

Error in the Propagation of Error Formula

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In a paper by Park and Himmelblau (1980), the authors draw the attention to the fact that the widely used formula for error propagation may give systematic errors in the estimation of the mean and the variance of a variable. Their formula for the propagation of errors is a simple truncation of a standard Taylor series, which has a validity as long as the approximation by the truncation is adequate for the application in question.

The phenomenon studied by these authors is mainly due to the curvature of the nonlinear relationship between the input and the response of an experiment and a mathematical model. The authors claim that the formula is in error, but the main reason for the discrepancy they observe, is that the propagation of error formula is used beyond its proper validity of approximation. The purpose of this short note is to draw some general conclusions as to the range of validity of the basic Taylor series approximation and to give some practical and more general advice to extend this range. For simplicity, a basic single-input, single-output system is considered.

Let the input variable to a nonlinear mathematical model be u and the output be x . Consider first a static situation where the model is given by the general nonlinear relationship:

$$x = f(u). \quad (1)$$

Now, let the probability distribution of the input u be a true Gaussian distribution, with constant mean and variance. The so-called propagation of error formula will only use the first two terms in a Taylor series expansion of $f(u)$, and calculate the expected value of x accordingly:

$$E(x) = f[E(u)]; \quad x \cong f[E(u)] + \frac{df}{du} [u - E(u)] \quad (2)$$

and consequently the expected variance in x ,

$$E\{[x - E(x)]^2\} = \left(\frac{df}{du}\right)^2 E\{[u - E(u)]^2\} \quad (3)$$

where the derivative of f is calculated at the expected value of u .

It is well known that a first-order Taylor series expansion is not a valid approximation if the standard deviation in the input variable is large and the second- and higher-order derivatives with respect to u are significant (Asbjornsen, 1975). Therefore, in those cases a simple and efficient improvement of the mean and variance estimation may be obtained by a simple extension of the Taylor series (Asbjornsen, 1975; Marketos, 1975).

Let a general Taylor series apply to the region $[E(u) - \Delta u, E(u) + \Delta u]$. Then:

$$x = f[E(u)] + \sum_{i=1}^{\infty} \frac{d^i f}{du^i} \frac{1}{i!} [u - E(u)]^i. \quad (4)$$

Since the probability distribution in u is assumed to be Gaussian, all uneven moments in $[u - E(u)]$ will vanish. The expected value of x may therefore be written:

$$E(x) = f[E(u)] + \sum_{i=1}^{\infty} \frac{d^{2i} f}{du^{2i}} \frac{1}{(2i)!} E\{[u - E(u)]^{2i}\}. \quad (5)$$

Similarly, the expected variance in x may be written as:

$$\begin{aligned} E\{[x - E(x)]^2\} &= E\left\{\left(\sum_{i=1}^{\infty} \frac{d^i f}{du^i} \frac{1}{i!} [u - E(u)]^i\right)^2\right\} \\ &= E\left\{\sum_{i=1}^{\infty} \frac{d^{2i} f}{du^{2i}} \frac{1}{(2i)!} E\{[u - E(u)]^{2i}\}\right\} \\ &= \sum_{k=1}^{\infty} \sum_{i=1}^{2k-1} \frac{d^i f}{du^i} \frac{d^{2k-i} f}{du^{2k-i}} \frac{1}{i!} \frac{1}{(2k-i)!} E\{[u - E(u)]^{2k}\} \\ &\quad - \sum_{k=2}^{\infty} \sum_{i=1}^{k-1} \frac{d^{2i} f}{du^{2i}} \frac{d^{2(k-i)} f}{du^{2(k-i)}} \frac{1}{(2i)!} \frac{1}{(2(k-i))!} \\ &\quad E\{[u - E(u)]^{2i}\} E\{[u - E(u)]^{2(k-i)}\} \end{aligned} \quad (6)$$

which again makes use of the fact that odd moments of $[u - E(u)]$ are zero.

This general analysis makes it possible to develop a more appropriate set of estimates of the expected values of the mean and the variance of x , once the mean and variance of the original Gaussian variable u are given. Furthermore, Eqs. 5 and 6 make it possible to judge what terms in the Taylor series approximation would be appropriate to include. The number of terms required will depend on the convergence properties of the Taylor series.

Take as an example the chemical equilibrium constant for the gaseous ammonia reaction (Hougen et al., 1959), the case reported by Park and Himmelblau:

$$K = \exp(-\Delta F_o/RT). \quad (7)$$

Select a temperature of 1,000 K. Assume the formula of Hougen et al. for ΔF_o to apply. Then a temperature of 1,000 K gives a

value of $\Delta F_o = 61,588 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$, which is assumed to be the expected value of ΔF_o . Now, assume that the standard deviation in the estimate of ΔF_o is given by:

$$\text{var}(u) = \text{var}(\Delta F_o)/[E(\Delta F_o)]^2 = 0.01 \quad (8)$$

Then, Eq. 5 gives the series expansion of the expected value of the equilibrium constant:

