$\widehat{\text{Theo1}}$ Confidence Intervals

T.N. Tasset*, D.A. Howe*, and D.B. Percival†

ABSTRACT Theoretical variance #1 ($\widehat{\text{Theo1}}$) has been developed at NIST to improve the estimation of long-term frequency stability. Its square-root ($\widehat{\text{Theo1}}$-dev) has two significant improvements over the Allan deviation $\hat{\sigma}_y(\tau)$ (Adev) in estimating long-term frequency stability, in that (1) it can evaluate frequency stability at averaging times 50 % longer than those of Adev, and (2) it can estimate frequency stability with greater confidence than any other estimator. We discuss a method for determining the exact confidence intervals of $\widehat{\text{Theo1}}$, particularly useful for small sample sizes, using analytic techniques. The confidence intervals of $\widehat{\text{Theo1}}$ are narrower and less skewed (more symmetric) than confidence intervals based on chi-square.

I. Introduction and Summary

An important challenge of characterizing oscillators is accurately determining frequency stability at long-term averaging times. For a given data run of length T, the two-sample Allan deviation $\hat{\sigma}_y(\tau)$, or Adev, can estimate frequency stability only up to averaging times of T/2 and at that value with minimal confidence [1, 2, 3]. This paper is about $\widehat{\text{Theo1}}$, a special-purpose, multi-sample statistic that evaluates very-long-term frequency stability at τ intervals between $\frac{T}{2}$ and T whose average is $\frac{3T}{4}$, or a maximum stride of $\tau_s = 0.75(T-\tau_0)$, where τ_0 is the sampling period between adjacent observations. $\widehat{\text{Theo1}}$ was developed following studies of an improved estimator of Adev called Total deviation, or "Totdev" [3, 4, 5, 6, 7, 8]. Formerly, we have based confidence intervals for Totdev and $\widehat{\text{Theo1}}$ on a chi-square distribution with equivalent degrees of freedom, ν, where the equivalent degrees of freedom are found by simulation. Compared to Adev, Totdev has less skew in its confidence intervals [5, 7]. Presently, $\widehat{\text{Theo1}}$ has the highest confidence in estimating long-term frequency stability [9, 10]. In the study here, we found that $\widehat{\text{Theo1}}$'s distribution function is both narrower and more symmetric than that of chi-square. Confidence intervals computed analytically for various sample sizes are consistent with simulation studies.

*National Institute of Standards and Technology, Time and Frequency Division; email: `metrology@boulder.nist.gov`.

†University of Washington, Applied Physics Laboratory.

II. $\widehat{\text{Theo1}}$ Definition

It is common practice to measure samples of the time-error function $x(t)$ between two oscillators and then derive frequency stability [1, 2, 3]. Starting with a sequence of time-error samples $\{x_t : t = 1, 2, \ldots, n\}$ with a sampling period τ_0, $\widehat{\text{Theo1}}$ averages every permissible squared second difference of time errors in a given span or stride $\tau_s = 0.75k\tau_0$. τ_s has the same meaning as the traditional sampling interval τ in the $\hat{\sigma}^2_y(\tau)$, the traditional estimator of the Allan variance. Let us start with the equation for $\widehat{\text{Theo1}}$, the estimator of Theo1 [9, 10]:

$$\widehat{\text{Theo1}}(\tau = 0.75k\tau_0) = \frac{4}{3(n-k+1)(k\tau_0)^2}\sum_{t=k}^{n} \sum_{\delta=1}^{\frac{k}{2}} \frac{1}{\delta}[(x_t - x_{t-\delta}) - (x_{t-k+\delta} - x_{t-k})]^2, \quad (1)$$

where k is even. In this equation, $\widehat{\text{Theo1}}$ is in terms of phase data, and we have the usual relation to frequency data. We want to express $\widehat{\text{Theo1}}$ in a quadratic form [11, 12, 13]. We start by defining:

