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NOTES AND CORRESPONDENCE

A Novel Method for the Homogenization of Daily Temperature Series and Its Relevance for Climate Change Analysis

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ABSTRACT

Instrumental daily series of temperature are often affected by inhomogeneities. Several methods are available for their correction at monthly and annual scales, whereas few exist for daily data. Here, an improved version of the higher-order moments (HOM) method, the higher-order moments for autocorrelated data (HOMAD), is proposed. HOMAD addresses the main weaknesses of HOM, namely, data autocorrelation and the subjective choice of regression parameters. Simulated series are used for the comparison of both methodologies. The results highlight and reveal that HOMAD outperforms HOM for small samples. Additionally, three daily temperature time series from stations in the eastern Mediterranean are used to show the impact of homogenization procedures on trend estimation and the assessment of extremes. HOMAD provides an improved correction of daily temperature time series and further supports the use of corrected daily temperature time series prior to climate change assessment.

1. Introduction

The study of extreme events' nature and statistical properties in a future climate is of major importance for impact, adaptation, and mitigation studies. The assessment of extremes, such as heat waves, is a complex task involving analysis of index time series (e.g., Moberg et al. 2006) and application of tools from extreme value theory (Coles 2001). The accuracy of this assessment depends on the use of high-quality daily time series that are not affected by inhomogeneities (e.g., sudden changes of the mean and variance) caused by nonclimatic factors (e.g., caused

by station relocation, instrumentation, or land-use changes; see also Aguilar et al. 2003). These break points can be identified through metadata and/or statistical methods (e.g., Alexandersson and Moberg 1997; Caussinus and Mestre 2004). However, metadata are often incomplete and/or not available. The correction of the detected break points is generally performed by employing reference series that are highly correlated with the series to be homogenized. The correction of daily climate time series is still at an early stage of research and few approaches have considered daily temperature data (e.g., Vincent et al. 2002; Della-Marta and Wanner 2006, hereafter DW06). DW06 developed a method for adjusting the mean and higher-order moments (HOM) of daily time series, which was used to homogenize daily western European and western Mediterranean temperature time series (e.g., Della-Marta et al. 2007; Aguilar et al. 2008). HOM has notable advantages compared to other methods (e.g., Vincent et al. 2002), particularly when highly correlated reference temperature series are available. However, HOM depends on the choice of regression function parameters and it is affected by data autocorrelation. The correction of inhomogeneities affecting daily series is a delicate process. Therefore, it is essential to address potential sources of uncertainty in the adjustment estimations. On these grounds, we propose an improved version of HOM, the higher-order moments for autocorrelated data (HOMAD). In the following sections, HOMAD is described and evaluated relative to HOM using simulated series and three selected case studies (third section). We conclude by presenting the advantages of HOMAD with respect to HOM and providing applications of the proposed methodology.

2. Method description

Let $\{Y_t\}$ with $t = 1, \ldots, N$ be the candidate (i.e., the series to be adjusted) affected by K break points, located at $\{t_{l_1}, \ldots, t_{l_K}\}$. Focusing on the most recent detected inhomogeneity, two homogeneous subperiods (HSPs) can be identified: HSP1 (from t_N to t_{l_K}) and HSP2 (from t_{l_K} to $t_{l_{K-1}}$). Let $\{X_t\}$ be a series highly correlated to $\mathbf{Y}$ (i.e., a reference) with a homogeneous period overlapping both HSP1 and HSP2. HOM is based on a regression model between $\mathbf{Y}$ and $\mathbf{X}$ and the cumulative distribution function (CDF) estimation in the two HSPs. The former is performed with a LOESS model (Cleveland and Devlin 1988). As explained in DW06, the regression function is controlled by the smoothing parameter λ and the degree of the local fitted polynomial α. The parameter values are chosen subjectively, although DW06 provide suggestions for their selection. As for the distribution estimation, the CDFs are fitted applying the theory of L

moments (Hosking 1990), without consideration of data autocorrelation, and six a priori chosen distributions are tested. However, daily records present a significant autocorrelation that influences the CDF estimation. Moreover, the identification of an appropriate distribution is not trivial; DW06 apply a Kolmogorov–Smirnov test (Shao 2003) for this task, but they report a similar behavior of the different distributions.

