## Near-consistent robust estimations of moments for unimodal distributions

## **Tuban Lee**

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Descriptive statistics for parametric models currently heavily rely on the accuracy of distributional assumptions. Here, leveraging the invariant structures of unimodal distributions, a series of sophisticated, yet efficient estimators, robust to both gross errors and departures from parametric assumptions, are proposed for estimating mean and central moments with insignificant asymptotic biases for common unimodal distributions. This article also illuminates the understanding of the common nature of probability distributions and the measures of them.

orderliness | invariant | unimodal | adaptive estimation | U-statistics

he asymptotic inconsistencies between sample mean  $(\bar{x})$ and nonparametric robust location estimators in asymmetric distributions on the real line have been noticed for more than two centuries (1), yet remain unsolved. Strictly speaking, it is unsolvable as by trimming, some information about the original distribution is removed, making it impossible to estimate the values of the removed parts without distributional assumptions. Newcomb (1886, 1912) provided the first modern approach to robust parametric estimation by developing a class of estimators that gives "less weight to the more discordant observations" (2, 3). In 1964, Huber (4) used the minimax procedure to obtain M-estimator for the contaminated normal distribution, which has played a pre-eminent role in the later development of robust statistics. However, as previously demonstrated, under growing asymmetric departures from normality, the bias of the Huber M-estimator increases rapidly. This is a common issue in parameter estimations. For example, He and Fung (1999) constructed (5) a robust M-estimator for the two-parameter Weibull distribution, from which all moments can be calculated. Nonetheless, it is inadequate for the gamma, Perato, lognormal, and the generalized Gaussian distributions (SI Dataset S1). Another interesting approach is based on L-estimators, such as percentile estimators. Examples of percentile estimators for the Weibull distribution, the reader is referred to Menon (1963) (6), Dubey (1967) (7), Hassanein (1971) (8), Marks (2005) (9), and Boudt, Caliskan, and Croux (2011) (10)'s works. At the outset of the study of percentile estimators, it was known that they arithmetically utilize the invariant structures of probability distributions (6, 11, 12). Maybe such estimators can be named as I-statistics. Formally, an estimator is classified as an I-statistic if it asymptotically satisfies  $I(LE_1, \dots, LE_l) = (\theta_1, \dots, \theta_q)$  for the distribution it is consistent, where LEs are calculated with the use of LU-statistics (defined in Subsection B), I is defined using arithmetic operations and constants but may also incorporate transcendental functions and quantile functions, and  $\theta$ s are the population parameters it estimates. A subclass of I-statistics, arithmetic I-statistics, is defined as LEs are LU-statistics, I is solely defined using arithmetic operations and constants. Since some percentile estimators use the logarithmic function to transform all random variables before computing the L-estimators, a percentile estimator might not always be an arithmetic I-statistic (7). In this article, two subclasses of I-statistics are introduced, arithmetic I-statistics and quantile I-statistics. Examples of quantile I-statistics will be discussed later. Based on LU-statistics, I-statistics are naturally robust. Compared to probability density functions (pdfs) and cumulative distribution functions (cdfs), the quantile functions of many parametric distributions are more elegant. Since the expectation of an L-estimator can be expressed as an integral of the quantile function, I-statistics are often analytically obtainable. However, the performance of the aforementioned examples is often worse than that of the robust M-statistics when the distributional assumption is violated (SI Dataset S1). Even when distributions such as the Weibull and gamma belong to the same larger family, the generalized gamma distribution, a misassumption can still result in substantial biases for central moments, rendering the approach ill-suited (SI Dataset S1).