$$E(K) = \exp[-E(\Delta F_o)/RT] \left[1 + \frac{1}{2}y^2 + \frac{1}{8}y^4 + \frac{1}{48}y^6 + \dots \right] \quad (9)$$

where $y = [E(\Delta F_o)/RT]\sigma_{\Delta F_o}$. Inserting $\Delta F_o/RT = 7.4$, the series and the expected value of the equilibrium constant becomes:

$$E(K) = \exp[-E(\Delta F_o)/RT] [1 + 0.2738 + 0.03748 + 0.00342 + \dots] \cong 1.315 \exp[-E(\Delta F_o)/RT] \quad (10)$$

which is close to identical to the results obtained by Park and Himmelblau in their Figure 2. The analysis above shows that terms after the sixth derivative may be truncated, due to the convergence nature of the series.

The estimated variance in x is more complicated to evaluate, as more terms are envisaged necessary. The variance is more sensitive to higher-order terms in the Taylor series expansion, and one would expect the convergence for the series approximation to the variance to exhibit slower convergence than the series for the mean value. Taking the same values and definitions as above, the expression for the expected variance is:

$$E\{[K - E(K)]^2\} = y^2 + \frac{3}{2}y^4 + \frac{7}{6}y^6 + \frac{247}{576}y^8 + \dots \quad (11)$$

This agrees indeed with the point made above that the convergence is slower, as now the eighth derivative in the Taylor series has to be included. Inserting the value for y above gives the terms in the series:

$$E(\sigma_K) = y[1 + 0.8303 + 0.3498 + 0.0704 + \dots]^{1/2} \cong y[1.5] \quad (12)$$

which again agrees very well with the results obtained by Park and Himmelblau in their Figure 3.

If one now considers a similar system, but with the temperature as a stochastic input, this is a much more common situation in chemical engineering. The question now is how serious the systematic errors are in derived properties such as reaction rates or vapor pressure. The integrals for the expected values derived by Park and Himmelblau are no longer analytically solvable, since the exponent in the Arrhenius-type expression now is a nonlinear function of the independent stochastic variable, the temperature.

Take as an example, a vapor pressure thermometer shown schematically in Figure 1. The heat transfer and the heat balance of the thermometer act as a low-pass filter which will attenuate fluctuations in the temperature outside the thermometer. If the outside temperature has superimposed Gaussian noise, then the interior temperature will also have a low-pass filtered Gaussian noise.

The relationship between the interior and the exterior temperatures may be written:

$$\left(V_l \rho_l C_{pl} + V_g \rho_g \lambda \frac{\partial \rho_g}{\partial T} \right) \frac{dT}{dt} = AU(T_o - T) \quad (13)$$

when the heat capacity of the wall is neglected and the liquid phase is assumed to be perfectly mixed and always in equilib-

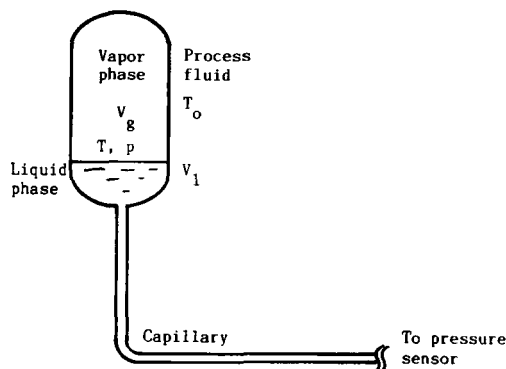


Figure 1. A simple vapor pressure thermometer.

rium with the vapor. The partial derivative of the density is therefore taken along the saturation curve of the vapor.

The low-pass filter in Eq. 13 may be expressed as an autoregressive model in discrete space:

$$T(k) = \alpha T(k-1) + (1-\alpha)T_o(k) \quad (14)$$

where the filter constant α is a function of the sampling time Δt and the thermometer time constant τ :

$$\tau = (V_l \rho_l C_{pl} + V_g \rho_g \lambda \partial \rho_g / \partial T) / A \cdot U \quad (15)$$

$$\alpha = \exp(-\Delta t / \tau)$$

For random fluctuations in T_o , the mean values in T_o and T are the same, since:

$$E(T) = \alpha E(T) + (1-\alpha)E(T_o) \quad (16)$$

as long as the stochastic variable T_o is stationary. However, the variance in T will be different, due to the effect of the low-pass filter:

$$\text{var}(T) = \frac{\alpha}{2-\alpha} \left[1 + 2 \sum_{i=1}^{\infty} (1-\alpha)^i r(i) \right] \quad (17)$$

where $r(i)$ is the autocorrelation coefficient of the exterior temperature fluctuations, given by:

$$r(i) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=1}^N T_o(k)T_o(k-i) / \text{var}(T_o) \quad (18)$$

Only when $\alpha = 1$ ($\tau = 0$), are the variances equal. If $\alpha = 0$ ($\tau = \infty$), then the variance of the interior temperature is zero.

