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On the transformation of colored random noise by the Kronig–Kramers integral transforms

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Abstract

The transformation of random noise present in impedance spectroscopy data by the important Kronig–Kramers integral-transform relations is investigated analytically. It is found that the standard deviation of the transformed noise may be smaller than the input noise under certain conditions. The output noise standard deviation depends critically on the details of the numerical quadrature procedure used for the Kronig–Kramers transformations, so the effects of several different numerical integration routines are investigated. In most cases of interest, it is proved that the standard deviation of the output noise is equal to that of the input noise, in agreement with earlier Monte Carlo results. It has been found possible not only to derive expressions for the limiting standard deviation of the transformed noise for several different integration procedures but also to obtain analytic expressions for their statistical distributions in the limit of an infinite number of discrete integration points. Finally, it is demonstrated that the integration routine may be adjusted to obtain either very small integration errors (in the absence of input noise) or smaller output noise with larger integration error. © 1997 Elsevier Science S.A.

Keywords: Colored random noise; Kronig–Kramers relations; Error transformations

1. Introduction

The Kronig–Kramers relations (KKR) are important coupled integral transforms connecting the real and imaginary (or magnitude and phase) parts of the small-signal frequency response of a physically realizable complex quantity, such as impedance or dielectric permittivity [1–7]. They are thus applicable to measurements of the linear electrical (or optical or mechanical) response of passive materials whose properties are time-invariant and satisfy causality. They have been widely used for a long time for analyzing situations where only a single part of a complex quantity is easily measured; then, in principle, one of the KKR may be used to calculate the other part of the complex quantity at any desired frequency. In addition, when both parts are available over a wide frequency range, they may be used to test whether the system is time-varying or not. This capability is particularly important for corrosion measurements. If any property variation is sufficiently small over the time required for immittance measurements, the resulting data may closely satisfy the KKR. Alternatively, when the application of a KKR to one part fails to predict the other measured part adequately, the data are inconsistent with the KKR conditions and should not be used for detailed analysis of the system.

There is, unfortunately, a practical limitation to the applicability of the KKR for obtaining accurate results. Their direct application requires integration over the full frequency range, $0 \leq \omega \leq \infty$, one that can only be approximated experimentally. Here ω is the angular frequency. It is thus common to use models of the expected high- and low-frequency responses for extrapolation outside of the measured range, a procedure which usually introduces unknown uncertainties in the results [6]. Recently, it has become common to avoid this problem by using complex non-linear least squares (CNLS) fitting of the data to a Voigt equivalent circuit, one made up of a series combination of parallel *RC*s ([8–13] and references cited therein).

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Such a circuit automatically satisfies the KKR. By using a sufficient number of elements, any conductive-system data consistent with these relations can be well fitted over its full range without the need for extrapolation. Again, lack of an adequate fit suggests that the system was not time-invariant during the measurement.

Orazem and co-workers [8,9,13] have found that, in many instances, the statistical variances of real- and imaginary-part response associated with stochastic measurement errors are approximately the same at each point of the measured frequency range. Although such behavior is probably associated with the specifics of the frequency response analyzer used for such measurements, and is thus unlikely to be an intrinsic property of immittance spectroscopy measurements, it has directed new attention to such errors and to the most appropriate weighting for CNLS fitting. It thus becomes worthwhile to investigate how stochastic errors are transformed by the KKR process.

Several years ago, the surprising result was demonstrated by Monte Carlo analysis that the variance of random noise transformed by either of the two KKR was equal to that of the untransformed noise at each point of the relevant frequency range [6]. Since any experimental data analyzed by the KKR or by the alternate Voigt fitting approach (called the 'measurement model approach' by Orazem and his co-authors) will involve stochastic errors (assumed here to consist of random, uncorrelated noise associated with a probability density such as a Gaussian), it is desirable to explore such noise behavior analytically in order to verify the above results if possible, and to obtain precise conditions for which they may apply.