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The majority of robust location estimators commonly used are symmetric, they are consistent for any symmetric distributions with finite second moments, owing to the prevalence of symmetric distributions. An asymmetric weighted L-statistic can achieve consistency for a semiparametric class of skewed distributions; but the lack of symmetry makes it suitable only for certain applications. From semiparametrics to parametrics, consider an estimator with a non-zero asymptotic breakdown point that is simultanously consistent for both a semiparametric class of distributions and a distinct parametric distribution with finite moments, such a robust location estimator is called an invariant mean. Based on the mean-weighted L-statistic- $\gamma$ -median inequality, the recombined mean is defined as

$$rm_{d,\epsilon,\gamma,n} := \lim_{c \to \infty} \left( \frac{(WL_{\epsilon,\gamma,n} + c)^{d+1}}{(\gamma m_n + c)^d} - c \right),$$

where d is the key factor for bias correction,  $\gamma m_n$  is the sample  $\gamma$ -median,  $\mathrm{WL}_{\epsilon,\gamma,n}$  is the weighted L-statistic. If  $\gamma$  is omitted,  $\gamma=1$  is assumed. The subsequent theorem shows the significance of this arithmetic I-statistic.

## **Significance Statement**

Bias, variance, and contamination are the three main errors in statistics. Consistent robust estimation is unattainable without parametric assumptions. Here, invariant moments are proposed as a means of achieving near-consistent and robust estimations of moments, even in scenarios where moderate violations of distributional assumptions occur, while the variances are sometimes smaller than those of the sample moments.

T.L. designed research, performed research, analyzed data, and wrote the paper. The author declares no competing interest.

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Theorem .1. Let  $BM_{\epsilon,n}$  be the WL,  $rm_{d\approx 0.103, \epsilon=\frac{1}{24}}$  is a consistent mean estimator for the exponential distribution, any symmetric distributions and the Pareto distribution with quantile function  $Q(p)=x_m(1-p)^{-\frac{1}{\alpha}}$ ,  $x_m>0$ , when  $\alpha\to\infty$ , provided that the second moments are finite.

*Proof.* Finding d and  $\epsilon$  that make  $rm_{d,\epsilon}$  a consistent 69 mean estimator is equivalent to finding the solution of 70  $E[rm_{d,\epsilon,n}] = E[X]$ . The quantile function of the expo-71 nential distribution is  $Q(p) = \ln\left(\frac{1}{1-p}\right)\lambda$ .  $E[X] = \lambda$ . 72  $E[m_n] = Q(\frac{1}{2}) = \ln 2\lambda$ . For the exponential distribution,  $E\left[{\rm BM}_{\epsilon=\frac{1}{24},n}\right] = \lambda \left(1 + \ln\left(\frac{26068394603446272\sqrt[6]{\frac{7}{247}}\sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)\right), \text{ the detailed formula is given in the SI Text. Since } rm_{d,\epsilon} =$  $\lim_{c\to\infty} \left( \frac{(\mathrm{BM}_{\epsilon}+c)^{d+1}}{(m+c)^{d}} - c \right) = (d+1)\,\mathrm{BM}_{\epsilon} - dm = \mu. \quad \mathrm{So},$  $d \; = \; \frac{\mu - \mathrm{BM}_{\epsilon}}{\mathrm{BM}_{\epsilon} - m} \; = \; \frac{\lambda - \lambda \left(1 + \ln \left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)\right)}{\lambda \left(1 + \ln \left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)\right) - \ln 2\lambda}$  $\frac{\ln\left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6} 101898752449325\sqrt{5}}\right)}{1-\ln(2)+\ln\left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6} 101898752449325\sqrt{5}}\right)}$  $\approx 0.103$ . The proof of the second assertion follows directly from the coincidence property. For any symmetric distribution with a fi-80 nite second moment,  $E[BM_{\epsilon,n}] = E[m_n] = E[X]$ . Then 81  $E\left[rm_{d,\epsilon,n}\right] = \lim_{c \to \infty} \left(\frac{(E[X]+c)^{d+1}}{(E[X]+c)^d} - c\right) = E\left[X\right]. \text{ The proof}$ 82 for the Pareto distribution is more general. The mean of 83 the Pareto distribution is given by  $\frac{\alpha x_m}{\alpha - 1}$ . Since any weighted L-statistic can be expressed as an integral of the quantile function as shown in Theorem A.1, the  $\gamma$ -median is also a percentile, replacing the WL and  $\gamma m$  in the d value with two 87 arbitrary percentiles  $p_1$  and  $p_2$ , for the Pareto distribution. 88  $d_{Perato} = \frac{\mu - Q(p_1)}{Q(p_1) - Q(p_2)} = \frac{\frac{\alpha x_m}{\alpha - 1} - x_m (1 - p_1)^{-\frac{1}{\alpha}}}{x_m (1 - p_1)^{-\frac{1}{\alpha}} - x_m (1 - p_2)^{-\frac{1}{\alpha}}}. \quad x_m \text{ can}$  be canceled out. For the exponential distribution,  $d_{exp} = \frac{1}{\alpha} - \frac$ 89  $\frac{\mu - Q(p_1)}{Q(p_1) - Q(p_2)} = \frac{\lambda - \ln\left(\frac{1}{1 - p_1}\right)\lambda}{\ln\left(\frac{1}{1 - p_1}\right)\lambda - \ln\left(\frac{1}{1 - p_2}\right)\lambda} = -\frac{\ln(1 - p_1) + 1}{\ln(1 - p_1) - \ln(1 - p_2)}.$ Since  $\lim_{\alpha \to \infty} \frac{\frac{\alpha}{\alpha - 1} - (1 - p_1)^{-1/\alpha}}{(1 - p_1)^{-1/\alpha} - (1 - p_2)^{-1/\alpha}} = -\frac{\ln(1 - p_1) + 1}{\ln(1 - p_1) - \ln(1 - p_2)},$ the d value for the Pareto distribution approach that of 93 the exponential distribution, as  $\alpha \to \infty$ , regardless of the type 94 of weighted L-statistic used. This completes the demonstra-95 tion. 

