Non-parametric Kernel-Based Estimation and Simulation of Precipitation Amount

Andrew Pavlides*, Vasiliki D. Agou†, and Dionissios T. Hristopulos‡

1School of Mineral Resources Engineering, Technical University of Crete, Chania, Crete 73100, Greece
2School of Electrical and Computer Engineering, Technical University of Crete, Chania, Crete 73100, Greece

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Abstract

The probability distribution of precipitation amount strongly depends on geography, climate zone, and time scale considered. Closed-form parametric probability distributions are not sufficiently flexible to provide accurate and universal models for precipitation amount over different time scales. In this paper we derive non-parametric estimates of the cumulative distribution function (CDF) of precipitation amount for wet periods. The CDF estimates are obtained by integrating the kernel density estimator leading to semi-explicit CDF expressions for different kernel functions. We investigate an adaptive plug-in bandwidth (KCDE), using both synthetic data sets and reanalysis precipitation data from the Mediterranean island of Crete (Greece). We show that KCDE provides better estimates of the probability distribution than the standard empirical (staircase) estimate and kernel-based estimates that use the normal reference bandwidth. We also demonstrate that KCDE enables the simulation of non-parametric precipitation amount distributions by means of the inverse transform sampling method.

Keywords— precipitation, kernel estimation, simulation, non-Gaussian, reanalysis data, non-parametric estimate

*apavlidis@isc.tuc.gr
†vagou@isc.tuc.gr
‡dchristopoulos@ece.tuc.gr; Corresponding author
1 Introduction

Precipitation is a key component of the hydrologic cycle. It is particularly important for the health of ecosystems and the well-being of human societies, since it helps to recharge aquifers and surface water bodies thus contributing to economic activity and the preservation of biodiversity. On the other hand, modeling precipitation is not an easy task. Features such as the intensity and duration of precipitation vary significantly depending on geographic location, climate zone, season, and local topography. There are also strong interannual variations in the amount of precipitation over any given geographical area.

Since precipitation is an inherently stochastic process, its properties are modeled by means of probability distributions. Reflecting the highly variable features of precipitation, such probability distributions vary significantly depending on the location and the time scales of the measurements, as well as the modalities by means of which the data are obtained (e.g., rain gauges, satellite sensors, radar-based estimates, reanalysis methods).

To further complicate the situation, climate change has an impact on the precipitation patterns globally. It affects the duration and rate of precipitation events, the return periods, and the total amount of precipitation received by an area. This is a major cause of concern, since altered precipitation patterns can destabilize ecosystems, cause significant economic damage due to extreme events, and ruin local economies. The risk is greater in certain vulnerable areas of the globe which include the Mediterranean basin. Precipitation plays a crucial role in the life of the major Mediterranean islands (e.g., Sicily, Sardinia, Cyprus, Corsica, and Crete). Changes in the intensity and total amount of precipitation, in combination with increased demand for water due to tourism and agricultural activities, can lead to soil erosion, depletion of groundwater aquifers, extinction of flora and fauna, increased flooding, salt water intrusion into aquifers, and eventually desertification. Developing accurate, quantitative, data-based models for precipitation is crucial for predicting climate change impacts and proposing effective policies to mitigate them.

The intensity (rain rate) and total amount of precipitation over a specified aggregation time window are often modeled using parametric approaches. Time windows of one hour, one day during the wet period, an entire month, an entire season, or one year are used. Common parametric models include the exponential, mixed exponential, gamma, lognormal, generalized gamma, Weibull, generalized extreme value (GEV), as well as hybrid mixtures of exponential with a Pareto tail [1, 2].

The gamma distribution is a popular choice, regardless of the observation time window over which data were aggregated [2]. It has been used to model daily rain rates [3], as well as monthly and seasonal precipitation anomalies [4, 5]. It adequately models the variation of precipitation amounts in wet periods with a scale parameter proportional to the number of days and a shape parameter independent of the length of the observation window [6]. Zero precipitation values are taken into account in the gamma model using Type I censoring of the distribution on the left [4]. Left censoring implies that the number of values below a given threshold is considered known, but the exact values are not. The same approach can also be used for the other distributions discussed below. However, recent studies have highlighted that the tails of the gamma distribution are not sufficiently heavy for heavy rain events [7, 8]. This is due to the fact that the exponential part of the gamma tail dominates the power-law term, and thus in many cases the gamma tail behaves similarly to the exponential.

The lognormal distribution has been used to approximate rain-rate [9, 10, 11], cumulus cloud populations [12], hourly precipitation [13], storm height distribution over the tropical oceans [14], amount of precipitable water [15, 16], and the estimated average rain rate from satellite observations [17]. A recent study of the lognormal and gamma distributions concluded that both fit satisfactorily TRMM data (obtained from the Tropical Rainfall Measuring Mission research satellite which operated from 1997 to 2015) of daily average rain-rate [3].

The Generalized Extreme Value (GEV) distribution has been applied to modeling of precipitation amount and extremes over different time scales, such as maximum one-day rainfall [18, 19], k-day extreme precipitation (for k ranging between 1 and 30) [20], daily precipitation forecasts [21], annual maximum precipitation [22], monthly return levels and their annual cycle [23],
and seasonal extremes using ensembles of climate models \[24\]. Distribution models that allow more flexible tail behavior than the GEV are considered in \[25, 26, 27\].

Parametric models offer the advantage of closed-form expressions for the probability density function, and in most cases for all the main probability functions (i.e., cumulative distribution, survival, and hazard rate functions). In addition, they are motivated by theoretical arguments. For example, the Fisher–Tippett–Gnedenko theorem states that the maximum of a sample of independent, identically distributed random variables (after suitable affine transformation) converges in distribution to the GEV family (which includes the Gumbel, Fréchet, and reverse Weibull models) \[28, 29\]. A recent analysis based on stochastic modeling of the competing factors in the atmospheric moisture budget justifies the use of the gamma distribution for precipitation intensity \[30\].

In spite of their considerable advantages, parametric models have a number of shortcomings. One of them is their limited flexibility. For example, a recent study of daily precipitation values over Europe showed that the gamma distribution is not supported by rigorous statistical testing at more than 40% of the examined stations \[31\]. In certain cases, a parametric expression of the cumulative distribution function (CDF) cannot be easily deduced. Such an example is the amount of monthly precipitation in semi-arid Mediterranean areas \[32\].

Standard parametric probability models (e.g., exponential, gamma distribution) may also fail to capture both the low-value (left tail) and high-value (right tail) regimes of the data distribution. This has motivated the introduction of hybrid models, which combine more than one distribution types. A different approach considers flexible three-parameter distributions that allow independent control of both tails \[27\]. Another problem is that parametric models often assume stationarity, i.e., that the parameters of the distribution remain constant during the time of observation. However, in light of the accelerating effects of climate change on meteorological variables such as temperature and precipitation \[33\], the stationarity assumption is not easily justified \[34\]. Moreover, parametric models that have proved satisfactory in the past may not adequately capture precipitation patterns in future climate. This concern is fueled by the expected increase of extreme precipitation events \[34\], as well as climate model simulations predicting changes in the statistical patterns of daily precipitation extremes \[35\].

Non-parametric approaches that estimate the probability distribution from the data without reference to a specific mathematical form provide a useful alternative to parametric models. The simplest non-parametric estimator is the empirical CDF, which has the form of a non-decreasing step function (a staircase). However, the empirical CDF is discontinuous. This is unsatisfactory for continuously-valued variables such as the rain rate, especially for limited sample size. In addition, the staircase estimate is not suitable for the simulation of continuous variables.

Kernel density (KDE) estimation (known as the Parzen Rosenblatt window method) is a non-parametric method which constructs approximations of the probability density function (PDF) without step discontinuities \[36, 37\]. Kernel density estimators employ a bandwidth parameter \( h \) which determines the range of the kernel function and controls the smoothness of the estimated PDF \[38\]. Selection of an optimal KDE bandwidth is an important problem in statistics \[39, 40, 41\]. Plug-in bandwidths rely on \textit{a priori} assumptions about the probability distribution of the data; they are derived by minimizing the Asymptotic Mean Integrated Square Error between the KDE and the unknown PDF \[42, 40, 41, 38\]. For example, if the data follow the normal probability distribution \( \mathcal{N}(m, \sigma^2) \), the normal reference rule (rule of thumb) bandwidth \( h \) for the Gaussian kernel is \( h = 1.06\sigma N^{-1/5} \), where \( N \) is the data size \[43\].