We shall consider two forms of the KKR for an electrical impedance, $Z(\omega) = Z'(\omega) + jZ''(\omega)$, where $Z(\omega)$ is a general impedance function and $j = \sqrt{-1}$. The standard form is [3]

$$Z'(\omega) \equiv Z'(\infty) + \frac{2}{\pi}\int_0^\infty \frac{[xZ''(x) - \omega Z''(\omega)]\,dx}{x^2 - \omega^2} \tag{1}$$

and

$$Z''(\omega) \equiv -\frac{2\omega}{\pi}\int_0^\infty \frac{[Z'(x) - Z'(\omega)]\,dx}{x^2 - \omega^2} \tag{2}$$

Note that the first of these relations does not allow one to estimate $Z'(\infty)$ from knowledge of $Z''(\omega)$, so its value must be determined separately. When the KKR are transformed to apply over the range from 0 to 1, one obtains [6]

$$Z'(\omega) \equiv Z'(\infty) + \frac{2}{\pi\omega}\int_0^1 \frac{[\omega y Z''(\omega y) - (\omega/y)Z''(\omega/y)]\,dy}{1 - y^2} \tag{3}$$

and

$$Z''(\omega) \equiv -\frac{2}{\pi}\int_0^1 \frac{[Z'(\omega y) - Z'(\omega/y)]\,dy}{1 - y^2} \tag{4}$$

The Monte Carlo study cited above was entirely numerical and dealt only with discrete values of the quantities involved in the above expressions. Numerical integration of Eqs. (1) and (2) was accomplished using equal intervals in the logarithm of the x variable, while that for Eqs. (3) and (4) involved equal intervals in y [6]. Noise samples $\epsilon(x)$ were drawn independently from a random, stationary Gaussian distribution with zero mean. Because of the linearity of the KKR, in the present noise study we need only to consider the KK transformations of the noise

$$I'(\omega) \equiv \frac{2}{\pi}\int_0^\infty \frac{x\epsilon(x)f(x)\,dx}{x^2 - \omega^2} \tag{5}$$

and

$$I''(\omega) \equiv -\frac{2\omega}{\pi}\int_0^\infty \frac{\epsilon(x)f(x)\,dx}{x^2 - \omega^2} \tag{6}$$

and their Eqs. (3) and (4) equivalents. There is no reason to expect $I'(\omega)$ and $I''(\omega)$ to be parts of a causal, analytic complex variable. Here $f(x)$ is an arbitrary continuous function used to 'color' the noise samples, so that their frequency behavior need not be necessarily homoscedastic. Since $f(x)$ is arbitrary, the two expressions above are essentially equivalent as far as noise transformation is concerned, a fact exploited in Appendix A. We assume that the $\epsilon(x)$ is a white noise, so that for every x, x', $x \neq x'$, random variables $\epsilon(x)$ and $\epsilon(x')$ are independent and identically distributed with expectations zero and variances σ^2.

The present analysis, like the Monte Carlo study in Ref. [6], deals with discrete-quadrature approximations to the KKR integrals. If one defines a step size h and a total number of discrete points for the approximation as N, then in order to obtain high accuracy for the transformations in Ref. [6], it was necessary to use a large N (often greater than 1000) and a correspondingly small h (when it was taken constant for a given integration). In the present work, we shall consider the limits $h \to 0$ and $N \to \infty$, with hN not necessarily tending to infinity. It will be shown that the transformation of errors by numerical integration of an integrand involving a pole of order less than unity leads, in the limit, to output errors with zero standard deviation (i.e. no error), while that involving a pole of order greater than unity yields output errors with infinite standard deviation! Thus, only transformations such as those of the KKR, which involve order-1 poles, are interesting and physically sensible.

In order to explore KKR error transformations adequately, it is worthwhile to consider a number of different cases. In the work below, we shall explore the following: (a) standard KKR and transformed KKR equations; (b) proportional and additive errors (as in Ref. [6]); (c) endpoint and midpoint integration routines; (d) equal step size, geometric spacing, and smoothed geometric step size. These different choices are further discussed in Section 2. As the reader will see, detailed analysis of these different choices confirms the results of the Monte Carlo study in Ref. [6] in most cases. In addition, however, we derive, for the first time, expressions for the distribution of the output noise for each of the above transformation possibilities, as well as its standard deviation.