$$y_t = \frac{x_t - x_{t-1}}{\tau_0}, \quad t = 1, 2, \ldots, n \quad (2)$$

$$\overline{y}_t(\delta) = \frac{1}{\delta}\sum_{j=0}^{\delta-1} y_{t-j}. \quad t = \delta, \delta+1, \ldots, n \quad (3)$$

$$= \frac{x_t - x_{t-\delta}}{\delta\tau_0}. \quad (4)$$

Then we can write (1) as

$$\widehat{\text{Theo1}}(\tau = 0.75k\tau_0) = \frac{4}{3(n-k+1)k^2}\sum_{t=k}^{n} \sum_{\delta=1}^{\frac{k}{2}} \delta[\overline{y}_t(\delta) - \overline{y}_{t-k+\delta}(\delta)]^2. \quad (5)$$

Next, define

$$\overline{z}_t(k,\delta) = \sqrt{\frac{2\delta}{3k}}(\overline{y}_t(\delta) - \overline{y}_{t-k+\delta}(\delta)), \quad \delta = 1, 2, \ldots, \frac{k}{2}. \quad (6)$$

Then we have

$$\widehat{\text{Theo1}}(\tau = 0.75k\tau_0) = \frac{2}{k(n-k+1)} \sum_{t=k}^{n} \sum_{\delta=1}^{\frac{k}{2}} [\overline{z}_t(k,\delta)]^2$$

$$= \frac{1}{m} \sum_{t=k}^{n} \sum_{\delta=1}^{\frac{k}{2}} [\overline{z}_t(k,\delta)]^2, \qquad (7)$$

where $m \equiv (n-k+1) \times \frac{k}{2}$.

III. Determining the Confidence Interval

Notice that the $\overline{z}_t(k,\delta)$'s are a collection of m random variables. Stack them into a single vector:

$$\overline{\mathbf{Z}} \equiv \begin{bmatrix} \overline{z}_k(k,1) \\ \overline{z}_k(k,2) \\ \vdots \\ \overline{z}_k(k,\frac{k}{2}) \\ \overline{z}_{k+1}(k,1) \\ \overline{z}_{k+1}(k,2) \\ \vdots \\ \overline{z}_{k+1}(k,\frac{k}{2}) \\ \vdots \\ \overline{z}_n(k,1) \\ \overline{z}_n(k,2) \\ \vdots \\ \overline{z}_n(k,\frac{k}{2}) \end{bmatrix}.$$

We assume that $\overline{\mathbf{Z}}$ is multivariate normal with covariance matrix $\Sigma_{\overline{\mathbf{Z}}}$, i.e., the $(r,s)^{\text{th}}$ element of $\Sigma_{\overline{\mathbf{Z}}}$ is the covariance between the rth and sth members of $\overline{\mathbf{Z}}$. If $\overline{Z_l}$ is the lth element of $\overline{\mathbf{Z}}$, then we can write

$$\widehat{\text{Theo1}}(\tau = 0.75k\tau_0) = \frac{1}{m} \sum_{l=1}^{m} \overline{Z}_l^2. \qquad (8)$$

The expected value of this estimator defines a population quantity that we denote as Theo1:

$$\text{Theo1}(\tau = 0.75k\tau_0) \equiv E\{\widehat{\text{Theo1}}(\tau = 0.75k\tau_0)\} \qquad (9)$$

$$= \frac{1}{m} \sum_{l=1}^{m} E\{\overline{Z}_l^2\}. \qquad (10)$$

Define

$$Q_m = \frac{m\widehat{\text{Theo1}}(\tau = 0.75k\tau_0)}{\text{Theo1}(\tau = 0.75k\tau_0)} = \frac{\sum_{l=1}^{m} \overline{Z_l}^2}{\text{Theo1}(\tau = 0.75k\tau_0)}. \qquad (11)$$