Non-parametric approaches have been used in precipitation studies. For instance, \[44, 45\] reported on KDE and its application in the simulation of daily precipitation. The study \[46\] reports on non-parametric precipitation distribution modeling using the Gaussian kernel and numerical integration of the density. The normal reference rule bandwidth with the interquartile range as measure of scale \[43\] and the Sheather-Jones plug-in bandwidth \[42\] were tested and returned comparable results.

We propose a non-parametric, kernel-based estimator (KCDE) which targets the CDF instead of the PDF. We analytically evaluate the kernel integrals which form the KCDE building blocks for selected kernel functions with both compact and infinite support. Based on synthetic data sets,
we show that KCDE equipped with the plug-in BGK bandwidth derived by Botev, Grotowski, and Kroese [47] estimates the data probability distribution more accurately than the normal reference bandwidth which is typically used in KDE. In addition, KCDE allows the efficient simulation of precipitation amounts from the non-parametric CDF by means of the inverse transform sampling method. We test KCDE performance against the empirical CDFs for several kernel functions.

Our analysis employs synthetic precipitation data motivated by rain gauge measurements as well as ERA5 reanalysis products for the Mediterranean island of Crete (Greece). Crete is a major Mediterranean island (fifth in size overall and the largest island of Greece), where the combination of adverse climate change forecasts, and increasing tourist and agricultural activities poses serious threats to the sustainability of the island’s water resources [48, 49, 50].

The remainder of this paper is structured as follows: Section 2 describes the methods used and a short synopsis of the investigated probability distribution models. Section 3 presents the theoretical developments proposed in this work. The KCDE is derived and the integrals involved in kernel-based CDF estimates, \(\hat{F}_k(z)\), are evaluated for selected kernel functions in Sections 3.1-3.2 (with more details in A). The BGK plug-in bandwidth estimation by [47] is reviewed in Section 3.3 (algorithmic details are given in B). Finally, a simulation method for precipitation amounts based on KCDE is proposed in Section 3.4. Section 4 presents applications of KCDE (using the BGK bandwidth) to synthetic data (Section 4.1 and C) and to ERA5 reanalysis data (Section 4.2 and D). Discussion, conclusions and suggestions for further studies are given in Section 5.

2 Methodology

2.1 Stochastic modeling of precipitation amount

In the following, we assume that the precipitation rate is a continuous-time, stationary stochastic process \(R(t;\omega)\) defined over a probability space \((\Omega, F, P)\), where \(\omega \in \Omega\) is the state index in the sample space \(\Omega\), \(F\) is a \(\sigma\)-algebra of events, and \(P\) is the probability measure for these events [51, 52].

The data comprise precipitation amounts \((z_1, z_2, \ldots, z_N)\) observed at times \(t_1, t_2, \ldots, t_N\). The times \(t_n = n\delta t\) are multiples of a characteristic time step \(\delta t\), corresponding to one day, week, month, season, or year. The amounts \(z_n\) represent the cumulative amount of precipitation over the time interval \([t_{n-1}, t_n)\). We focus on wet time intervals, i.e., \(z_n > 0\) for all \(n\). The cumulative precipitation represents samples of the following stochastic integral (for definition see [51]):

\[
Z_N(t_n;\omega) = \int_{t_{n-1}}^{t_n} dt R(t;\omega), \quad n = 1, \ldots, N.
\]

In the following, for brevity we refer to \(Z_N(t_n;\omega)\) as \(Z(t;\omega)\). However, \(Z(t;\omega)\) implicitly depends on the averaging window \(\delta t\). Multiple samples from the same probability model will be distinguished by means of the index \(m = 1, \ldots, M\), i.e., \(Z^{(m)} = (z_1^{(m)}, z_2^{(m)}, \ldots, z_N^{(m)})^\top\), where \(\top\) denotes the transpose of a matrix or vector.

Different probability models will be distinguished by means of the integer subscript \(j\), i.e., \(\varphi_{N,j}^{(m)}\), \(j = 1, \ldots, J\) and \(J\) is the number of models tested. The marginal CDF of \(Z(t;\omega)\) is defined by \(F(z) = \text{Prob}(Z \leq z)\) and the marginal PDF by \(f(z) = \frac{dF(z)}{dz}\).

2.2 Probability distribution estimation

The respective estimates of the CDF and PDF from the data are denoted by \(\hat{F}_k(z)\), \(\hat{f}_k(z)\) if the estimates are based on KDE and \(\hat{F}_s(z)\), \(\hat{f}_s(z)\) if the estimates are obtained by means of the empirical staircase function.

A smoothing kernel is a real-valued, non-negative function \(K(z - z'; h) = K\left(\frac{z - z'}{h}\right)\), which respects the properties of symmetry, i.e., \(K(u) = K(-u)\) and normalization, i.e.,
We investigate four non-Gaussian probability distributions commonly associated with precipitation modeling [16]: the gamma (GAM), the Generalized Extreme Value (GEV), the lognormal (LGN), and the Weibull (WBL) models. The PDFs of these distributions are given in Eq. (1) below.

\[ f(z; \xi, \sigma) = \frac{z^{\xi-1} e^{-\frac{z}{\sigma}}}{{\sigma}^\xi \Gamma(\xi)}, \quad z > 0 \text{ and } \xi, \sigma > 0, \]  

\[ \text{GEV: } f(z; \mu, \sigma, \xi) = \frac{1}{\sigma} y(z)^{\xi+1} \exp\left(-y(z)\right), \quad z \in \mathbb{S}(\xi), \]  

where \( y(z) = \begin{cases} 1 + \xi \left(\frac{z - \mu}{\sigma}\right)^{-1/\xi} & \xi \neq 0, \\ \exp(-\frac{z - \mu}{\sigma}) & \xi = 0, \end{cases} \)  

\[ \text{lognormal: } f(z; \mu, \sigma) = \frac{1}{z\sigma \sqrt{2\pi}} \exp\left\{ -\frac{(\log z - \mu)^2}{2\sigma^2} \right\}, \quad z > 0, \sigma > 0, \]  

\[ \text{Weibull: } f(z; \sigma, \xi) = \begin{cases} \left(\frac{\xi}{\sigma}\right)^{\xi-1} e^{-(z/\sigma)^\xi}, & z \geq 0, \\ 0, & z < 0, \end{cases} \]  

In the above equations, \( \mu \in \mathbb{R} \) is the location parameter, \( \sigma > 0 \) is the scale parameter that controls the dispersion of the distribution, and \( \xi \) is a shape parameter. \( \Gamma(\cdot) \) is the gamma function. Note that for \( \xi = 1 \), the gamma distribution defaults to the exponential model.

In the case of the GEV distribution, \( \xi \) determines which type (I, II, or III) is represented. The Gumbel distribution (type I) is obtained for \( \xi = 0 \), the Fréchet distribution (type II) for \( \xi < 0 \), and the Reverse-Weibull distribution (type III) for \( \xi > 0 \) [53]. For \( \xi \in (-0.278, 1) \) the GEV distribution is positively skewed; it also has a finite mean given by \( m = \mu + \sigma \Gamma(\xi+1) \) for \( \xi \neq 0 \), and \( m = \mu + \sigma \gamma_E \) for \( \xi = 0 \), where \( \gamma_E \approx 0.57721 \) is the Euler-Mascheroni constant [21]. The support \( \mathbb{S}(\xi) \) of the GEV distribution is \( \mathbb{S}(\xi) = [\mu - \sigma/\xi, \infty) \) for \( \xi > 0 \), \( \mathbb{S}(\xi) = (-\infty, \infty) \) for \( \xi = 0 \), and \( \mathbb{S}(\xi) = (-\infty, \mu - \sigma/\xi) \) for \( \xi < 0 \).