Theorem .1 implies that for the Weibull, gamma, Pareto, lognormal and generalized Gaussian distribution,  $rm_{d\approx 0.103,\epsilon=\frac{1}{24}}$  is consistent for at least one particular case. The biases of  $rm_{d\approx 0.103,\epsilon=\frac{1}{24}}$  for distributions with skewness between those of the exponential and symmetric distributions are tiny (SI Dataset S1).  $rm_{d\approx 0.103,\epsilon=\frac{1}{24}}$  exhibits excellent performance for all these common unimodal distributions (SI Dataset S1).

Besides introducing the concept of invariant mean, the purpose of this paper is to demonstrate that, in light of previous works, the estimation of central moments can be transformed into a location estimation problem by using U-statistics, the central moment kernel distributions possess desirable properties, and a series of sophisticated yet efficient robust estimators can be constructed whose biases are typically smaller than

the variances (as seen in Table  $\ref{Table}$  for n=4096) for unimodal distributions.

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## **Background and Main Results**

**A. Invariant mean.** It is well established that a theoretical model can be adjusted to fit the first two moments of the observed data. A continuous distribution belonging to a location–scale family, parametrized by a location parameter  $\mu$  and a scale parameter  $\lambda$ , takes the form  $F(x) = F_0\left(\frac{x-\mu}{\lambda}\right)$ , where  $F_0$  is a standard distribution without any shifts or scaling. Therefore,  $F(x) = Q^{-1}(x) \to x = Q(p) = \lambda Q_0(p) + \mu$ . Thus, for a location-scale distribution, any WA $(\epsilon, \gamma)$  can be expressed as  $\lambda$ WA $_0(\epsilon, \gamma) + \mu$ , where WA $_0(\epsilon, \gamma)$  is an integral of  $Q_0(p)$  according to the definition of the weighted average. The following theorem shows that the  $whl_k$  kernel distribution is always a location-scale distribution if the original distribution is a location-scale distribution with the same location and scale parameters. The proof is given in the SI Text.

**Theorem A.1.** 
$$whl_k (x_1 = \lambda x_1 + \mu, \dots, x_k = \lambda x_k + \mu) = \lambda whl_k (x_1, \dots, x_k) + \mu.$$

Let WeHLM<sub>0</sub>( $\epsilon, \gamma$ ) denote the expected value of a weighted Hodges-Lehmann mean for the standard distribution, then for a location-scale family of distributions parametrized by a location parameter  $\mu$  and a scale parameter  $\lambda$ , the WeHLM can also be expressed as  $\lambda$ WeHLM<sub>0</sub>( $\epsilon, \gamma$ ) +  $\mu$ . Since Theorem A.1 also proved the  $w_i \neq 1$  case, this form is valid for all weighted L-statistics. The simultaneous cancellation of  $\mu$  and  $\lambda$  in  $\frac{(\lambda \mu_0 + \mu) - (\lambda W L_0(\epsilon, \gamma) + \mu)}{(\lambda W L_0(\epsilon, \gamma) + \mu) - (\lambda \gamma m_0 + \mu)}$  assures that d is always a constant for a location-scale distribution.