2. The variance of random errors transformed by the KKR using numerical integration

In the present work, emphasis is on the effects of errors in data, and extrapolation error is avoided by dealing only with a continuous function defined over the entire $0 \le \omega \le \infty$ range or its Eqs. (3) and (4) equivalent, $0 \le y \le 1$. Since the actual numerical integrations required for KK transformation were carried out in Ref. [6] using open integration formulas, we study here primarily procedures of this type described in Ref. [14]. In general terms, the procedures may be described as

$$\int_{x_1}^{x_N} g(x)\,\mathrm{d}x \simeq h[c_1 g_1 + \ldots + c_N g_N] \tag{7}$$

for endpoint formulas or as

$$\int_{x_1}^{x_N} g(x)\,\mathrm{d}x \simeq h[c_1 g_{3/2} + \ldots c_{N-1} g_{N-1/2}] \tag{8}$$

for midpint formulas. Here $h = x_{k+1} - x_k$, $g_k = g(x_k)$, $g_{k+1/2} = g(x_k + h/2)$, $k = 1,2,\ldots$, and the weight coefficients c_k take a variety of values. For example, for $c_1 = \ldots = c_N = 1$ Eq. (8) describes *the extended midpoint rule*, an open analog of the trapezoidal rule, with an accuracy of integration of $O(N^{-2})$. If in Eq. (7) one sets $c_1 = 0$, $c_2 = \frac{23}{12}$, $c_3 = \frac{7}{12}$, $c_4 = \ldots = c_{N-3} = 1$, $c_{N-2} = \frac{7}{12}$, $c_{N-1} = \frac{23}{12}$, $c_N = 0$, the accuracy for a smooth enough g is $O(N^{-4})$ (see Ref. [14], p. 109). This second example suggests, as well as most of the algorithms described in Ref. [14], a rather complicated notation $c_k = c_k(N)$ because several last members of the sequence $\{c_k, k = 1,\ldots,N\}$ actually depend on N. In non-confusing cases we shall omit the argument N. From this point on we shall assume that the weights $c_k(N)$ stabilize as N becomes large: for any fixed number k, beginning with some large N, $c_k(N) = c_k$, so that they do not depend on N. This is valid for all the algorithms described in Ref. [14].

Most of results presented in Ref. [6] were obtained with the midpoint routine applied to the transformed KKR, that is to the integrals in Eqs. (3) and (4), but Gauss–Legendre and Gauss–Chebyshev quadrature routines were also used.

Further, for data extending over a wide range of frequencies, say several decades or more, such as the responses considered in Ref. [6], it is generally more efficient to use geometric intervals in x_k, for example, $x_{k+1}/x_k = [x_N/x_1]^{1/(N-1)}$. We study such extensions of the algorithms as well; see Table 1 and the discussion below. To do so, we use the more general notation $w_k = x_{k+1} - x_k$, so that $w_k = h$ in Eqs. (7) and (8).

Now we discuss how to introduce random errors into quadrature formulas for Eqs. (3) and (4). In accordance with Eqs. (1) and (2) and Eqs. (5) and (6), since points ωy and ω / y are different, the random errors should be introduced separately

Table 1
Numerical integration parameters

	Endpoints y_k	w_k	Midpoints y_k
Geometric	$e^{-(N-k+1)h}$	$e^{-(N-k)h} - e^{-(N-k+1)h}$	$e^{-(N-k+1/2)h}$
Equal	$1-(N-k+1)h$	h	$1-(N-k+1/2)h$
Geometric smoothed	$e^{-(N-k+1)h}$	$\frac{1}{2}[e^{-(N-k-1)h} - e^{-(N-k+1)h}]$ for $k = 2,\ldots,N-1$, $w_1 = e^{-(N-1)h} - e^{-Nh}$, $w_N = 1 - e^{-h}$	$e^{-(N-k+1/2)h}$