The respective CDFs of the gamma, GEV, lognormal and weibull models are given below:

\[ F(z; \xi, \sigma) = \int_0^z f(u; \xi, \sigma) \, du = \frac{\gamma(\xi; \frac{z}{\sigma})}{\Gamma(\xi)}, \]  

\[ \text{GEV: } F(z; \mu, \sigma, \xi) = \exp\left(-y(z)\right), \quad z \in \mathbb{S}(\xi), \]  

\[ \text{lognormal: } F(z; \mu, \sigma) = \frac{1}{2} \left\{ 1 + \text{erf}\left(\frac{\log z - \mu}{\sigma \sqrt{2}}\right) \right\}, \quad \text{for } z > 0, \]  

\[ \text{Weibull: } F(z; \sigma, \xi) = 1 - e^{-(z/\sigma)^\xi}, \quad \text{for } z > 0. \]  

In Eq. (2), the function \( y(z) \) is defined in Eq. (1b), \( \gamma(\xi; \cdot) \) represents the lower incomplete gamma function, and \( \text{erf}(\cdot) \) is the error function [54]. Note that for the gamma and lognormal distributions \( F(0; \cdot, \cdot) = 0 \), while for the GEV finite values of the CDF are possible for negative values of \( z \). Since \( z < 0 \) is not acceptable for precipitation amounts, typically one sets \( F(z < 0) = 0 \) [21].
3 Theory and Calculations

In this section we derive a non-parametric, kernel-based method for CDF estimation from the data, and we propose a simulation method for precipitation amounts from the kernel-based CDF estimate. Since we focus on cumulative precipitation amounts over specific time windows, we only take account of non-zero precipitation values.

3.1 Kernel-based CDF estimation

Let \( z_i \) represent the \( i \)-th value of the ordered sample, which satisfies the following properties: for any given \( i \in \{1, \ldots, N\} \) there exists \( j \in \{1, \ldots, N\} \) such that \( z_i = z_j \) and \( z_1 \leq z_2 \leq \ldots \leq z_N \).

The standard PDF kernel density estimator (KDE) is given by

\[
\hat{f}_K(z) = \frac{1}{Nh} \sum_{i=1}^{N} K \left( \frac{z - z_i}{h} \right),
\]

where \( h \) is the kernel bandwidth of the kernel \( K(\cdot) \).

Non-parametric estimates (KCDE) of the CDF based on kernel functions \( K(u) \) can also be obtained. These estimates are given by the following weighted sum

\[
\hat{F}_K(z) = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{N} \tilde{K} \left( \frac{z - z_i}{h} \right).
\]

In Eq. (4), \( \tilde{K}(\cdot) \) is the CDF kernel step defined by means of the integral

\[
\tilde{K} \left( \frac{z - z_i}{h} \right) = \frac{1}{h} \int_{-\infty}^{z} K \left( \frac{z' - z_i}{h} \right) \, dz'.
\]

The CDF kernel steps are smoothed versions of the rectangular steps used in the empirical (staircase) CDF estimation. Equation (4) is obtained from Eq. (3) using the integral \( \hat{F}_K(z) = \int_{-\infty}^{z} \hat{f}_K(z') \, dz' \). Table 1 lists commonly used kernel functions and their respective CDF steps.

The CDF step of the Gaussian kernel is evaluated in Section 3.2, while the CDF steps of other commonly used kernels can be found in A.

A suitable kernel bandwidth \( h \) can be estimated by (i) minimizing specific cost functions such as the Root Mean Square Error (RMSE) or the Kullback–Leibler divergence (KLD) between \( \hat{F}_K(\cdot) \) and \( F(\cdot) \) using leave-one-out cross validation (LOOCV) or (ii) explicit (plug-in) bandwidth formulas based on parametric assumptions [55, 38]. The use of plug-in bandwidths produces similar or better PDF estimates for non-uniformly distributed data than bandwidths estimated with LOOCV [46, 56]. The optimal bandwidth in practice depends on the CDF shape and the data density (i.e., the spacing between measured values) [57]. Our preliminary investigations which compared \( \hat{F}_K(z) \) based on (i) the BGK bandwidth and (ii) the LOOCV bandwidth for synthetic data exhibited superior performance of the BGK bandwidth. Hence, we use the plug-in BGK bandwidth [47] (see Section 3.3).

In KDE, boundary values may require special treatment. For example, large bandwidths can lead to \( \hat{F}_K(z) > 0 \) for \( z < 0 \), which is not meaningful for precipitation amounts. Various solutions have been proposed for density estimation near the boundary [58, 59]. Note that it is not permissible to set the PDF equal to zero for \( z < 0 \), because it would violate the normalization of the PDF. Instead, we modify the CDF so that if \( \hat{F}_K(0) = p > 0 \), we set \( \hat{F}_K(z) = 0 \) for \( z < 0 \) and \( \hat{F}_K(0) = p \). This assignment implies zero probability for \( z < 0 \) and a discontinuous jump at \( z = 0 \), while it maintains normalization, i.e., \( \hat{F}_K(z \to \infty) = 1 \).
Table 1: Kernel functions $K(z)$ and respective CDF kernel steps, $\tilde{K}(u)$, as defined by means of Eq. (5). $h$ is the kernel bandwidth. $I(|z| \leq 1)$ is an indicator function used for compactly supported kernels: $I(|z| \leq 1) = 1$ when $|z| \leq 1$ and $I(|z| \leq 1) = 0$ otherwise. $\text{sgn}(u) = u/|u|$ is the sign function. The following kernel models are used: Ga: Gaussian, Ex: Exponential, Ep: Epanechnikov, Bp: Bitriangular, Tr: Triweight, Sp: Spherical, Un: Uniform. For compact support kernels (i.e., all but the exponential and Gaussian) the equations for $\tilde{K}(u)$ are valid for $-1 \leq u \leq 1$; for $u < -1$ it holds that $\tilde{K}(u) = 0$, while for $u > 1$ one gets $\tilde{K}(u) = 1$.

| Kernel | $K(z)$ | $\tilde{K}(u)$ (for compact kernels $|u| \leq 1$) |
|--------|--------|-----------------------------------------------|
| Ga     | $\exp(-z^2)$ | $\frac{1}{2} [1 + \text{erf}(u)]$ |
| Ex     | $\exp(|z|)$ | $\text{sgn}(u) \frac{1 - e^{-|u|}}{2} + \frac{1}{2}$ |
| Ep     | $\frac{3}{4}(1 - z^2) I(|z| \leq 1)$ | $\frac{3}{4} \left( u + \frac{2}{3} \right)$ |
| Bp     | $\frac{3}{2}(1 - |z|)^2 I(|z| \leq 1)$ | $\frac{3}{2} \left( \frac{u^3}{3} - u^2 \text{sgn}(u) + u + \frac{1}{3} \right)$ |
| Tr     | $(1 - z^2)^3 I(|z| \leq 1)$ | $\frac{35}{32} \left( u - u^3 + \frac{3u^5}{5} - \frac{u^7}{7} + \frac{16}{35} \right)$ |
| Sp     | $(1 - 1.5|z| + 0.5|z|^3) I(|z| \leq 1)$ | $\frac{4}{3} \left( \text{sgn}(u) \frac{u^2 - 6}{8} u^2 + u + \frac{13}{8} \right)$ |
| Un     | $\frac{z}{2} I(|z| \leq 1)$ | $\frac{1}{2} (u + 1)$ |

3.2 CDF step for Gaussian kernel function

The Gaussian (squared exponential) kernel, defined by $K(u) = \frac{1}{\sqrt{2\pi}} \exp(-u^2)$, is an infinitely extended function which has wide-ranging applications in data analysis, machine learning, regression and other fields [60, 61, 62].

Using the change of variable $u_i = (z - z(i))/h$ it follows that $dz = h du_i$. Subsequently, the CDF kernel step $\tilde{K}(u)$ is evaluated by means of the integral

$$\tilde{K}(u_i) = \int_{-\infty}^{u_i} dx K(x) = \frac{1}{2} \left[ \text{erf}(u_i) + 1 \right],$$

where $\text{erf}(\cdot)$ is the Gauss error function

$$\text{erf}(u_i) = \frac{2}{\sqrt{\pi}} \int_0^{u_i} e^{-x^2} dx.$$

The CDF kernel step obtained from Eq. (6) is illustrated in Fig. 1 for different $h$ values. As shown in these plots, the CDF kernel step tends to the discontinuous step function as $h \to 0$; then KCDE tends to the empirical staircase estimator. As $h$ increases, the bandwidth becomes smoother.