The performance in heavy-tailed distributions can be further improved by constructing the quantile mean as

$$qm_{d,\epsilon,\gamma,n} := \hat{Q}_n \left( \left( \hat{F}_n \left( WL_{\epsilon,\gamma,n} \right) - \frac{1}{1+\gamma} \right) d + \hat{F}_n \left( WL_{\epsilon,\gamma,n} \right) \right),$$

provided that  $\hat{F}_n(WL_{\epsilon,\gamma,n}) \geq \frac{1}{1+\gamma}$ , where  $\hat{F}_n(x)$  is the empirical cumulative distribution function of the sample,  $\hat{Q}_n$  is the sample quantile function. When  $\hat{F}_n(WL_{\epsilon,\gamma,n}) < \frac{1}{1+\gamma}$ ,  $qm_{d,\epsilon,\gamma,n}$  is defined as  $\hat{Q}_n\left(\hat{F}_n\left(\mathrm{WL}_{\epsilon,\gamma,n}\right) - \left(\frac{1}{1+\gamma} - \hat{F}_n\left(\mathrm{WL}_{\epsilon,\gamma,n}\right)\right)d\right)$ . Without loss of generality, in the following discussion, only the case where  $\hat{F}_n\left(\mathrm{WL}_{\epsilon,\gamma,n}\right) \geq \frac{1}{1+\gamma}$  is considered. Moreover, in extreme right-skewed heavy-tailed distributions, the calculated percentile can exceed  $1 - \epsilon$ , the percentile will be modified to  $1 - \epsilon$  if this occurs. A widely used method for calculating the sample quantile function involves employing linear interpolation of modes corresponding to the order statistics of the uniform distribution on the interval [0, 1], i.e.,  $\hat{Q}_n(p) = X_{\lfloor h \rfloor} + (h - \lfloor h \rfloor) \left( X_{\lceil h \rceil} - X_{\lfloor h \rfloor} \right), \ h = (n-1) p + 1.$ To minimize the finite sample bias, here, the inverse function of  $\hat{Q}_n$  is deduced as  $\hat{F}_n(x) := \frac{1}{n-1} \left( cf - 1 + \frac{x - X_{cf}}{X_{cf+1} - X_{cf}} \right)$ , where  $cf = \sum_{i=1}^{n} \mathbf{1}_{X_i \leq x}$ ,  $\mathbf{1}_A$  is the indicator of event A. The quantile mean uses the location-scale invariant in a different way as shown in the following proof.

**Theorem A.2.** Let  $BM_{\epsilon,n}$  be the WL,  $qm_{d\approx 0.088, \epsilon=\frac{1}{24}}$  is a consistent mean estimator for the exponential, Pareto  $(\alpha \to \infty)$  and any symmetric distributions provided that the second moments are finite.

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163 Proof. The cdf of the exponential distribution is F(x) = 1164  $1 - e^{-\lambda^{-1}x}$ ,  $\lambda \ge 0$ ,  $x \ge 0$ . Recall that the expecta165 tion of  $BM_{\epsilon,n}$  can be expressed as  $\lambda BM_0(\epsilon)$ , so  $F(BM_{\epsilon})$  is
166 free of  $\lambda$ , as are  $F(\mu)$  and F(m). When  $\epsilon = \frac{1}{24}$ ,  $d = \frac{1}{24}$ 

free of 
$$\lambda$$
, as are  $F(\mu)$  and  $F(m)$ . When  $\epsilon = \frac{1}{24}$ ,  $d = \frac{F(\mu) - F(BM_{\epsilon}) - \frac{1}{2}}{F(BM_{\epsilon}) - \frac{1}{2}} = \frac{-e^{-1} + e^{-\left(1 + \ln\left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)\right)}{-\left(1 + \ln\left(\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)\right)} = \frac{101898752449325\sqrt{5} \sqrt[6]{\frac{247}{7}} \sqrt[3]{11}}{2e^{-\left(\frac{1}{2}\right)} \sqrt[6]{\frac{26068394603446272 \sqrt[6]{\frac{7}{247}} \sqrt[3]{11}}{391^{5/6}101898752449325\sqrt{5}}\right)}$ 