and statistically independently into both of the terms of differences in square brackets. We denote by ϵ_{1k}, ϵ_{2k} independent identically distributed random variables with zero means and variances equal to σ^2. That is

$$Z'_e(\omega)-Z'_e(\infty)\equiv\frac{2}{\pi\omega}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[\omega y_k Z''(\omega y_k)-(\omega/y_k)Z''(\omega/y_k)]}{1-y_k^2}$$
$$+\frac{2\beta}{\pi\omega}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[\omega y_k Z''(\omega y_k)\epsilon_{1k}-(\omega/y_k)Z''(\omega/y_k)\epsilon_{2k}]}{1-y_k^2}$$
$$+\frac{2(1-\beta)}{\pi\omega}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[\omega y_k\epsilon_{1k}-(\omega/y_k)\epsilon_{2k}]}{1-y_k^2} \tag{9}$$

and

$$Z''_e(\omega)\equiv-\frac{2}{\pi}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[Z'(\omega y_k)-Z'(\omega/y_k)]}{1-y_k^2}-\frac{2\beta}{\pi}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[Z'(\omega y_k)\epsilon_{1k}-Z'(\omega/y_k)\epsilon_{2k}]}{1-y_k^2}$$
$$-\frac{2(1-\beta)}{\pi}\sum_{k=1}^{N}\frac{c_{N-k+1}w_k[\epsilon_{1k}-\epsilon_{2k}]}{1-y_k^2} \tag{10}$$

Here and in the following, since there is a pole at $y=1$, this point is of most interest, and we number the integration coefficients c_k from right to left. We study the stochastic errors of the numerical integration in two cases: $\beta=1$, that is proportional random errors, and $\beta=0$, that is additive random errors.

Now we specify other parameters of numerical integration; they are the points y_k and steps w_k. Table 1 summarizes all the cases we study. For the equal spaced points y_k the parameter h should be chosen to be $1/N$. For geometric points it should be chosen to be much larger as one approaches the right end of the interval (0,1), as discussed later. But everywhere it is required that in the limits $h\to 0$, $N\to\infty$, Nh tends to a constant.

The direct numerical integration of the KKR in standard form, Eqs. (1) and (2), is possible also. Here we consider the most natural specification of the y_k and the w_k. Namely, we consider geometrically spaced points

$$x_{k+1}/x_k=[x_N/x_1]^{1/(N-1)}$$

that is, $x_k=x_1\,e^{hk}$ and $h=\log(x_{k+1}/x_k)$. We suppose that ω is one of the points x_k. After the substitutions of variables to obtain the reduced transformations of Eqs. (3) and (4), it is easy to see that this numerical integration procedure corresponds to the case of geometric points described by Table 1, with a slight variation of the points and interval lengths around the ω point. Thus, considering the cases from Table 1, we simultaneously consider some direct numerical integrations of Eqs. (1) and (2).

3. Summary of results

3.1. Stabilization of the output standard deviations

Since the differences in square brackets in Eqs. (9) and (10) are statistically independent either for $\beta=1$ or $\beta=0$, we can apply the general evaluations given in Appendix A.

3.1.1. Geometric, geometric smoothed and equal intervals using endpoints (see Table 1)

In these cases, by Eq. (A-8), the limits of the output standard deviations are equal to

$$\pi^{-1}\sigma\sqrt{2}|Z'(\omega)|\sqrt{\sum_{l=1}^{\infty}c_l^2 l^{-2}}\ \text{and}\ \pi^{-1}\sigma\sqrt{2}|Z''(\omega)|\sqrt{\sum_{l=1}^{\infty}c_l^2 l^{-2}} \tag{11}$$

for proportional random errors and

$$\pi^{-1}\sigma\sqrt{2}\sqrt{\sum_{l=1}^{\infty}c_l^2 l^{-2}} \tag{12}$$

for additive random errors.