Results for the CDF kernel steps corresponding to other kernel functions are presented in Table 1; they are based on the calculations in A. For compactly supported kernels, the step $\tilde{K}(u)$ is zero for $u < -1$, it is given by the expressions listed in Table 1 for $|u| \leq 1$, and it is equal to one for $u > 1$. For kernels with infinite support (e.g., Gaussian, exponential), the kernel step approaches zero and one asymptotically as $u \to -\infty$ and $u \to \infty$ respectively.
3.3 BGK bandwidth estimation

The standard bandwidth selection in KDE aims to minimize the Asymptotic Mean Integrated Square Error (AMISE) [38, 43, 57]. Assume a Gaussian kernel $K(\cdot)$ and a PDF $f(z)$ which is at least twice differentiable, i.e., $f'(z)$ and $f''(z)$ are finite numbers for all $z$. Botev, Grotowski and Kroese [47] (henceforward BGK), have shown that the bandwidth which minimizes AMISE is given by

$$h = \left( \frac{1}{2^{2/5} \pi N G[f']} \right)^{1/3},$$

where $G[f'] = \int_{-\infty}^{\infty} dz [f''(z)]^2$ is a functional of $f(z)$.

Equation (7) in theory provides the BGK plug-in bandwidth. However, in practice it requires knowledge of the PDF $f(z)$, which is in general unknown a priori. BGK approximates $f(z)$ by means of $\hat{f}_a(z)$, which is the KDE based on an auxiliary bandwidth $a$. The latter is calculated by means of an iterative algorithm after several repetitions [47]. The details of the algorithm are described in B. Note that in BGK different bandwidths are proposed for PDF versus CDF estimation. Our approach explicitly integrates the PDF kernel density estimates; so, it uses the PDF bandwidth formula.

For data that deviate from the normal distribution, the normal reference rule can lead to significant PDF oversmoothing [47, 38, 63, 42]. Another popular method of bandwidth estimation involves using LOOCV to minimise KLD or RMSE between $\hat{F}_K(\cdot)$ and $F(\cdot)$. LOOCV bandwidth estimates require time consuming numerical optimization and often yield small bandwidths that tend to produce peakedness (high kurtosis) in the density [64, 46].

The BGK algorithm has two significant advantages over other plug-in methods: It does not require normal data, and it is computed efficiently without the need for numerical optimization [47]. Even though the BGK bandwidth is optimized for the Gaussian kernel, our tests with synthetic data in Section 4.1 show that it also performs well with compact-support kernels.

3.4 KCDE-ITS simulation algorithm for precipitation amount

Time series of precipitation amounts that respect KCDE-derived distributions can be simulated using the inverse transform sampling (ITS) method [52]. Given a time series of precipitation amounts...
(z₁, z₂, ..., zₙ), the goal is to generate an ensemble of time series, \( \left( z₁^{(m)}, z₂^{(m)}, ..., zₙ^{(m)} \right) \), where \( m = 1, \ldots, M \) is the state index, that share the same probability distribution as the sample. Henceforth we drop the index \( (m) \) to abbreviate notation.

The ITS method is based on the law of conservation of probability under nonlinear, monotonic transformations: If \( Z(\omega) \) is a random variable with CDF \( \hat{F}_Z(z) \) and \( U(\omega) \) is a uniformly distributed random variable, then

\[
\hat{F}_Z(z) = F_U(u) \Rightarrow z = \hat{F}_Z^{-1}(u),
\]

where \( F_U(\cdot) \) is the CDF of the uniform distribution [51, 52]. The inverse CDF \( \hat{F}_Z^{-1}(\cdot) \) can be calculated either by means of numerical optimization or a lookup table; we use the latter approach. For compactly supported kernel functions, ITS simulation involves the following steps:

1. The KCDE-based CDF of precipitation amount \( \hat{F}_Z(z) \) is derived from the sample by applying Eq. (4).
2. A lookup table is generated which comprises a set of \( L = 10,000 \) discretization points, i.e., \( \{(z_l, u_l)\}_{l=1}^{L} \) pairs.
3. The set \( \{z_l\}_{l=1}^{L} \) is obtained by uniformly distributing \( z_l \in [z_{\min}^{'}, z_{\max}^{'}, \ldots, z_{\max}'] \), where \( z_{\min}^{'}, z_{\max}^{'} = \max(\epsilon, z_{\min} + h), z_{\min}, z_{\max} \) are respectively the minimum and maximum values of the available sample, and \( h \) is the BGK bandwidth.
4. The set \( \{u_l\}_{l=1}^{L} \) is generated by setting \( u_l = \hat{F}_Z(z_l) \), for all \( l = 1, \ldots, L \) according to Eq. (8).
5. A set of uniform random numbers \( \{u_n\}_{n=1}^{N'} : u_n \sim U(0, 1) \) are generated.
6. For each \( u_n, n = 1, \ldots, N' \) the nearest neighbor \( u_{l|n} \) in the lookup table is found, and the simulated value \( z_n \) is set equal to \( z_{l|n} \), i.e., which is the pair of \( u_{l|n} \) in the lookup table.

4 Results

This section presents estimation of precipitation amount CDFs from synthetic and ERA5 reanalysis data using the proposed KCDE method. It also uses the KCDE-based simulation to generate and discuss probable scenarios of precipitation amounts.

4.1 KCDE application to synthetic data

We generate data from parametric probability distributions with statistical properties motivated by observations of monthly precipitation amounts on the Mediterranean island of Crete (Greece) [32, 49]. One hundred time series of independent values are generated from the gamma, GEV, Weibull and lognormal distributions discussed in Section 2.3. Samples of five different sizes \( (N=50, 100, 200, 500 \) and 1000 points) are generated from each distribution.

The studied probability distributions and their parameters are: \( \text{GAM}(\xi = 1, \sigma = 30), \text{GAM}(\xi = 0.35, \sigma = 40), \text{LGN}(\mu = 2, \sigma = 1.1), \text{GEV}(\xi = 0.25, \sigma = 8, \mu = 15), \text{GEV}(\xi = 0, \sigma = 18, \mu = 45), \text{GEV}(\xi = -0.25, \sigma = 30, \mu = 100), \text{and WBL}(\sigma = 15, \xi = 0.7). \) The respective theoretical CDFs and PDFs are shown in Fig. 2.

4.1.1 Comparisons of CDF estimates

The simulated precipitation amounts comprise the vectors \( Z_N^{(m)} \) of length \( N \in \{50, 100, 200, 500, 1000\} \). \( m = 1, \ldots, M \) \( (M = 100) \) denotes the sample index, and \( j = 1, \ldots, 7 \) marks the probability distribution model.

The CDF is estimated using the KCDE method with the BGK bandwidth (see Section 2). KCDE is performed with several compactly supported kernels (triweight, uniform, spherical, bitriangular, Epanechnikov) and the infinite-support Gaussian kernel. For comparison purposes, in
Figure 2: CDF (left) and PDF (right) plots for the six investigated probability models [see Eq. (2)]. GAM1: GAM(ξ = 1, σ = 30), GAM2: GAM(ξ = 0.35, σ = 40), LGN: LGN(m = 2, σ = 1.1), GEV1: GEV(ξ = 0.25, σ = 8, µ = 15), GEV2: GEV(ξ = 0, σ = 18, µ = 45), GEV3: GEV(ξ = −0.25, σ = 30, µ = 100), WBL: WBL(σ = 15, ξ = 0.7). The horizontal axis represents monthly precipitation amount (mm). The parameters ξ, σ, µ, λ, κ for each model are defined with reference to Eq. (1).

Figure 3: Cloud of 100 empirical (staircase) CDFs for four probability distribution models. GAM1: GAM(ξ = 1, σ = 30), GAM2: GAM(ξ = 0.35, σ = 40), GEV1: GEV(ξ = 0.25, σ = 8, µ = 15), LGN: LGN(m = 2, σ = 1.1). The CDF estimates are based on samples of length N = 75. The theoretical CDF curves are shown by the continuous line (red online).