The residual dependence in the regression model, $\mathbf{Y} = g(\mathbf{X}) + \boldsymbol{\epsilon}$ or $\mathbf{Y} \sim N[g(\mathbf{X}), \sigma_{\boldsymbol{\epsilon}}^2 \mathbf{R}]$ (where $\mathbf{R}$ and $\sigma_{\boldsymbol{\epsilon}}^2$ are unknown), affects the standard methods for the smoothing parameter choice (Opsomer et al. 2001). Therefore, a penalized spline smoothing (e.g., Currie and Durban 2002; Durban and Currie 2003) with a restricted maximum likelihood (REML) smoothing parameter estimate (Patterson and Thompson 1971; Harville 1977) that considers data autocorrelation is chosen to replace the LOESS method. Following Krivobokova and Kauermann (2007), $g(\mathbf{X}) = \boldsymbol{\chi}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}$, where $\boldsymbol{\chi}$ and $\mathbf{Z}$ have rows $\mathbf{X}_i = (1, x_i)$ and $\mathbf{Z}_i = [(x_i - \tau_1)_+, \ldots, (x_i - \tau_K)_+]$, respectively. In the $\mathbf{Z}_i$ definition, τ_i are fixed knots and $(x)_+ = \max(x, 0)$. The number of knots is not a crucial parameter and is calculated by using $\min(N/4, 40)$ (Ruppert 2002). The coefficients $\boldsymbol{\beta}$ and $\mathbf{u}$ are estimated with the penalized likelihood $l_p(\boldsymbol{\beta}, \mathbf{u}; \sigma_{\boldsymbol{\epsilon}}^2, \mathbf{R}, \lambda)$ and the smoothing parameter λ is given by minimizing a negative restricted maximum likelihood function (REML; see the appendix). Since the correlation matrix is usually unknown, the estimation is performed using a matrix $\hat{\mathbf{R}}$ that is assumed to approximate $\mathbf{R}$. We found satisfactory results with an autoregressive model of the first order (AR1); however, the user can modify this setting if a stronger correlation is evident. It is important to point out that Krivobokova and Kauermann (2007) proved the robustness of the REML approach against an incorrect specification of the matrix. Finally, in order to achieve numerical stability we have followed the suggestions of Krivobokova et al. (2008) by implementing the penalized spline.

With regard to the CDF estimation, we address the dependence of data and avoid the constraint of fixed a priori distributions by applying the nonparametric Parzen–Rosenblatt estimator with a Gaussian kernel. Assuming that observations are a realization of identically distributed random variables $\mathbf{X} = (X_1, \ldots, X_n)$, with a common distribution function F and probability density function f, an estimator of the latter is the Parzen–Rosenblatt kernel density estimator:

$$f_h(x) = n^{-1} \sum_{i=1}^{n} K_h(X_i - x),$$

where $K_h(\cdot) = h^{-1} K(\cdot/h)$ is the kernel function, that is, a symmetric density function (e.g., Gaussian) scaled by

a positive real parameter h called the bandwidth. Moreover, the distribution function is given by

$$F_h(x) = \frac{1}{n}\sum_{i=1}^{n} H\!\left(\frac{x - X_i}{h}\right),$$

where $H(x)$ is defined by $\int_{-\infty}^{x} K(t)\, dt$. Therefore, the pth quantile ξ_p is given by $F^{-1}(p) = \inf\{x \in \Re: F(x) \ge p\}$. The asymptotic behavior of this method was tested under various assumptions of data dependence. For instance, Estévez and Vieu (2003) and Wang (2007) studied the case of long memory processes, while the weakly dependent processes were considered by Bosq (1998). The outcome of these studies demonstrates that the more interesting properties of the kernel estimator still hold. In instances of independence, bandwidth selection is often made by applying the least squares cross validation (LSCV). Following the notation of Sköld (2001) and using the so-called integrated mean square error, the LSCV bandwidth is defined by $h_{\text{LSCV}} = \text{argmin}_h \text{ LSCV}(h)$, where

$$\text{LSCV}(h) = \int f_h^2(x)\, dx - 2n^{-1}\sum_{i=1}^{n} f_h^{(i)}(X_i).$$

In the above equation, $f_h^{(i)}$ is the leave-one-out kernel density estimator, which is robust against moderate dependence of data (Hart and Vieu 1990). However, as suggested by Hart and Vieu (1990), in case of dependence some improvements can be achieved by replacing $f_h^{(i)}$ with the leave-$(2p + 1)$-out estimator:

$$f_h^{(i,p)}(\cdot) = n_i^{-1}\sum_{k;|k-i|>p} K_h[(\cdot) - X_k],$$

where n_i is the cardinality of the set $\{k; |k - i| > p\}$. There is not a rule available for the choice of the p parameter. Therefore, autoregressive models [AR(p)] are fitted to the series and compared by using the corrected Akaike Information Criterion (AIC; Hurvich and Tsai 1989).