Let q_p be the p^{th} quantile of the distribution of Q_m:

$$F_m(q_p) \equiv \mathrm{P}\left[Q_m \le q_p\right] = p. \qquad (12)$$

Then a $(1-2p) \times 100\%$ confidence interval for Theo1 is given by

$$\left[\frac{m\widehat{\text{Theo1}}(\tau = 0.75k\tau_0)}{q_{1-p}}, \frac{m\widehat{\text{Theo1}}(\tau = 0.75k\tau_0)}{q_p}\right]. \qquad (13)$$

The random variable Q_m is a quadratic form in m normal variables. We can determine the distribution once we transform it into the standardized form,

$$Q_m = \sum_{l=1}^{m} \lambda_l {U_l}^2, \qquad (14)$$

where the U_l's are independent chi-square random variables, each with one degree of freedom, and the λ_l's are the eigenvalues of a normalized version of $\Sigma_{\overline{\mathbf{Z}}}$.

Once the covariance matrix has been normalized and the eigenvalues are known, we can numerically evaluate $F_m(x)$ in one of two ways. Expanding $F_m(x)$ in terms of the sums of the distribution function of central chi-square random variables works well for small n [12]. As n gets large, a more efficient means is by numerical inversion of the characteristic function [13].

IV. Example Calculation

We let $n = 6$, $k = 4$, and assume that our data are random walk frequency modulation (RWFM). We have

$$\overline{\mathbf{Z}} \equiv \begin{bmatrix} \overline{z}_4(4,1) \\ \overline{z}_4(4,2) \\ \overline{z}_5(4,1) \\ \overline{z}_5(4,2) \\ \overline{z}_6(4,1) \\ \overline{z}_6(4,2) \end{bmatrix},$$

and

$$\Sigma_{\overline{\mathbf{Z}}} = \left[\begin{matrix} E\{\overline{z}_4^2(4,1)\} & E\{\overline{z}_4(4,1)\overline{z}_4(4,2)\} & E\{\overline{z}_4(4,1)\overline{z}_5(4,1)\} \\ E\{\overline{z}_4(4,2)\overline{z}_4(4,1)\} & E\{\overline{z}_4^2(4,2)\} & E\{\overline{z}_4(4,2)\overline{z}_5(4,1)\} \\ E\{\overline{z}_5(4,1)\overline{z}_4(4,1)\} & E\{\overline{z}_5(4,1)\overline{z}_4(4,2)\} & E\{\overline{z}_5^2(4,1)\} \\ E\{\overline{z}_5(4,2)\overline{z}_4(4,1)\} & E\{\overline{z}_5(4,2)\overline{z}_4(4,2)\} & E\{\overline{z}_5(4,2)\overline{z}_5(4,1)\} \\ E\{\overline{z}_6(4,1)\overline{z}_4(4,1)\} & E\{\overline{z}_6(4,1)\overline{z}_4(4,2)\} & E\{\overline{z}_6(4,1)\overline{z}_5(4,1)\} \\ E\{\overline{z}_6(4,2)\overline{z}_4(4,1)\} & E\{\overline{z}_6(4,2)\overline{z}_4(4,2)\} & E\{\overline{z}_6(4,2)\overline{z}_5(4,1)\} \end{matrix}\right.$$

$$\left.\begin{matrix} E\{\overline{z}_4(4,1)\overline{z}_5(4,2)\} & E\{\overline{z}_4(4,1)\overline{z}_6(4,1)\} & E\{\overline{z}_4(4,1)\overline{z}_6(4,2)\} \\ E\{\overline{z}_4(4,2)\overline{z}_5(4,2)\} & E\{\overline{z}_4(4,2)\overline{z}_6(4,1)\} & E\{\overline{z}_4(4,2)\overline{z}_6(4,2)\} \\ E\{\overline{z}_5(4,1)\overline{z}_5(4,2)\} & E\{\overline{z}_5(4,1)\overline{z}_6(4,1)\} & E\{\overline{z}_5(4,1)\overline{z}_6(4,2)\} \\ E\{\overline{z}_5^2(4,2)\} & E\{\overline{z}_5(4,2)\overline{z}_6(4,1)\} & E\{\overline{z}_5(4,2)\overline{z}_6(4,2)\} \\ E\{\overline{z}_6(4,1)\overline{z}_5(4,2)\} & E\{\overline{z^2}_6(4,1)\} & E\{\overline{z}_6(4,1)\overline{z}_6(4,2)\} \\ E\{\overline{z}_6(4,2)\overline{z}_5(4,2)\} & E\{\overline{z}_6(4,2)\overline{z}_6(4,1)\} & E\{\overline{z}_6^2(4,2)\} \end{matrix}\right].$$