In addition to the KCDE, \( \hat{F}_K(z) \), we calculate the staircase CDF estimate, \( \hat{F}_s(z) \), and the theoretical CDF, \( F(z) \), at the test points (times) \( t_{k,N,j,m} \), where \( k = 1, \ldots, N_t \) (\( N_t = 500 \)). The times \( t_{k,N,j,m} \) are uniformly distributed between the minimum and maximum values for each sample.
vector $Z_{N,j}^{(m)}$. In the following, for ease of notation we drop the indices $\{N, j, m\}$ whenever possible.

The mean square error (MSE$_k$) between $F_k(\cdot)$ and the theoretical CDF $F(\cdot)$ is calculated for all the studied kernels and all the samples $Z_{N,j}^{(m)}$ based on the validation values at the test points. Similarly, the mean square error (MSE$_s$) of the staircase function $F_s(\cdot)$ with respect to $F(\cdot)$ is also calculated.

### 4.1.2 Assessing KCDE performance

The relative performance of KCDE and the staircase estimate is measured by means of the error ratio $RE_k = \frac{MSE_k}{MSE_s}$. If $RE_k < 1$, the kernel-based CDF $F_k(\cdot)$ is a better approximation of the theoretical CDF $\hat{F}(z)$ than the staircase function. The comparison is illustrated in the box plots of Fig. 4.

As evidenced in these plots, in most cases the KCDEs, $F_k(z)$, perform better than the staircase estimates $F_s(z)$. Hence, $F_k(z)$, especially for compact kernels, better approximates the CDF of non-Gaussian, skewed distributions than the staircase CDF $F_s(z)$. The exception is GAM($\xi = 0.35$, $\sigma = 40$), the PDF $f(z)$ of which exhibits a singularity at zero (see Fig. 2). This violates the BGK smoothness conditions which require the existence of $f'(z)$ and $f''(z)$. Based on Fig. 4, no single kernel is universally the top performer. The compactly supported kernels tend to outperform the Gaussian kernel. However, in certain cases the Gaussian kernel performs better than all the compact kernels, particularly for the GEV distribution.

The bitriangular and uniform kernels performed best among the compact kernels, with Bitriangular returning the smallest RE$_k$. The spherical kernel, while performing well compared to the step function (see Fig. 4), outperforms the other kernels in less than 1% of the experiments. However, the deviation of the spherical from other compact kernels in terms of MSE is within 2% (based on the average MSE over the 35 different sampling scenarios). In most cases in which the spherical kernel performs well, a different kernel performs slightly better (often the Bitriangular kernel).

The same analysis was performed using the plug-in bandwidth $r^{(m)}_{N,j}$ based on the normal reference rule:

$$r^{(m)}_{N,j} = 1.06 \tilde{\sigma}_j^{(m)} N^{-1/5}, \quad m = 1, \ldots, M, \quad j = 1, \ldots, 6, \quad (9)$$

where $\tilde{\sigma}_j^{(m)}$ is the standard deviation of the sample $Z_{N,j}^{(m)}$ [43]. The results (Fig. C1 in C) show that $F_k$ using the normal reference bandwidth performs similarly to the staircase estimate $F_s$ for the compact kernels. The BGK bandwidth $h_{N,j}^{(m)}$ outperforms the normal reference rule according to the error ratio $RE_k$. The results support the conclusions reached in [47].

The above analysis shows that KCDE equipped with the BGK bandwidth estimates the CDF of synthetic data more reliably than KCDE with the normal reference bandwidth and the empirical staircase estimators. The relative performance of different kernel functions on the estimate of the CDF $\hat{F}_k(z)$ should be further investigated.

### 4.1.3 KCDE-ITS simulations

One simulated state was generated for each probability model in Section 2.3, based on a single sample of length $N = 250$. The simulated time series involve $N' = 250$ points. The CDF $F_k(\cdot)$ was estimated using Eq. (4) with the spherical kernel (which has similar performance as the Bitriangular kernel; see Section 4.1.2).

Figure 5 shows the quantile-quantile (q-q) plots between the simulated series and the samples. The q-q pairs cluster around the diagonal line, indicating good agreement between the probability distributions of the sample and simulated state, except for a few points in the right tail of the distributions. This behavior signifies underestimation of the maxima by the ITS simulated time series. Given the skewness of the probability models, the bias stems from the fact that obtaining a simulated sample which contains a value close to the sample maximum requires generating a
Figure 4: Boxplots of $\text{RE}_{k-s}$ (MSE of KCDE $\hat{F}_K$ divided by the MSE of the staircase estimate $\hat{F}_s$) for all tested kernels. $N$ is the sample size. The abbreviations of the probability models (GAM1, GAM2, LGN, GEV1, GEV2, GEV3, WBL) are defined in the main text.

uniform random number close to one. This is more likely to happen for longer simulated series. Note that values higher than the sample maximum can also be obtained by ITS simulation and are more likely for high values of $N'$ compared to $N$ (this case is not shown herein). For compactly supported kernels such values do not exceed the limit $z_{\text{max}} + h$.

4.2 KCDE application to ERA5 reanalysis data

This section employs ERA5 reanalysis precipitation data (mm) downloaded from the Copernicus Climate Change Service [65]. The data set includes 23,300,610 values of hourly precipitation amounts for a period of 41 years (from 01-Jan-1979 06:00:00 to 31-Dec-2019 23:00:00) at the nodes of a $5 \times 13$ spatial grid (see Fig. 6) on and around the island of Crete (Greece). The average spatial resolution is $\approx 0.28$ degrees (grid cell size $\approx 31$ km), and 359,394 hourly precipitation
Figure 5: Quantile-quantile (q-q) plots between synthetic sample data and ITS simulated sequences of the same length. The kernel-based CDF estimate \( \hat{F}_k \) was constructed using the spherical kernel. Each synthetic sample includes 250 values drawn from the parametric probability distributions presented in Section 2.3.

Our analysis focuses on the wet period, i.e., from October to March [66]. Daily, weekly, monthly and annual precipitation sets were generated by aggregating the hourly values at each location over the respective time window. We kept only non-zero precipitation values for our analysis. Note that we also tested replacing zeros with small values as done in some studies [4, 67, 68]. Such replacement does not significantly affect the shape of the distributions at any time scale. The optimal model for the daily data sets (based on selection criteria of Table D2) in certain cases changes from Weibull (if zeros are excluded) to gamma (if zeros are replaced with small values are available at every node.
values), but in such cases the two models look quite similar.

Figure 6: Geomorphological map of Crete showing the 65 ERA5 grid locations (blue markers) on and around the island of Crete (Greece) used in this study [69]. The node on the fourth row and seventh column (red marker online) is the test location near the Messara valley.

4.2.1 CDF estimation for the ERA5 data

The KCDE analysis of precipitation data was performed for all 65 grid nodes. For brevity we mostly discuss results from a single representative node (see Fig. 6) which is located near the major agricultural area of Crete, i.e., the valley of Messara [70]. The coordinates (LAT, LON) of the test node in the World Geodetic System (WGS 84) are $35^\circ 0'0.00''$N and $25^\circ 0'0.00''$E. The probability distributions at 5 additional nodes, geographically dispersed over the island, are considered in the simulation study in Section 3.4.

Table 2 presents summary statistics of wet-period precipitation amounts for the four time scales along with the respective best-fit parametric models based on BIC. The optimal parametric models are all non-Gaussian distributions. More details are shown in Table D1 which reports the optimal parametric model based on Akaike’s Information Criterion (AIC), the Bayesian Information Criterion (BIC), and the negative log likelihood (NLL). The three criteria agree on the optimal distribution models for all time scales considered. For daily amounts the optimal fit is obtained by the Weibull, followed by the gamma, lognormal, GEV and the normal distribution. For weekly precipitation, the ranking of the probability distributions (from best to worst) is: gamma, Weibull, lognormal, GEV and normal. For the monthly data, the following ranking is obtained: Weibull, gamma, GEV, normal, and lognormal. Finally, for the annual data the best model is the Weibull distribution.