Supplementing the estimation steps of the procedure, HOMAD introduces an additional control on the series. As highlighted by DW06, the correlation between the candidate and the reference series is of major importance and ensures reliable correction. Furthermore, HOM and HOMAD rely on the stability of the regression function between $\mathbf{Y}$ and $\mathbf{X}$; in instances where this condition is not met the entire procedure could be compromised. In the case of two HSPs (one break point), the following relationships hold: $\mathbf{Y}^{\text{HSP1}} = f(\mathbf{X}^{\text{HSP1}}) + \boldsymbol{\epsilon}$ and $\mathbf{Y}_{\text{hom}}^{\text{HSP2}} = g(\mathbf{X}^{\text{HSP2}}) + \boldsymbol{\gamma}$, where $\mathbf{Y}_{\text{hom}}^{\text{HSP2}}$ is the homogeneous series (i.e., not altered by the inhomogeneity) in

TABLE 1. Simulation results with DW06 series and the new simulated series. True denotes the magnitude of the known inhomogeneity (°C).

DW06 simulated series			
10 years; true = 2.13		40 years; true = 2.11	
HOM	HOMAD	HOM	HOMAD
2.21 ± 0.094	2.17 ± 0.085	2.10 ± 0.046	2.10 ± 0.04
New simulated series			
10 years; true = 1.34		40 years; true = 2.29	
HOM	HOMAD	HOM	HOMAD
1.17 ± 0.109	1.34 ± 0.085	2.30 ± 0.042	2.28 ± 0.046

the second subperiod. The stability of the regression function implies that f is equal to g. Since the inhomogeneity is unknown, any strong departure from stationarity of $f(X_t) - \tilde{g}(X_t)$ (where $\tilde{g}$ is the regression function estimated by $\mathbf{Y}^{\text{HSP2}}$ and $\mathbf{X}$) in the HSPs implies a probable violation of the stability assumption. Therefore, HOMAD estimates this difference and tests the presence of a trend, enabling the user to decide whether a correction of the candidate series is appropriate or not.

3. Simulation and case studies

To evaluate HOMAD relative to HOM, two sets of simulations are carried out with an inhomogeneity (i.e., a Gaussian random variable with mean equal to 1.3σ, where σ refers to the candidate) and standard deviation equal to one. In the first set, we use simulated series of DW06, which give (for construction) independent residuals in the regression model (see previous section). We perform 1000 runs taking 10-yr candidate and reference daily series and two HSPs of the same length (i.e., a break point at the middle of the candidate series). This is followed by another 1000 runs using 40-yr daily series. In the second set of simulations, candidate and reference series are created following the approach of Wilks (1999), with a trend term and an autoregressive component. In this case, the regression model does not have independent residuals. As in the first set, 1000 runs are done with 10-yr series and another 1000 are done with 40-yr series. The results of both simulation sets are presented in Table 1. The performance of HOM and HOMAD is similar for the 40-yr runs, whereas HOMAD outperforms HOM for the 10-yr series. As expected, the two methods have the same behavior when applied on large samples.

