Hammond, J. L. (1975). Generation of Pseudorandom Numbers with Specified Univariate Distributions and Correlation Coefficients. IEEE Transactions on Systems, Man, and Cybernetics, SMC-5(5), 557–561. https://doi.org/10.1109/TSMC.1975.5408380

17. Liu, P.-L., & Der Kiureghian, A. (1986). Multivariate distribution models with prescribed marginals and covariances. Probabilistic Engineering Mechanics, 1(2), 105– 112. https://doi.org/10.1016/0266-8920(86)90033-0

18. Macke, J. H., Berens, P., Ecker, A. S., Tolias, A. S., & Bethge, M. (2009). Generating spike trains with specified correlation coefficients. Neural Computation, 21(2), 397–423.

19. Mandelbrot, B. B. (1971). A Fast Fractional Gaussian Noise Generator. Water Resour. Res., 7(3), 543–553.

20. Mielke, P. W., & Johnson, E. S. (1974). Some generalized beta distributions of the second kind having desirable application features in hydrology and meteorology. Water Resources Research, 10(2), 223–226. https://doi.org/10.1029/WR010i002p00223 21. Nataf, A. (1962). Statistique mathematique-determination des distributions de probabilites dont les marges sont donnees. COMPTES RENDUS HEBDOMADAIRES DES SEANCES DE L ACADEMIE DES SCIENCES, 255(1), 42.

22. Papalexiou, S.M. (2010). Stochastic modelling demystified. 10.13140/RG.2.2.34889.60008.https://www.researchgate.net/publication/333323778_Stochastic_modelling_demystified 23. Papalexiou, S. M. (2017). A unified theory for exact stochastic modelling of univariate and multivariate processes with continuous, mixed type, or discrete marginal distributions and any correlation structure. ArXiv:1707.06842 [Math, Stat]. Retrieved from http://arxiv.org/abs/1707.06842

24. Papalexiou, S. M. (2018). Unified theory for stochastic modelling of hydroclimatic processes: Preserving marginal distributions, correlation structures, and intermittency. Advances in Water Resources, 115, 234–252. https://doi.org/10.1016/j.advwatres.2018.02.013

25. Papalexiou, S. M., Markonis, Y., Lombardo, F., AghaKouchak, A., & Foufoulaâ˘AR˘ Georgiou, E. (2018). Precise Temporal Disaggregation Preserving Marginals and Correlations (DiPMaC) for Stationary and Nonstationary Processes. Water Resources Research. https://doi.org/10.1029/2018WR022726

26. Park, J.-S., Seo, S.-C., & Kim, T. Y. (2009). A kappa distribution with a hydrological application. Stochastic Environmental Research and Risk Assessment, 23(5), 579– 586. https://doi.org/10.1007/s00477-008-0243-5

27. Schreiber, null, & Schmitz, null. (1996). Improved Surrogate Data for Nonlinearity Tests. Physical Review Letters, 77(4), 635–638. https://doi.org/10.1103/PhysRevLett.77.635

28. Serinaldi, F., & Lombardo, F. (2017). General simulation algorithm for autocorrelated binary processes. Physical Review. E, 95(2–1), 023312. https://doi.org/10.1103/PhysRevE.95.023312

29. Venema, V., Meyer, S., García, S. G., Kniffka, A., Simmer, C., Crewell, S., et al. (2006). Surrogate cloud fields generated with the iterative amplitude adapted Fourier transform algorithm. Tellus A, 58(1), 104–120. https://doi.org/10.1111/j.16000870.2006.00160.x

30. Xiao, Q. (2014). Evaluating correlation coefficient for Nataf transformation. Probabilistic Engineering Mechanics, 37(Supplement C), 1–6. https://doi.org/10.1016/j.probengmech.2014.03.010

References used in the answers to the reviewers

Embrechts, P., McNeil, A.J., Straumann, D., 2010. Correlation and dependence in risk management: Properties and pitfalls, in: Dempster, M.A.H. (Ed.), Risk Management. Cambridge University Press, Cambridge, pp. 176–223. https://doi.org/10.1017/cbo9780511615337.008

Hosking, J.R.M., 1994. The four-parameter kappa distribution. IBM J. Res. Dev. 38, 251–258.

Keylock, C.J., 2012. A resampling method for generating synthetic hydrological time series with preservation of cross-correlative structure and higher-order properties. Water Resour. Res. 48, 1–18. https://doi.org/10.1029/2012WR011923

Keylock, C.J., 2007. A wavelet-based method for surrogate data generation. Phys. D Nonlinear Phenom. 225, 219–228. https://doi.org/10.1016/j.physd.2006.10.012

Kleiber, C., 2008. A auide to the Dagum distributions, in: Chotikapanich, D. (Ed.), Modeling Income Distributions and Lorenz Curves. Springer, Berlin-New York, pp. 97–117. https://doi.org/10.1007/978-0-387-72796-7_6

Mehrotra, R., Sharma, A., 2006. A nonparametric stochastic downscaling framework for daily rainfall at multiple locations. J. Geophys. Res. Atmos. 111, 1–16. https://doi.org/10.1029/2005JD006637

Mielke, P.W., 1973. Another family of distributions for describing and analyzing precipitation data. J. Appl. Meteorol. 12, 275–280.

Nguyen, H., Mehrotra, R., Sharma, A., 2019. Correcting systematic biases across multiple atmospheric variables in the frequency domain. Clim. Dyn. 52, 1283–1298. https://doi.org/10.1007/s00382-018-4191-6

Papalexiou, S.M., 2018. Unified theory for stochastic modelling of hydroclimatic processes: Preserving marginal distributions, correlation structures, and intermittency. Adv. Water Resour.

115, 234–252. https://doi.org/10.1016/j.advwatres.2018.02.013
Salas, J.D., Lee, T., 2010. Nonparametric simulation of single-site seasonal streamflows. J. Hydrol. Eng. 15, 284–296. https://doi.org/10.1061/(ASCE)HE.1943-5584.0000189
Tsoukalas, I., Efstratiadis, A., Makropoulos, C., 2018. Stochastic periodic autoregressive to anything (SPARTA) modeling and simulation of cyclostationary processes with arbitrary marginal distributions. Water Resour. Res. 54, 161–185. https://doi.org/10.1111/j.1752-1688.1969.tb04897.x