Note that for $c_l\equiv 1$, the sum is the Riemann zeta-function of 2, that is $\pi^2/6$ (see Ref. [15], eq. 0.233), and the limits equal $\sigma|Z'(\omega)|/\sqrt{3}$ and $\sigma|Z''(\omega)|/\sqrt{3}$ for the proportional errors and $\sigma/\sqrt{3}$ for the additive errors. Thus, for this situation the output errors are actually smaller than the input errors.

3.1.2. Geometric, geometric smoothed, and equal intervals using midpoints (see Table 1)

By Eq. (A-10), the limiting standard deviations equal

$$\frac{2\sqrt{2}\,\sigma|Z'(\omega)|}{\pi}\sqrt{\sum_{l=1}^{\infty}\frac{c_l^2}{(2l-1)^2}} \text{ and } \frac{2\sqrt{2}\,\sigma|Z''(\omega)|}{\pi}\sqrt{\sum_{l=1}^{\infty}\frac{c_l^2}{(2l-1)^2}} \tag{13}$$

for proportional errors, and

$$2\pi^{-1}\sqrt{2}\,\sigma\sqrt{\sum_{l=1}^{\infty}c_l^2(2l-1)^{-2}} \tag{14}$$

for additive errors.

For $c_l \equiv 1$ the sum is equal to $\pi^2/8$ (see Ref. [15], eq. 0.324), and the limits thus equal $\sigma|Z'(\omega)|$ and $\sigma|Z''(\omega)|$ in the proportional errors case and just σ in the additive errors case. Thus, the results obtained in Ref. [6] by the Monte Carlo approach are verified by the present analytic study.

3.2. Stabilization of the output error distributions

The hypothesis of stabilization (the existence of the limit as $h \to 0$) of the output error distributions was suggested in Ref. [6]. Now, using Eqs. (A-13) and (A-14) for the endpoints cases, and Eq. (A-15) for the midpoints cases, we summarize the results as follows.

In the endpoint cases, the distributions of the output errors tend to the distributions of the random variables

$$K\sum_{l=1}^{\infty}c_l(\epsilon_{1l}-\epsilon_{2l})l^{-1}$$

where K is either $2\sigma|Z'(\omega)|/\pi$ and $2\sigma|Z''(\omega)|/\pi$ for proportional errors or $2\sigma/\pi$ for additive errors.

In the midpoint cases, the distributions of the output errors tend to the distributions of the random variables

$$K\sum_{l=1}^{\infty}c_l(\epsilon_{1l}-\epsilon_{2l})(2l-1)^{-1}$$

where K takes the same respective values as above.

Particularly for the extended midpoint rule, the stabilization is around the distribution of the random variables

$$K\sum_{l=1}^{\infty}(\epsilon_{1l}-\epsilon_{2l})(2l-1)^{-1}$$

The results hold for both equal and geometric integrating intervals.

The present analysis, together with the corresponding evaluations in Appendix A, show that for Eqs. (3) and (4) output stochastic errors are generated in a small neighborhood of the pole at $y = 1$. To reduce the stochastic error, one should space the points of integration thinner around the pole. Consider an example. Let us use the midpoint rule, $c_1 = \ldots = c_N = 1$, with a modification so that the integration points are $y_k = 1-(N-k+1/2)h$ for $k = m, m+1, \ldots, N$, so that the intervals lengths are equal to $w_1 = mh$, $w_2 = w_3 = \ldots = h$. It is easy to see that the limit of stochastic error is then proportional to

$$X = \sqrt{\sum_{l=m}^{\infty}(2l-1)^{-2}}$$

with the same coefficients as in Eqs. (13) and (14). With $m = 2,3,4$, we find decreases in the output-error standard deviation by 0.48, 0.35, and 0.29 times respectively. On using the trapezoidal integration rule, $X \simeq \sqrt{m}/(2m-1)$, this leads to the close approximations 0.47, 0.35 and 0.29.