 $\frac{\frac{101898752449325\sqrt{5}\sqrt{6}\sqrt{\frac{247}{7}}391^{5/6}}{\frac{26068394603446272\sqrt[3]{11}e}{\frac{1}{2} - \frac{101898752449325\sqrt{5}\sqrt{6}\sqrt{\frac{247}{7}}391^{5/6}}{\frac{26068394603446272\sqrt[3]{11}e}{\sqrt[3]{11}e}} \approx 0.088. \text{ The proof of the}$ 

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symmetric case: since for any symmetric distribution with a finite second moment,  $F(E[BM_{\epsilon,n}]) = F(\mu) = \frac{1}{2}$ . Then, the expectation of the quantile mean is  $qm_{d,\epsilon} = F^{-1}(F(\mu) - \frac{1}{2})d + F(\mu) = F^{-1}(0 + F(\mu)) = \mu$ .

For the assertion related to the Pareto distribution, the cdf of it is  $1-\left(\frac{x_m}{x}\right)^{\alpha}$ . Similar to Theorem .1, replacing the  $F(\mathrm{WL}_{\epsilon,\gamma})$  and  $\frac{1}{1+\gamma}$  in the d value with two arbitrary percentiles  $p_1$  and  $p_2$ ,

$$d_{Pareto} = \frac{1 - \left(\frac{x_m}{\frac{\alpha x_m}{\alpha - 1}}\right)^{\alpha} - \left(1 - \left(\frac{x_m}{x_m(1 - p_1)^{-\frac{1}{\alpha}}}\right)^{\alpha}\right)}{\left(1 - \left(\frac{x_m}{x_m(1 - p_1)^{-\frac{1}{\alpha}}}\right)^{\alpha}\right) - \left(1 - \left(\frac{x_m}{x_m(1 - p_2)^{-\frac{1}{\alpha}}}\right)^{\alpha}\right)} = 0$$

78  $\frac{1-\left(\frac{\alpha-1}{\alpha}\right)^{\alpha}-p_1}{p_1-p_2}$ . When  $\alpha \to \infty$ ,  $\left(\frac{\alpha-1}{\alpha}\right)^{\alpha}=\frac{1}{e}$ , so in this case,  $d_{Pareto}$  is identical to that of the exponential distri-

bution, since 
$$d_{exp} = \frac{\left(1 - e^{-1}\right) - \left(1 - e^{-\ln\left(\frac{1}{1 - p_1}\right)}\right)}{\left(1 - e^{-\ln\left(\frac{1}{1 - p_1}\right)}\right) - \left(1 - e^{-\ln\left(\frac{1}{1 - p_2}\right)}\right)}$$

 $\frac{1-\frac{1}{e}-p_1}{p_1-p_2}$ . Therefore, same logic as in Theorem .1, their d values are always identical, regardless of the type of weighted L-statistic used. All results are now proven.

The definitions of location and scale parameters are such that they must satisfy  $F(x; \lambda, \mu) = F(\frac{x-\mu}{\lambda}; 1, 0)$ . By recalling  $x = \lambda Q_0(p) + \mu$ , it follows that the percentile of any weighted L-statistic is free of  $\lambda$  and  $\mu$ , which guarantees the validity of the quantile mean. The quantile mean is a quantile I-statistic. Specifically, an estimator is classified as a quantile I-statistic if LEs are percentiles of a distribution obtained by plugging LU-statistics into a cumulative distribution function and I is defined with arithmetic operations, constants and quantile functions.  $qm_{d\approx 0.088,\epsilon=\frac{1}{24}}$  works better in the fat-tail scenarios (SI Dataset S1). Theorem .1 and A.2 show that  $rm_{d\approx 0.103,\epsilon=\frac{1}{24}}$ and  $qm_{d\approx 0.088,\epsilon=\frac{1}{24}}$  are both consistent mean estimators for any symmetric distribution and a skewed distribution with finite second moments. It's obvious that the breakdown points of  $rm_{d\approx 0.103,\epsilon=\frac{1}{24}}$  and  $qm_{d\approx 0.088,\epsilon=\frac{1}{24}}$  are both  $\frac{1}{24}$ . Therefore they are all invariant means.