For completeness, Table D2 reports the frequency (total number of ERA5 nodes) with which a parametric model is selected as the optimal probability distribution for each time scale. As in the case of the test location, all three criteria agree on the optimal model except for the annual time scale. On the daily scale, the Weibull model is selected at 56 nodes, followed by the gamma model at 9 nodes. For the weekly scale the gamma distribution is the optimal model at all 65 nodes. For the monthly scale, the Weibull distribution is the optimal model at most nodes according to all three criteria (the number of nodes differs depending on the criterion). Finally, for the annual precipitation AIC and BIC select the gamma model at 28 nodes, the normal at 18 nodes, the lognormal at 14 nodes and the Weibull at 5 nodes. For the annual data, the Weibull distribution
Table 2: Summary statistics for the daily, weekly, monthly and annual precipitation amounts for the wet period (October to March) (from ERA5 reanalysis data) for the test location on the island of Crete. The coordinates (LAT, LON) of the node are 35°0′0.00″N and 25°0′0.00″E in the World Geodetic System (WGS 84). N: Number of records analyzed, N\textsubscript{z}: number of zero records removed, \bar{z}: mean value, \textbar{z}_{0.50}: median, \textbar{z}_{\text{min}}, \text{minimum}, \text{\textbar{z}}_{\text{max}}, \text{maximum}, σ\textsubscript{z}: standard deviation, cov: coefficient of variation, s\textsubscript{z}: skewness, k\textsubscript{z}: kurtosis. “Model” is the best-fit distribution based on the Bayesian Information Criterion (BIC).

| Scale | N   | N\textsubscript{z} | \bar{z} | \textbar{z}_{0.50} | \textbar{z}_{\text{min}} | \text{\textbar{z}}_{\text{max}} | σ\textsubscript{z} | cov | s\textsubscript{z} | k\textsubscript{z} | Model       |
|-------|-----|---------------------|---------|---------------------|--------------------------|-----------------------------|----------------|-----|----------------|----------------|-------------|
| Daily | 5,664 | 1,808               | 2.0884  | 4.7684 × 10^{-4}   | 56.1037                 | 4.4048                      | 2.1091         | 4.3233 | 28.6750       | Weibull       |
| Weekly | 1,055 | 13                  | 11.2781 | 6.3763              | 84.3720                 | 12.6180                     | 1.1188         | 1.5697 | 5.4716         | gamma         |
| Monthly | 246   | 0                   | 48.0850 | 44.3109             | 142.1008                | 29.4220                     | 0.6119         | 0.6378 | 3.0325         | Weibull       |
| Annual | 41    | 0                   | 288.5103| 303.1404            | 415.0781                | 66.7700                     | 0.2314         | -0.1206 | 2.5123         | Weibull       |

provides the best fit at the test location (and its four nearest nodes in the south), while the gamma distribution is selected at the majority of the ERA5 sites.

4.2.2 Estimates of precipitation amount at different time scales

From the analysis above it follows that the optimal parametric model depends on both the time scale considered and the geographic location. This variability motivates the use of non-parametric estimates of the underlying probability distribution. This section presents KCDEs of precipitation amount at the test location over the daily, weekly, monthly and annual time windows.

The KCDEs are calculated with the Bitriangular kernel which performed best (among the studied compact kernels) on synthetic data, as discussed in Section 4.1. The sample size for each time window is shown in Table 2. Figure 7 compares the empirical (staircase), and KCDE estimates with the best-fit parametric models for each time scale. As is evident in these plots, the continuous KCDE curves are closer to the empirical estimates than the parametric models. The behavior reflects the fact that parametric models are not flexible enough to capture the natural stochasticity of precipitation. The differences between the three curves are smallest in the case of the annual data, which are closer to the normal distribution (see Table D2). The respective BGK bandwidths for the Bitriangular kernel are h\textsubscript{d} = 0.0017, h\textsubscript{w} = 0.027, h\textsubscript{m} = 14.898, and h\textsubscript{a} = 40.824 (all in mm) for the four different time scales. These results show that the BGK bandwidth adapts to the shape and scale of the underlying distribution. The inset plots in Fig. 7 demonstrate that KCDE provides estimates closer to the empirical CDF than the optimal parametric models. Note that the BGK bandwidth for the monthly wet-season data is h\textsubscript{m} = 14.898 mm while the respective bandwidth for the monthly entire-season data set is h\textsubscript{m} = 0.1413 mm (the analysis for the entire season is not reported herein). This difference is due to the presence of a large number of low values in the full data set and illustrates the ability of the BGK bandwidth to adapt to the data distribution.

4.2.3 KCDE-ITS simulation study based on ERA5 reanalysis data

Wet-period ERA5 daily precipitation data from 1979 to 2019 at six geographically dispersed nodes are used to demonstrate the application of the ITS simulation method. The selected locations are listed in Table 3.

The time series Z\textsubscript{N,s,t}, where t = 1, ..., 41, and s = 1, ..., 6 denotes the precipitation amount for the wet period of a specific year (indexed by t = year − 1978) at a specific node (denoted by s). For example, the time series Z\textsubscript{182,4,1} comprises N = 182 values corresponding to the wet-period days at location s = 4 for the year 1979. Aggregate time series, Z\textsubscript{N,s}, comprise the wet-period data for the entire 41-year window at each location.
Figure 7: Empirical–staircase (step function, blue online) and KCDE with Bitriangular kernel (smooth line, red online) CDF estimates for the daily (upper left), weekly (upper right), monthly (bottom left) and annual (bottom right) precipitation amount reanalysis data for the wet period (October to March). The dashed line (green online) corresponds to CDFs of the optimal parametric models based on the Bayesian Information Criterion (BIC). Based on BIC, the optimal models are Weibull (daily), gamma (weekly), Weibull (monthly), and Weibull (annual) scales respectively.

Table 3: List of the selected ERA5 nodes. The node coordinates (LAT, LON) are shown in the World Geodetic System (WGS 84).

| Index s | Node | Area Name                  | (LAT, LON)                |
|---------|------|-----------------------------|---------------------------|
| s = 1   | N12  | Chania                      | (35°30'0.00" N, 24°00'0.00" E) |
| s = 2   | N13  | Lefka Ori (White Mountains) | (35°15'0.00" N, 24°00'0.00" E) |
| s = 3   | N18  | Askifou plateau            | (35°15'0.00" N, 24°15'0.00" E) |
| s = 4   | N28  | Psiloritis mountain        | (35°15'0.00" N, 24°45'0.00" E) |
| s = 5   | N34  | Vagionia                   | (35°00'0.00" N, 24°00'0.00" E) |
| s = 6   | N49  | Ierapetra                  | (35°00'0.00" N, 25°45'0.00" E) |

The CDF estimates $\hat{F}_{K,s}(z)$ for $Z_{N,s,t}$ and $\tilde{F}_{K,s,t}(z)$ for $Z_{N,s,t}$, for $s = 1, \ldots, 6$ and $t = 1, \ldots, 41$ were calculated using the Bitriangular kernel with the BGK bandwidth (which are henceforth used). The results are shown in Fig. 8. All CDFs have similar shapes which are quite different from the S-shaped normal CDF. The CDFs exhibit significant probability mass for small
values and extended right tails. The maximum amounts differ slightly between locations.

Figure 8: CDF $\hat{F}_{K,s,t}(z)$ clouds for precipitation amount of individual years (blue lines) and $\hat{F}_{K,s}(z)$ for the aggregate precipitation (red lines) at six ERA5 nodes. The Bitriangular kernel with BGK bandwidth was used for CDF estimation.

To test the ITS simulation method we used the following study design. For each of the years 2015–2019 ($t = 37, \ldots, 41$), the time series $Z_{N,s,t}$ for the years $t = 1, \ldots, T - 1$ were used as the training set. The precipitation time series $Z_{N,s,T}$ for the year $t = T$ were considered as the validation set. For each year, an aggregate time series $Z_{N,s}$ was constructed based on the data of the respective training set. Based on the latter, 1000 times series for the year $T$ were simulated using ITS. The simulated time series are denoted by $Z_{N,s,t}^{(m,T)}$, where $t = 1, \ldots, T - 1$, $m = 1, \ldots, 1000$ is the state index, $s = 1, \ldots, 6$ and $T = 37, \ldots, 41$ is the index of the validation year.
4.2.4 Analysis of simulation results

Figures 9-10 present boxplots of total precipitation during the wet period of the validation year (on the left column) as well as the maximum daily precipitation (on the right column). These boxplots are based on the 1000 simulated states for each node $s$ and validation year $T$. The respective wet-period total and maximum daily precipitation validation values for each year $T$ are also shown (using longer horizontal line segments).