In addition to these simulations, three daily maximum temperature series—Bozkurt (Turkey), Goztepe/Istanbul (Turkey), and Corfu (Greece)—are chosen to evaluate the behavior of HOMAD relative to HOM. These series are selected according to quality, completeness, and
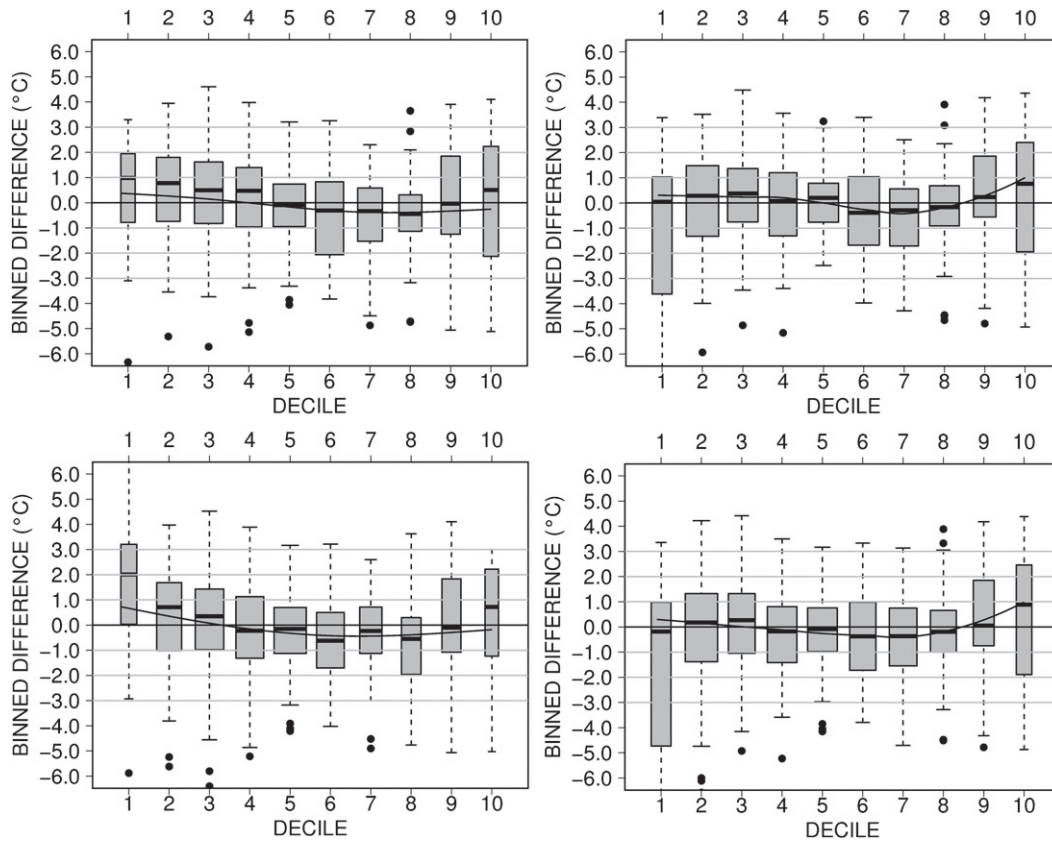
FIG. 1. (left) HOMAD and (right) HOM decile adjustments and smoothed adjustments (black solid line) for the series of Bozkurt (September). The upper plots refer to the inhomogeneity of 1976. The lower plots refer to 1981.

abundance of highly correlated neighboring series for correction. The inhomogeneities are detected by comparing the series with a set of highly correlated time series and validated by applying to the annual series the penalized maximal t (PMT) tests (Wang 2008; Wang et al. 2007) and the test of Caussinus and Mestre (2004) [for details, see also Kuglitsch et al. (2009)]. For Bozkurt (daily temperature time series from 1960 to 2006), two break points are detected in 1976 and 1981, resulting in three homogeneous subperiods. The series of Goztepe/ Istanbul (daily data from 1930 to 2006) is affected by two break points in 1984 and 1988. The series of Corfu is affected by one inhomogeneity in 1989 during the period 1960–2006. Decile adjustments and smoothed adjustments for the series are shown in Figs. 1–3 for each series. Although the adjustments appear similar (as expected, since HOMAD is based on HOM), they highlight the different corrections estimated by the two methods. To determine the potential impact of the different corrections, the mean annual summer (June– August) series are calculated for all the series (raw and corrected) and a trend analysis is performed. The results (Table 2) point out the important effects of the