We need to determine the entries of $\Sigma_{\overline{\mathbf{Z}}}$. We note first that if we define

$$z_t(k-\delta) = \sum_{i=0}^{k-\delta-1} z_{t-i}, \qquad (15)$$

where $\{z_t\}$ is the first difference of our frequency data, then we can write

$$\overline{z}_t(k,\delta) = \sqrt{\frac{2}{3\delta k}} \sum_{j=0}^{\delta-1} z_{t-j}(k-\delta) = \sqrt{\frac{2}{3\delta k}} \sum_{j=0}^{\delta-1} \sum_{i=0}^{k-\delta-1} z_{t-j-i}. \qquad (16)$$

Hence, we have

$$\overline{z}_4(4,1) = \frac{\sqrt{2}}{2\sqrt{3}} \sum_{i=0}^{2} z_{4-i} = \frac{\sqrt{2}}{2\sqrt{3}}(z_2 + z_3 + z_4),$$

$$\overline{z}_4(4,2) = \frac{\sqrt{2}}{2\sqrt{6}} \sum_{j=0}^{1}\sum_{i=0}^{1} z_{4-j-i} = \frac{\sqrt{2}}{2\sqrt{6}}(z_2 + 2z_3 + z_4),$$

etc. Since we are assuming that y_t is a random-walk process, then z_t is Gaussian white noise with zero mean and unit variance; i.e.,

$$E\{z_t z_{t'}\} = \begin{cases} 1, & t = t' \\ 0, & t \neq t' \end{cases} .$$

We can evaluate the covariances of $\Sigma_{\overline{\mathbf{Z}}}$ easily; for example,

$$\begin{aligned} &E\{\overline{z}_4(4,1)\overline{z}_4(4,2)\} \\ &= \left(\frac{\sqrt{2}}{2\sqrt{3}}\right)\left(\frac{\sqrt{2}}{2\sqrt{6}}\right) E\{(z_2+z_3+z_4)(z_2+2z_3+z_4)\} \\ &= \frac{1}{6\sqrt{2}} E\{{z_2}^2 + 2{z_3}^2 + {z_4}^2 + 3z_2z_3 + 2z_2z_4 + 3z_3z_4\} \\ &\quad = \frac{1}{6\sqrt{2}}(1+2+1+0+0+0) = \frac{4}{6\sqrt{2}} = \frac{4\sqrt{2}}{12}. \end{aligned}$$

Continuing in this manner we obtain

$$\Sigma_{\overline{\mathbf{Z}}} = \frac{1}{12}\begin{bmatrix} 6 & 4\sqrt{2} & 4 & 3\sqrt{2} & 2 & \sqrt{2} \\ 4\sqrt{2} & 6 & 3\sqrt{2} & 4 & \sqrt{2} & 1 \\ 4 & 3\sqrt{2} & 6 & 4\sqrt{2} & 4 & 3\sqrt{2} \\ 3\sqrt{2} & 4 & 4\sqrt{2} & 6 & 3\sqrt{2} & 4 \\ 2 & \sqrt{2} & 4 & 3\sqrt{2} & 6 & 4\sqrt{2} \\ \sqrt{2} & 1 & 3\sqrt{2} & 4 & 4\sqrt{2} & 6 \end{bmatrix}.$$