![Boxplots of wet-period total and maximum daily precipitation](image)

(a) Year 2015
(b) Year 2016
(c) Year 2017

Figure 9: Boxplots of wet-period total (left column) and maximum daily (right column) precipitation based on 1000 ITS simulations at six ERA5 nodes: $s_1$: Chania, $s_2$: Lefka Ori, $s_3$: Askifou, $s_4$: Psiloritis, $s_5$: Vagionia, $s_6$: Ierapetra. Dotted horizontal lines extending outside the boxes represent the total (black, left column) and maximum daily (red, right column) ERA5 precipitation values for the validation years 2015-2017.

In most cases, the validation values are within the distributions generated by KCDE-ITS
Figure 10: Boxplots of wet-period total (left column) and maximum daily (right column) precipitation based on 1000 ITS simulations at six ERA5 nodes: \( s_1 \): Chania, \( s_2 \): Lefka Ori, \( s_3 \): Askifou, \( s_4 \): Psiloritis, \( s_5 \): Vagionia, \( s_6 \): Ierapetra. Dotted horizontal lines extending outside the boxes represent the total (black, left column) and maximum daily (red, right column) ERA5 precipitation values for the validation years 2018-2019.

Simulation. For the wet-season total precipitation, the simulations generated reliable predictions at all locations with the exception of the year 2019 (\( T = 41 \)). In 2019 the data at the first three stations, which are located on the Western side of the Crete, exceed the range generated by KCDE-ITS. The year 2019 was marked by extremely heavy precipitation on Crete [71], and the western part of the island typically receives most of the precipitation. Hence, it is not surprising that the simulation, which was trained on previous years of less intense precipitation, did not adequately capture the behavior for 2019.

Regarding estimates of the expected daily maximum precipitation, the 95% percentile of the ITS simulations seems adequate. For the six studied locations and the five validation years, the validation ERA5 maximum value exceeded the 95% interval only in Chania (\( s = 1 \)) during 2019 (\( T = 41 \)).

Note that precipitation estimates at different locations are spatially correlated. Thus, 2016 was a rather dry year while 2019 a particularly wet year across the island. Furthermore, the failure to adequately capture the rainfall amounts during 2019 at some of the test locations demonstrates a limitation of non-parametric methods—the extrapolation outside the range of the dataset can be poor. According to [72], in order to reduce extrapolation errors samples longer than 50 years should be used.
5 Discussion and Conclusions

We propose the KCDE approach for estimating the CDF of skewed probability distributions. Such distributions typically describe the amount of precipitation received by a geographical area over a given interval. KCDE uses a non-parametric estimate of the CDF which is obtained by means of explicit integration of underlying kernel functions. We showed that KCDE equipped with the BGK plug-in bandwidth [47] estimates skewed probability distributions more accurately than the empirical staircase estimator or KDE with the normal reference rule (Section 4.1 and C). These results suggest that the BGK bandwidth, which is based on rigorous statistical theory, can efficiently adapt to the shape of different data probability distributions. To our knowledge this is the first application of the BGK bandwidth in the non-parametric analysis of precipitation. As shown in Section 4.1.2 the flexible BGK bandwidth in combination with compactly supported kernels in several cases out-performs the infinitely extended Gaussian kernel in the CDF estimation of skewed probability distributions.

A different non-parametric estimator of the distribution of precipitation amount was used in [46]. This work employed the Gaussian kernel with simpler plug-in bandwidths. The latter in most cases do not perform as well as the BGK bandwidth according to [47] and our analysis in Section 4.1. The non-parametric approach in [46] also uses CDF estimates, which are obtained by integrating numerically the kernel density estimates. In our approach, we explicitly integrate the kernel functions and provide analytical expressions for the CDF steps for different kernels, both compactly supported and infinitely extended.

Our analysis and validation of KCDE employed synthetic data from parametric probability distributions and ERA5 reanalysis data. We did not include observation data in this study because the available record for Crete is very sparse, with a large fraction of missing values [49]. In the reanalysis data sets we focused on the wet season for Crete. Hence, we did not attempt to model the occurrence of precipitation. This can be achieved with Markov chain methods [73], or by means of censored latent Gaussian processes [74, 75]. However, it is not necessary if the goal is to model the precipitation amount over a certain period.

Taking advantage of the explicit equations for the CDF kernel steps, we formulated an ITS simulation algorithm based on KCDE which is suitable for non-Gaussian distributions. KCDE-ITS is a flexible and easy to use simulation method which can adapt to different distribution shapes. In its current form, KCDE-ITS does not account for correlations between precipitation amounts at different times. Precipitation data, however, exhibit short-range correlations (e.g., over a couple of days for the daily amounts) as evidenced in the variogram function (not shown herein). Such dependence can be introduced in the simulations a posteriori: A Monte Carlo approach can be used in which simulated values are shuffled aiming to optimize a correlation cost functional. This procedure is computationally expensive and also unnecessary for estimating total precipitation amounts over a given period of time. For methods that introduce space-time correlations in precipitation simulations we refer readers to [76]. Regarding the use of KCDE-ITS simulations to design protective measures against extreme precipitation, our investigations show the 95% percentile of maximum daily precipitation predicted by KCDE-ITS based on 1000 simulated states provides an adequate estimate for most years.

It is generally accepted that in non-parametric estimation no single kernel function or bandwidth estimate is optimal for all purposes. We have found that the BGK bandwidth has advantages for the probability models studied. However, this finding cannot be generalized to all possible models of distribution functions without further studies to determine optimality conditions for the BGK bandwidth. Finally, to successfully apply KCDE for simulation purposes, training data over a long observation window are needed in order to capture rare events. This is exemplified by the unsatisfactory performance of the KCDE-ITS simulation for the extreme-precipitation year 2019 as discussed in Section 4.2.4. The issue of adequate sample size becomes even more pertinent in light of climate change which is expected to significantly influence precipitation patterns in the Mediterranean basin.

The proposed KCDE method for non-parametric estimation of probability distributions and the associated KCDE-ITS simulation method can be applied to precipitation amounts in different
geographical areas and climates. The reanalysis data used in this study focused on precipitation modeling for the Mediterranean island of Crete. However, the synthetic data were based on probability distributions that are commonly used in studies of precipitation. The KCDE method can also be applied to other non-Gaussian hydrological variables (e.g., annual mean river flows, flood frequency, and droughts). An open goal (common to all non-parametric methods) is the enhancement of KCDE with improved extrapolation capability outside the range of the observation dataset.

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A Integrals for CDF kernel steps

The change of variables \((z - z[i])/h \to u_i\) implies \(dz = h \, du_i\). Then, the CDF kernel step defined by Eq. (5) is expressed as

\[
\tilde{K}(u_i) = \int_{-\infty}^{u_i} du' K(u').
\]  

(10)

Compact kernels are of the general form \(K(u) = g(u) I(|u| \leq 1)\), where \(I(|u| \leq 1)\) is the indicator function: \(I(|u| \leq 1) = 1\) if \(|u| \leq 1\) and \(I(|u| \leq 1) = 0\) otherwise. For compact kernels, Eq. (10) is expressed as follows

\[
\tilde{K}(u_i) = I(u_i > -1) \int_{-1}^{u_i} du' g(u'),
\]  

(11)

where \(\tilde{u}_i = \min(1, u_i)\). The above implies that the CDF kernel step vanishes if \(u_i < -1\) for compact kernels. This reflects the fact that the sample value \(z[i]\) does not contribute to the CDF at \(z\), since the latter is more than one bandwidth less than \(z[i]\). Below we explicitly calculate the integrals (11) for the Epanechnikov and Bitriangular kernels. The CDF steps for other kernels are similarly calculated (see also Table 1).