Notice that the numerical integration error will have, for fixed m, the same order as N becomes large. To investigate both kinds of error carefully, it is necessary to optimize the density of the y_k around the pole. In other words, one must choose between optimizing the procedure for either small integration error (many points near the pole) or small transformed noise error (few points near the pole).

4. Note added proof

Since this paper was accepted, one which deals in part with the same subject has recently appeared (M Durbha, M.E. Orazem and L.H. Garcia-Rubio, *J. Electrochem. Soc.*, *144* (1997) 48). One of the present authors (JRM) provided a long, detailed review in April 1996 of the original version of this paper, and recommended that the MS be accepted only after extensive revision because its analytical proof of KKR noise-transformation was incorrect. However, the Orazem work prompted the present authors to subsequently develop a completely different and correct proof. The present paper is the result, and a preprint of it (identical to the present accepted version) was sent to Dr. Orazem in June 1996, along with the identification of JRM as one of the reviewers of the original version.

The new proof in the revised Orazem paper, which was received by the journal near the end of September 1996 but not seen by the present authors until its publication, is quite different from their original one and is less general and more approximate than that presented here. It is noteworthy that, in the Orazem paper, neither are the referees thanked for their comments and suggestions nor is the early receipt of, or existence of, the present work acknowledged. Nevertheless, on comparing the final version of the Orazem paper with this one, it is obvious that their proof involves many crucial elements first introduced in the present work. In particular: (a) the basic idea of proving the equality of the input and output error variances using the rules and constraints of numerical integration; (b) the essence of their Eqs. (13), (14), (15), (27), and (28); and (c) the recognition that output stochastic errors are generated in the immediate neighborhood of the pole in the integrand. Their proof does not contain specific definitions of the placement of their integration points, y_m, or of their weights, yet the present work shows that the transformed variances depend sensitively on such details as the specific form of the numerical integration procedure. Thus their proof is both derivative and sufficiently incomplete to preclude its application to actual numerical integration without further information. The Orazem work introduces a Taylor expansion, stated to be valid when the error variance is continuous at the pole position. However, such an expansion requires the existence of two-times differentiability (with a continuous second derivative), conditions not mentioned. Further, all the proofs in the present work require no differentiability conditions, are valid for non-constant but continuous variance, and do not require the assumption of a particular error structure.

Finally, the Orazem paper contains incorrect and inappropriate criticisms of the original JRM Monte-Carlo work (Ref. [6] herein), ones absent from their original version, but perhaps related to the recommendation in the JRM review that their actual references to the earlier work were misleading and misplaced and that the results of the earlier work should be recognized as the justification for developing an analytic proof of the noise transformation relations. After reading the above discussion of the history of these matters, the reader will not be surprised to learn that this recommendation was not implemented.

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Appendix A. Numerical integration around a pole in the presence of random errors

We study the sum which generalizes all introduced stochastic errors:

$$\Xi = \sum_{k=1}^{N} \frac{c_{N-k+1} w_k f(y_k) \epsilon_k}{1 - y_k^2} \tag{A-1}$$

where f is a continuous function on [0,1], and the ϵ_k are independent identically distributed random variables with $\mathbf{E}[\epsilon_k] \equiv 0$, $\mathbf{var}[\epsilon_k] \equiv \sigma^2$.

A.1. Stabilization of the output standara deviations

We begin with the calculation of the limit of the variance of Ξ as $h \to 0$ and $N \to \infty$. Since the ϵ_k are independent, the variance of the sum is equal to

$$\mathbf{var}[\Xi] = \sigma^2 \sum_{k=1}^{N} \frac{f(y_k)^2 c_{N-k+1}^2 w_k^2}{\left(1 - y_k^2\right)^2} \tag{A-2}$$

Take a sufficiently small $\delta > 0$ specified below and split the sum in Eq. (A-2) into two parts:

$$\mathrm{var}[\Xi] = \sigma^2 \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2 f(y_k)^2}{(1-y_k^2)^2} + \sigma^2 \sum_{k:y_k < 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2 f(y_k)^2}{(1-y_k^2)^2} \quad \text{(A-3)}$$