Table 1: Quantiles for RWFM noise

n	k	$q_{0.025}$	$q_{0.050}$	$q_{0.159}$	$q_{0.841}$	$q_{0.950}$	$q_{0.975}$
4	2	0.2158	0.3519	0.8353	5.181	7.815	9.349
4	4	0.01731	0.03604	0.1392	3.912	7.521	9.819
8	2	1.690	2.167	3.445	10.56	14.07	16.01
8	4	1.126	1.563	3.001	16.98	26.57	32.43
8	8	0.04927	0.08475	0.2753	7.830	15.06	19.66
16	2	6.262	7.261	9.653	20.35	25.00	27.49
16	4	6.994	8.602	12.94	39.05	52.99	60.97
16	8	3.641	4.993	9.726	62.12	100.4	124.2
16	16	0.09317	0.1594	0.5288	15.68	30.18	39.14
32	2	17.54	19.28	23.22	38.78	44.99	48.23
32	4	25.07	28.66	37.39	78.60	97.50	107.8
32	8	24.76	30.74	47.28	152.7	210.9	244.5
32	16	12.39	17.22	34.53	236.7	388.3	483.3
32	32	0.1769	0.3066	1.039	31.38	60.42	78.55
64	2	42.95	45.74	51.85	74.15	82.53	86.83
64	4	69.92	76.44	91.37	152.6	178.0	191.4

From equation (10), we also have Theo1$(\tau = 0.75k\tau_0) = 1/2$; i.e., this is given by the diagonal elements of $\Sigma_{\overline{\mathbf{Z}}}$. We obtain

$$Q_m = \frac{\sum_{l=1}^{m} {\overline{Z}_l}^2}{\mathrm{Theo1}(\tau = 0.75k\tau_0)} = 2\sum_{l=1}^{m} {\overline{Z}_l}^2.$$

The next step is to determine the eigenvalues of $\Sigma_{\overline{\mathbf{Z}}}$, and once that is done we use one of the aforementioned numerical techniques to calculate the quantiles $q_{0.159} = 1.252$ and $q_{0.841} = 10.69$. The $(1 - 2(0.159)) \times 100\ \% = 68.2\ \%$ confidence interval is thus

$$\begin{aligned} &\left[\frac{6\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0)}{q_{0.841}}, \frac{6\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0)}{q_{0.159}}\right] \\ &= \left[0.561\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0), 4.79\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0)\right]. \end{aligned}$$

Quantiles corresponding to 68.2 %, 90 %, and 95 % confidence intervals and for various sample sizes are shown in Table 1 and are consistent with simulation studies.

V. Comparison to Chi-Square

Traditionally, the confidence intervals of $\widehat{\mathrm{Theo1}}$ and similar statistics have been approximated by assuming a chi-square distribution with equivalent degrees of freedom, ν, where the equivalent degrees of freedom are found by simulation. Equations for the number of degrees of freedom for $\widehat{\mathrm{Theo1}}$ can be found in [8] and for Adev in [14, 15]. With this approximation, a $(1 - 2p) \times 100\ \%$ confidence interval is given by

$$\left[\frac{\nu\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0)}{\chi^2_{\nu;1-p}}, \frac{\nu\widehat{\mathrm{Theo1}}(\tau = 0.75k\tau_0)}{\chi^2_{\nu;p}}\right],$$

where $\chi^2_{\nu;p}$ represents the p^{th} quantile of the distribution of a chi-square random variable with ν degrees of freedom. We find that the exact confidence intervals of $\widehat{\mathrm{Theo1}}$ are less skewed than confidence intervals based on chi-square. Ratios of the exact confidence to the approximation are shown in Table 2 for the case of RWFM.

Table 2: Ratio of lengths of confidence intervals for RWFM noise and various n and k. Notice that for each n, as k gets large, the chi-square approximation becomes increasingly inaccurate.

n	k	Ratio
32	2	0.93
32	4	0.88
32	8	0.74
64	2	0.97
64	4	0.93
64	8	0.86

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