The vapor pressure p in the thermometer is usually taken as a measure of the temperature T , and the relationship between p and T (which is practically instantaneous) is of a nonlinear nature (the Clausius-Clapeyron model):

$$p = k \exp(-\lambda/RT) = f(T). \quad (19)$$

Hence, the analysis of mean and variance for a general nonlinear relationship will apply here, as shown above. One will now get slightly modified derivatives:

$$\frac{df}{dT} = \kappa f[E(T)]/E(T); \quad \kappa = [-\lambda/RE(T)]$$

$$\frac{d^2 f}{dT^2} = \kappa(\kappa - 2) f[E(T)]/[E(T)]^2 \quad (20)$$

$$\frac{d^3 f}{dT^3} = [2(\kappa - 1) + \kappa^2(\kappa - 2)] f[E(T)]/[E(T)]^3$$

and further for higher derivatives. However, if one considers the example below, the third derivative will be sufficient.

Let the outside temperature have uncorrelated white noise (all $r(i)$ terms are zero). Assume a thermometer time constant of 10 s and a sampling interval of 2 s. Assume that the variance of the exterior temperature is 1,600 K² ($\sigma_{T_o} = 40$ K), then the variance of the temperature of the liquid inside the thermometer is:

$$\sigma_T^2 = \frac{\alpha}{2 - \alpha} \sigma_{T_o}^2 = 160 \text{ K}^2 \quad (21)$$

Assume further, that $E(T) = E(T_o) = 400$ K and that $\lambda/RT = 10$. Then the relationship between the expected pressure and the expected temperature of the thermometer is:

$$E(P) = f[E(T)] [1.04] \quad (22)$$

Similarly, by the use of the general expression Eq. 6 and the derivatives in Eq. 20, the relationship between the expected variance in the pressure and the temperature is:

$$E\{[P - E(P)]^2\} = \left(\frac{df}{dT}\right)^2 E\{[T - E(T)]^2\} [1.13] \quad (23)$$

The reverse estimation is now possible, where one is interested in the estimation of the real mean value and variance of the process. Then:

$$E(T_o) = E(T) \equiv f^{-1}[E(P)/1.04] \quad (24)$$

$$\sigma_{T_o} \approx \frac{2 - \alpha}{\alpha} \sigma_T = \left|\frac{df}{dT}\right|^{-1} \frac{1}{1.13} \frac{2 - \alpha}{\alpha} \sigma_P \quad (25)$$

The problem of nonlinear characteristics and their effects on the estimation of mean and variance is a very significant one in instrumentation (Asbjornsen, 1975), in particular in mass or energy flow metering, where even small systematic errors in the mean value estimate may have very large effects financially, due to the large production, consumption, or export quantities. The general analysis shown here, even extended to multiple inputs, helps in the evaluation of such errors.

In an attempt to illustrate some of the phenomena arising from nonlinear characteristics, the example above elucidates a number of points:

1. The Arrhenius type of nonlinear relationship has very large higher-order derivatives with respect to temperature or activation energy, which are the main reasons for the phenomenon described by Park and Himmelblau. An analysis based on an extended Taylor series expansion will be more generally applicable as shown, and normally fully adequate. A judgment can then be made at which term the Taylor series approximation could be truncated.

2. The most likely variable to exhibit random fluctuations in the Arrhenius expression is the temperature. The variance in this variable is usually small enough to justify a second- or third-order Taylor series approximation for the mean and the variance. Therefore, the practical implications of Parks and Himmelblau's rigorous analysis are not so pronounced as their article may seem to indicate. Furthermore, it is not applicable to temperature fluctuations.

3. In most practical cases, the primary stochastic variable is exposed to a linear low-pass filter before it enters the nonlinear expression. Hence, the filter reduces the variance and the problem. The effects of systematic errors caused by a neglect of higher-order derivatives in the Taylor series approximation

are reduced accordingly. In computer control, the inverse transformation $u = f^{-1}(x)$ may compensate for the nonlinearity, whereby the problem disappears completely.

4. When the nonlinearity has an inflection point (in the Arrhenius case $\lambda/RT = 2$ for temperature), the systematic error in the mean value shifts sign. The systematic error in the estimates of both mean and variance has a minimum in the inflection point, which is intuitively obvious.

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NOTATION

A	= heat transfer surface
C_{pi}	= specific heat capacity of liquid
$E(\cdot)$	= expectation operator
$f(\cdot)$	= nonlinear function
ΔF_o	= Gibbs free energy
i	= counting index
k	= preexponential factor
K	= equilibrium constant
p	= pressure
$r(i)$	= correlation coefficient
R	= gas constant
Δt	= sampling time
T	= temperature
u	= input variable
U	= heat transfer coefficient
V_g	= gas volume (constant)
V_l	= liquid volume (constant)
x	= output variable
y	= dimensionless variable, explained in the text

Greek Letters

α	= filter factor
κ	= dimensionless variable, explained in the text
λ	= latent heat of evaporation
ρ_g	= gas density
ρ_l	= liquid density
τ	= time constant, explained in the text

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