homogenization procedure on trend estimation. The raw series of Istanbul has no trend, whereas the HOMAD/ HOM corrected series have a significant positive trend, with a slope equal to $0.13 \pm 0.05°C$ decade^{-1} and $0.1 \pm 0.05°C$ decade^{-1}, respectively. For the raw series of Bozkurt and Corfu, the trends have erroneous slope. In Bozkurt the slope is underestimated whereas in Corfu the slope is overestimated. An extremes analysis is also performed on summer daily temperature and a declustered peak over threshold (dePOT) model (Davison and Smith 1990) is applied to the raw and the HOMAD/HOM corrected series. The results (Table 3) show that in all three cases the correction influences the extreme distribution parameters (i.e., shape and scale of the generalized Pareto distribution) and, therefore, the characterization of extremes. HOM corrected series consistently have higher 5-yr and 25-yr return values. However, as shown in Table 3, the differences between the raw and the HOMAD/HOM corrected series are minimal, mainly because of the presence of a finite right end point (the shape parameters are always negative). It is important to note that more complex extreme models (e.g., with time-dependent parameters) could be influenced by homogenization in
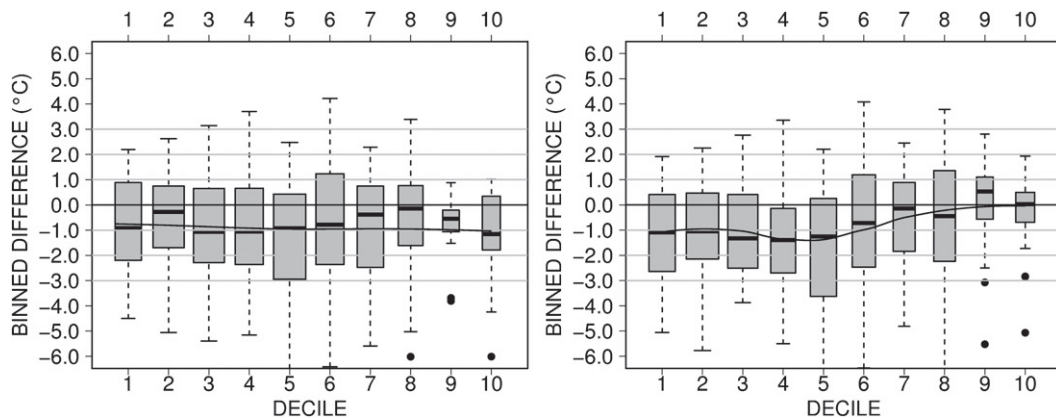
FIG. 2. (left) HOMAD and (right) HOM decile adjustments and smoothed adjustments (black solid line) for the series of Gozpete/Istanbul (June). The figure refers to the inhomogeneity of 1984.

a higher degree, because (as seen for mean summer temperature series) the correction influences the trend estimation. The comparison of raw and corrected time series, as shown by the case studies, reveals the necessity for homogenization prior to climate change analysis. The different results from HOMAD and HOM highlight the importance of using reliable methods to detect and correct inhomogeneities. The evaluation of HOMAD relative to HOM reveals the importance of the potential uncertainties during the homogenization procedure that are related with data autocorrelation and the subjective choice of regression parameters (and of the distributions to be tested).

4. Conclusions

The homogenization procedure is an essential step for climate change analyses based on observations (e.g., extreme value analysis). We propose a new methodology

(HOMAD), which builds on the method of DW06 by addressing data autocorrelation and providing an objective choice of regression parameters. Since the complexity of a real inhomogeneity is not easily reproducible, the evaluation of correction methods can be performed in simple situations (e.g., Gaussian random term added to the series after a certain point). Our simulations show that HOMAD outperforms HOM when applied to small samples, whereas the two methods provide similar results for larger ones. We acknowledge that further investigation is necessary to address other sources of uncertainty; however, our results provide valuable information on HOMAD/HOM behavior and the relevance of autocorrelation and an objective selection of regression parameters. Three daily temperature series from the Mediterranean have been used to compare the performance of HOMAD and HOM. Differences between the adjustments suggested by the two methods have been found in all three cases. These differences influence the outcome of analyses performed on the homogenized series
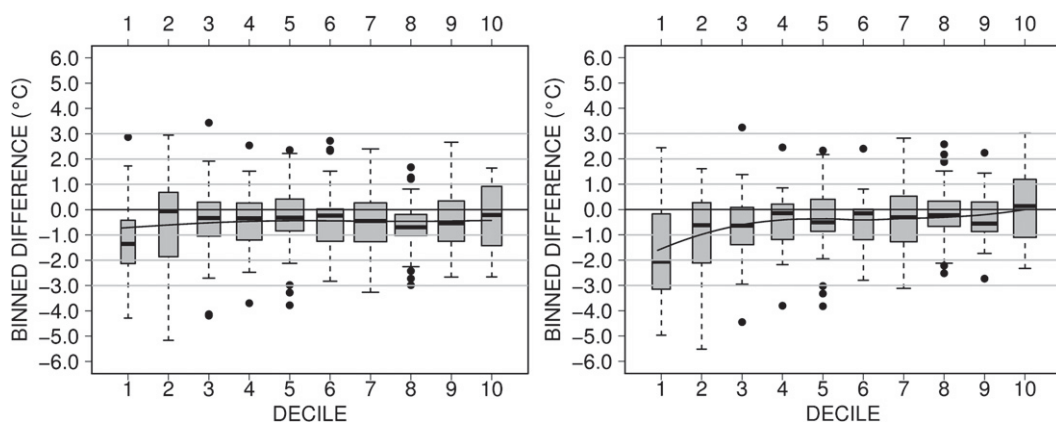

FIG. 3. (left) HOMAD and (right) HOM decile adjustments and smoothed adjustments (black solid line) for the series of Corfu (December).