A.1 Epanechnikov kernel

The Epanechnikov kernel is defined by means of the equation

\[
K(u) = \frac{3}{4} (1 - u^2) I(|u| \leq 1).
\]  

(12)

Thus, the CDF kernel step for \(u_i > -1\) is given by

\[
\tilde{K}(u_i) = \frac{3}{4} \int_{-1}^{\tilde{u}_i} (1 - u^2) du = \frac{3}{4} \left[ u - \frac{u^3}{3} \right]_{-1}^{\tilde{u}_i} = \frac{3}{4} \left( \tilde{u}_i - \frac{1}{3} \tilde{u}_i^3 + \frac{2}{3} \right).
\]  

(13)

A.2 Bitriangular kernel

The Bitriangular kernel is defined by means of the equation,

\[
K(u) = \frac{3}{2} (1 - |u|^2) I(|u| \leq 1)(u).
\]  

(14)

Thus, the CDF kernel step for \(u_i > -1\) is given by

\[
\tilde{K}(u_i) = \frac{3}{2} \int_{-1}^{\tilde{u}_i} (1 - |u|^2) du = \frac{3}{2} \left( u^3 - u_i |u_i| + u_i \right)_{-1}^{\tilde{u}_i} = \frac{3}{2} \left[ \tilde{u}_i^3 - \tilde{u}_i^2 \text{sgn}(u_i) + \tilde{u}_i + \frac{1}{3} \right].
\]  

(15)
This appendix reviews the details of BGK bandwidth estimation. The estimate employs an auxiliary bandwidth \( \hat{a}_1 \), which is obtained from a sequence of bandwidths \( a_{j,n} \), \( j = l, l-1, \ldots, 1 \). The index \( n = 0, 1, \ldots, n^* \) counts the number of repetitions until convergence is achieved, while \( l \) is a pre-selected recursion depth (usually \( l = 7 \)).

The sequence is initialized by arbitrarily setting \( a_{l+1,0} \) equal to the machine precision; the \( a_{j,n} \) for given \( n \) are generated by means of the following recursive expression

\[
a_{j,n}^2 = \frac{1 + 2^{-(j+1/2)} \prod_{k=1}^{j} (2k-1)}{3} \left( \frac{N}{\pi^{1/2} \hat{f}^{(j+1)}(z)} \right)^{2/(2j+3)}, \quad j = l, l-1, \ldots, 1.
\]

In the above, \( \hat{f}^{(j+1)}(\cdot) \) is defined in Eq. (7), and \( \hat{f}^{(j+1)}(\cdot) \) is the kernel-based PDF estimate with bandwidth \( a_{j+1,n} \); the latter requires recursive calculation of \( \hat{f}^{(j+2)}(\cdot) \). If \( a_{j=m,n} \) is known, then \( G[\hat{f}^{(j)}(z)] \) is also known, and the \( a_{j,m}, l > j \geq 1 \) follow by iterative application of Eq. (16) for progressively smaller \( j \).

For \( n = 0 \) it is assumed that the initial bandwidth \( a_{l,0} \) is estimated using as \( \hat{f}^{(l+1)}(\cdot) \) in Eq. (16) a Gaussian PDF with mean and variance estimated from the data. One can then estimate the auxiliary bandwidth from Eq. (16) for \( n = 0 \) without further repetition. However, as shown in [47], if the true distribution deviates significantly from the normal, suboptimal estimates of \( h \) are obtained from this initial condition. Better results are obtained by progressively refining the auxiliary bandwidth estimates.

For \( n \geq 1 \) Eq. (16) is initialized using as PDF (for \( j = l \)) the kernel density estimate with bandwidth \( a_{1,n-1} \), i.e., the PDF \( \hat{f}^{(1)}(\cdot) \) from the previous stage. The repetition counter increases up to \( n^* \) such that \( |a_{1,n^*} - a_{1,n^*-1}| < \epsilon \). Finally, by setting \( \hat{a}_1 = a_{1,n^*} \) the BGK bandwidth \( h \) is calculated from Eq. (7) and \( \hat{a}_1 \).

This appendix presents boxplots of the mean square error ratios that compare the performance of KCDE using the normal reference rule for bandwidth selection (see Section 4.1.1). The plots in Fig. C1 illustrate that the CDF estimated with the normal reference rule does not significantly improve the estimation compared to the staircase function.
Figure C1: Boxplots of $\text{RE}_{k_{	ext{opt}}} (\text{MSE of } \hat{F}_{K} \text{ divided by the MSE of the staircase estimate } \hat{F}_{s})$ using the Normal Reference Rule as bandwidth instead of the BGK. $N$ is the sample size. Abbreviations are defined in the main text.
## D Exploratory Analysis of ERA5 Precipitation

Table D1: Best-fit probability distribution models for the daily, weekly, monthly and annual precipitation amounts for the wet period (October to March) (from ERA5 reanalysis data) for the selected node near Messara valley. Measures of fit: Akaike’s Information Criterion (AIC), the Bayesian Information Criterion (BIC), and the negative log-likelihood (NLL). Measures of fit for the optimal models are boldfaced.

| Method | Model | Normal | Weibull | Gamma | GEV | LGN |
|--------|-------|--------|---------|-------|-----|-----|
| **Daily precipitation** | | | | | | |
| AIC | 3.2873 ×10^4 | **1.0878 ×10^4** | 1.1104 ×10^4 | 1.2876 ×10^4 | 1.1434 ×10^4 |
| BIC | 3.2886 ×10^4 | **1.0892 ×10^4** | 1.1117 ×10^4 | 1.2896 ×10^4 | 1.1447 ×10^4 |
| NLL | 1.6434 ×10^4 | **5.4372 ×10^3** | 5.5501 ×10^3 | 6.4352 ×10^3 | 5.7149 ×10^3 |
| **Weekly precipitation** | | | | | | |
| AIC | 8.3461 ×10^3 | 6.9989 ×10^3 | **6.9412 ×10^3** | 7.4841 ×10^3 | 7.4278 ×10^3 |
| BIC | 8.3560 ×10^3 | 7.0089 ×10^3 | **6.9511 ×10^3** | 7.4900 ×10^3 | 7.4377 ×10^3 |
| NLL | 4.1710 ×10^3 | 3.4975 ×10^3 | **3.4686 ×10^3** | 3.7391 ×10^3 | 3.7119 ×10^3 |
| **Monthly precipitation** | | | | | | |
| AIC | 2.3649 ×10^3 | **2.3276 ×10^3** | 2.3428 ×10^3 | 2.3406 ×10^3 | 2.3996 ×10^3 |
| BIC | 2.3719 ×10^3 | **2.3346 ×10^3** | 2.3467 ×10^3 | 2.3531 ×10^3 | 2.4066 ×10^3 |
| NLL | 1.1832 ×10^3 | **1.1618 ×10^3** | 1.1678 ×10^3 | 1.1673 ×10^3 | 1.1988 ×10^3 |
| **Annual precipitation** | | | | | | |
| AIC | 463.8558 | **463.4259** | 465.4719 | 467.1305 | 465.8434 |
| BIC | 467.2829 | **466.8531** | 468.8991 | 470.8069 | 470.6502 |
| NLL | 230.7360 | **229.7130** | 231.5652 | 229.9199 | 229.9217 |
Table D2: Number of times \( \in \{0, 1, 2, \ldots, 65\} \) each parametric model is selected as the optimal distribution for the daily, weekly, monthly and annual precipitation amounts for the wet period (October to March) for the 65 ERA5 nodes around Crete. Measures of fit: Akaike’s Information Criterion (AIC), the Bayesian Information Criterion (BIC), and the negative log-likelihood (NLL). Measures of fit for the optimal models are boldfaced.

| Method | Model   | Normal | Weibull | Gamma | GEV | LGN |
|--------|---------|--------|---------|-------|-----|-----|
|        | Daily precipitation |        |         |       |     |     |
| AIC    | 0       | 56     | 9       | 0     | 0   |     |
| BIC    | 0       | 56     | 9       | 0     | 0   |     |
| NLL    | 0       | 56     | 9       | 0     | 0   |     |
|        | Weekly precipitation |        |         |       |     |     |
| AIC    | 0       | 0      | 65      | 0     | 0   |     |
| BIC    | 0       | 0      | 65      | 0     | 0   |     |
| NLL    | 0       | 0      | 65      | 0     | 0   |     |
|        | Monthly precipitation |        |         |       |     |     |
| AIC    | 0       | 61     | 4       | 0     | 0   |     |
| BIC    | 0       | 61     | 4       | 0     | 0   |     |
| NLL    | 0       | 59     | 1       | 5     | 0   |     |
|        | Annual precipitation |        |         |       |     |     |
| AIC    | 18      | 5      | 28      | 0     | 14  |
| BIC    | 18      | 5      | 28      | 0     | 14  |
| NLL    | 3       | 2      | 7       | 52    | 1   |