First we establish that the second term plays a negligible role in generating the limiting output standard deviation errors. Moreover, since this term is the variance of

$$\Xi_2 = \sum_{k:y_k < 1-\delta}^{N} \frac{c_{N-k+1} w_k f(y_k) \epsilon_k}{1-y_k^2} \quad \text{(A-4)}$$

we thus establish as well that this latter sum plays a negligible role in producing the limiting output error distributions. Using the inequality

$$w_k^2 \le w_k \max_k [w_k]$$

and the trivial identity $\sum_{k=1}^{K} w_k = y_N - y_1$, we obtain that for any positive δ

$$\mathrm{var}[\Xi_2] = \sigma^2 \sum_{k:y_k < 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2 f(y_k)^2}{(1-y_k^2)^2} \le C^2 \sigma^2 \delta^{-2} \max_k [w_k] \max_{y \in [0,1]} f(y)^2 \to 0 \quad \text{(A-5)}$$

as $h \to 0$, uniformly in N, with C bounding the coefficients c_k.

Consider the first term in Eq. (A-3), which is the variance of

$$\Xi_1 = \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1} w_k f(y_k) \epsilon_k}{1-y_k^2} \quad \text{(A-6)}$$

Given $\kappa > 0$ but arbitrarily small, choose the δ so small that

$$|f(y)^2 - f(1)^2| \le \kappa \text{ for any } y \ge 1-\delta$$

Then

$$\sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2 f(y_k)^2}{(1-y_k^2)^2} \begin{array}{l} \le \left(f(1)^2 + \kappa\right) \displaystyle\sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2}{(1-y_k^2)^2} \\ \ge \left(f(1)^2 - \kappa\right) \displaystyle\sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2}{(1-y_k^2)^2} \end{array} \quad \text{(A-7)}$$

Now for all cases described in Table 1 we shall calculate the limits of the last sum and show that they do not depend on δ. Since $\kappa > 0$ was arbitrary, it follows that one will obtain the same limit as that of the sum in Eq. (A-2).

A.1.1. Geometric, geometric smoothed, and equal intervals using endpoints, see Table 1

We have for the geometric cases

$$\sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2}{(1-y_k^2)^2} = \sum_{k:e^{-(N-k+1)h} \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 e^{-2(N-k+1)h}(e^h-1)^2}{[1-e^{-2(N-k)h}]^2} = \sum_{l=1}^{l:e^{-lh} \ge 1-\delta} \frac{c_l^2 e^{-2lh}(e^h-1)^2}{(1-e^{-2lh})^2}$$

where $l = N-k+1$.

Since for small enough δ and for all l such that $e^{-lh} \ge 1-\delta$

$$1 - e^{-2lh} \ge lh/2 \text{ and } 1 - e^{-h} \le h$$

the summand in the last sum is at most $4C^2/l^2$, where C is the constant bounding the c_l. Therefore this sum is bounded by the converging series

$$\sum_{l=1}^{\infty} 4C^2 l^{-2}$$

Further, as $h \to 0$, for any fixed l, the limit of the lth summand equals $c_l^2/(4l^2)$. Thus, by the Lebesgue–Fatou Lemma (Ref. [16], p. 17)

$$\lim_{h\to 0} \mathrm{var}[\Xi] = \sigma^2 f(1)^2 \lim_{h\to 0} \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}^2 w_k^2}{(1-y_k^2)^2} = \frac{\sigma^2 f(1)^2}{4} \sum_{l=1}^{\infty} \frac{c_l^2}{l^2} \quad \text{(A-8)}$$

In the important case $c_l \equiv 1$, we have from the Riemann zeta function of 2

$$\lim_{h\to 0} \mathrm{var}[\Xi] = \sigma^2 f(1)^2 \pi^2/24 \tag{A-9}$$

(see Ref. [15], eq. 0.233).

For equally spaced points, calculations are easier, and the result is still the same. For the smoothed cases, all analysis and evaluations are still the same. Only the first term of the final sums is different, but it is easy to show that the limit is the same.