To study the impact of the choice of WAs in rm and qm, it is constructive to recall that a weighted average is a linear combination of quantile averages. While using a less-biased weighted average can generally enhance performance (SI Dataset S1), there is a greater risk of violation in the semiparametric framework. However, the mean-WA $_{\epsilon,\gamma}$ - $\gamma$ -median inequality is robust to slight fluctuations of the QA function of the underlying distribution. Suppose the QA function is generally decreasing in [0,u], but increasing in  $[u,\frac{1}{1+\gamma}]$ , since  $\frac{1}{1+\gamma}-\gamma\epsilon$  of the quantile averages will be included in the computation of WA $_{\epsilon,\gamma}$ ,

as long as  $\frac{1}{1+\gamma} - u \ll \frac{1}{1+\gamma} - \gamma \epsilon$ , and other portions of the QA function satisfy the inequality constraints that define the  $\nu$ th  $\gamma$ -orderliness on which the WA<sub> $\epsilon,\gamma$ </sub> is based, the mean- $WA_{\epsilon,\gamma}$ - $\gamma$ -median inequality will still hold. This is due to the violation being bounded (13) and therefore cannot be extreme for unimodal distributions. For instance, the SQA function is non-monotonic when the shape parameter of the Weibull distribution  $\alpha > \frac{1}{1-\ln(2)} \approx 3.259$  as shown in the previous article, the violation of the third orderliness starts near this parameter as well, yet the mean-BM  $_{\frac{1}{24}}\text{-median}$  inequality is still valid when  $\alpha \leq 3.387$ . Another key factor in determining the risk of violation is the skewness of the distribution. Previously, it was demonstrated that in a family of distributions differing by a skewness-increasing transformation in van Zwet's sense, the violation of orderliness, if it happens, often only occurs when the distribution is nearly symmetrical (14). When  $\gamma = 1$ , the over-corrections in rm and qm are dependent on the  $SWA_{\epsilon}$ -median difference, which can be a reasonable measure of skewness (15, 16), implying that the over-correction is often tiny with a moderate d. The same logic can be applied to other weighted L-statistics. This qualitative analysis provides another perspective, in addition to the bias bounds (13), that rm and qm based on the mean-WL $_{\epsilon,\gamma}$ - $\gamma$ -median inequality are generally safe for unimodal distributions.

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B. Robust estimations of the central moments. In 1979, Bickel and Lehmann, in their final paper of the landmark series Descriptive Statistics for Nonparametric Models (17), generalized a class of estimators called "measures of spread," which "does not require the assumption of symmetry." From that, a popular efficient scale estimator, the Rousseeuw-Croux scale estimator (18), was derived in 1993, but the importance of tackling the symmetry assumption has been greatly underestimated. While they had already considered one version of the trimmed standard deviation in the third paper of that series (19), in the final section of the fourth paper (17), they explored another two possible versions, which were modified here for comparison,

$$\left[n\left(\frac{1}{2} - \epsilon\right)\right]^{-\frac{1}{2}} \left[\sum_{i=\frac{n}{2}}^{n(1-\epsilon)} \left[X_i - X_{n-i+1}\right]^2\right]^{\frac{1}{2}}, \quad [1] \quad {}_{24}$$

and 248

$$\left[ \binom{n}{2} \left( 1 - \epsilon - \gamma \epsilon \right) \right]^{-\frac{1}{2}} \left[ \sum_{i = \binom{n}{2} \gamma \epsilon}^{\binom{n}{2} (1 - \epsilon)} \left( X - X' \right)_i^2 \right]^{\frac{1}{2}}, \quad [2] \quad {}_{24}$$

**Data Availability.** Data for Table ?? are given in SI Dataset S1. All codes have been deposited in GitHub.

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