TABLE 2. Trend estimations for the three case studies. Only the significant values (°C decade^{-1}) are reported.

Time series	Raw	HOMAD	HOM
Corfu	0.20 ± 0.08	0.16 ± 0.07	0.16 ± 0.08
Istanbul	—	0.13 ± 0.05	0.10 ± 0.05
Bozkurt	0.22 ± 0.10	0.27 ± 0.09	0.26 ± 0.10

(e.g., trend assessment or return levels estimation). Based on the theoretical improvements and the promising results of HOMAD, we suggest the application of this method to future daily temperature homogenization exercises. Moreover, we encourage the use of HOMAD in the evaluation efforts of the homogenization methodologies (e.g., COST Action ES0601 "Advances in homogenization methods of climate series: An integrated approach—HOME", and other national or international programs). An R-FORTRAN software package is available for scientific use through the first author.

APPENDIX

Penalized and Restricted Likelihood Functions

The penalized likelihood function is given by

$$l_p(\boldsymbol{\beta}, \mathbf{u}; \sigma_\epsilon^2, \mathbf{R}, \lambda) = -2^{-1}\{N\log(\sigma_\epsilon^2) + \log|\mathbf{R}|$$
$$+ (\mathbf{Y} - \mathbf{C}\boldsymbol{\theta})^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{Y} - \mathbf{C}\boldsymbol{\theta})\sigma_\epsilon^{-2}\}$$
$$- \lambda 2^{-1}\sigma_\epsilon^{-2}\mathbf{u}^{\mathrm{T}}\mathbf{D}\mathbf{u}, \tag{A1}$$

where $\mathbf{C} = (\mathbf{X}, \mathbf{Z})$, $\boldsymbol{\theta} = (\boldsymbol{\beta}^{\mathrm{T}}, \mathbf{u}^{\mathrm{T}})^{\mathrm{T}}$, and $\mathbf{D}$ is usually chosen equal to the $\mathbf{I}_K$. The smoothing parameter is obtained minimizing the negative REML:

$$-2\text{REML}(\mathbf{R}, \lambda) = (N - p)\log(\hat{\sigma}_{\epsilon,MM}^2) + \log|\mathbf{V}_{\mathbf{R},\lambda}|$$
$$+ \log|\mathbf{X}^{\mathrm{T}}\mathbf{V}_{\mathbf{R},\lambda}^{-1}\mathbf{X}|, \tag{A2}$$

where p is equal to the dimension of $\boldsymbol{\beta}$, $\hat{\sigma}_{\epsilon,MM}^2 = (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^{\mathrm{T}}\mathbf{V}_{\mathbf{R},\lambda}^{-1}(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})/(N - p)$. Moreover, $\mathbf{V}_{\mathbf{R},\lambda} = \mathbf{R} + \mathbf{Z}\mathbf{D}^-\mathbf{Z}^{\mathrm{T}}\lambda^{-1}$, and $\mathbf{D}^-$ is the generalized inverse of $\mathbf{D}$. For a complete description the reader is referred to Eilers and Marx (1996), Currie and Durban (2002), and Krivobokova and Kauermann (2007).

TABLE 3. Results of the extreme analysis: GPD parameters and 5(25)-yr return levels (values in °C).

Time series	Raw	HOMAD	HOM
Corfu			
Shape	-0.11 ± 0.079	-0.20 ± 0.065	-0.20 ± 0.078
Scale	1.98 ± 0.239	2.34 ± 0.250	2.47 ± 0.301
r5	38.7 ± 0.72	38.8 ± 0.70	39.1 ± 0.70
r25	40.9 ± 1.34	40.6 ± 1.11	41.1 ± 1.12
Istanbul			
Shape	-0.12 ± 0.058	-0.15 ± 0.058	-0.06 ± 0.07
Scale	2.25 ± 0.207	2.41 ± 0.224	2.03 ± 0.219
r5	37.1 ± 0.72	37.1 ± 0.73	37.5 ± 0.78
r25	39.4 ± 1.28	39.3 ± 1.24	40.1 ± 1.60
Bozkurt			
Shape	-0.13 ± 0.056	-0.10 ± 0.062	-0.04 ± 0.078
Scale	2.99 ± 0.267	2.76 ± 0.266	2.46 ± 0.286
r5	36.8 ± 0.90	36.2 ± 0.98	36.5 ± 1
r25	39.6 ± 1.58	39.2 ± 1.82	40.0 ± 2.15

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