A.1.2. Geometric, geometric smoothed and equal intervals using midpoints, see Table 1

By the reason given in the previous paragraph, we need to consider only the non-smoothed case. Again, differences with the previous cases are minimal. The bounding series is

$$\sum_{l=1}^{\infty} C^2(2l-1)^{-2}$$

and the limit as $h \to 0$ of a summand in the final sum is equal to $c_l^2/(2l-1)^2$, so again using Lebesgue–Fatou Lemma

$$\lim_{h\to 0} \mathrm{var}[\Xi] = \sigma^2 f(1)^2 \sum_{l=1}^{\infty} c_l^2(2l-1)^{-2} \tag{A-10}$$

In the important case $c_l \equiv 1$, we have

$$\lim_{h\to 0} \mathrm{var}[\Xi] = \sigma^2 f(1)^2 \pi^2/8 \tag{A-11}$$

(see Ref. [15], eq. 0.324).

A.2. Stabilization of the output error distributions

By virtue of Eq. (A-5) we need only study the sum Ξ_1, (Eq. (A-6)). Setting in Eq. (A-7) $f_1(y) \equiv f(y) - f(1)$, we get

$$\mathrm{var}\left[\Xi_1 - f(1) \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}(N) w_k \epsilon_k}{1-y_k^2}\right] \le \kappa \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}(N)^2 w_k^2}{\left(1-y_k^2\right)^2} \tag{A-12}$$

and by Section A.1.2 the multiplier of κ is bounded for all considered cases. We are thus now in a position to calculate a limit of the second term under the **var** sign. It follows from Eq. (A-12) that if the limit does exist and it does not depend on δ, the sum Σ tends in quadratic mean to the same limit.

A.2.1. Endpoint cases

Consider the sum

$$\xi_1 = (f(1)/4) \sum_{l=1}^{\infty} c_l \epsilon_l l^{-1} \tag{A-13}$$

which obviously converges in square mean, so the random variable ξ_1 is well defined. Since the ξ_k are independent, we easily calculate that

$$\begin{aligned}
&\mathrm{var}\left[f(1) \sum_{k:y_k \ge 1-\delta}^{N} \frac{c_{N-k+1}(N) w_k \epsilon_k}{1-y_k^2} - \frac{f(1)}{4} \sum_{k:e^{-(N-k+1)h} \ge 1-\delta}^{N} \frac{c_{N-k+1}\epsilon_k}{N-k+1}\right] \\
&= \mathrm{var}\left[f(1) \sum_{l=1}^{l:y_{N-l+1} \ge 1-\delta} \frac{c_l(N) w_{N-l+1} \epsilon_{N-l+1}}{1-y_{N-l+1}^2} - \frac{f(1)}{4} \sum_{l=1}^{l:e^{-lh} \ge 1-\delta} \frac{c_l \epsilon_{N-l+1}}{l}\right] \\
&= f(1)^2 \sum_{l=1}^{l:e^{-lh} \ge 1-\delta} \left[\frac{c_l(N) w_{N-l+1}}{1-y_{N-l+1}^2} - \frac{c_l}{4l}\right]^2
\end{aligned} \tag{A-14}$$

By the assumptions on the $c_l(N)$ for a constant C_1 and for all N

$$\sum_{1}^{N} [c_l(N) - c_l]^2 \le C_1$$

Using this inequality, it is straightforward to show that the sum in the right-hand part of Eq. (A-14) tends to zero as $h \to 0$ Since the variables ϵ_l and ϵ_{N-l+1} have the same distribution, the distribution of the output error stabilizes to the distribution of ξ_1.

In the smoothed case we again find stabilization to the same distribution of ξ_1.

A.2.2. Midpoint cases

Following the same reasoning, we get the stabilization of the output error to the distribution of the random variable ξ_2, given by

$$\xi_2 = f(1) \sum_1^{\infty} c_l \epsilon_l (2l-1)^{-1} \tag{A-15}$$

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