Investigating Entropic Concepts in Control Charts Based on Shewhart's Ideas

João Teotônio Manzi[a], José Jaílson Nicácio[a], Heleno Bispo[a*]

[a] *Federal University of Campina Grande, Department of Chemical Engineering, Campina Grande - PB, Brasil*
[*] *heleno.bispo@eq.ufcg.edu.br*

ABSTRACT

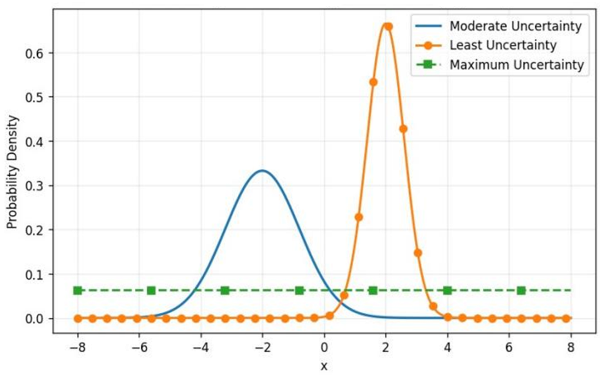
This article addresses entropic concepts and the analysis of dispersion or variance applied to process monitoring, both measures of uncertainty, although they are treated by different metrics. Entropy is discussed in more depth as it deals with irreversibility, while variance refers to dispersion around a central tendency index. Consequently, an analysis from an entropic point of view can offer a more realistic and in-depth perspective. This paper uses the concept of maximum entropy, which corresponds to the maximum uncertainty or irreversibility generated by the system. This strategy was compared to that provided by SPC (Statistical Process Control), more specifically through Shewhart control charts. From a process monitoring perspective, analytical results show that both strategies generate equivalent results, since Shewhart's choice for the limits of the control charts is based on the analysis of different probability distributions within the $\pm 3\sigma$ limits, including the normal distribution. The distribution which maximizes the entropy under the fixed expected value and variance is also the normal distribution. Therefore, the conclusion that can be drawn is that both procedures generate equivalent results with advantages for the control chart strategy due to simplicity, and because it is easy for, mainly, practitioners to understand, and also because of the analysis of the results per se.

Keywords: Entropy; Control Charts; Statistical Process Control; Process Monitoring.

1 Introduction

The concept of entropy plays a fundamental role in all branches of science and, simultaneously, arouses fascination and fear. In closed systems, it has been shown that entropy always increases and this occurs in our universe which is considered closed. Thus, the task to involve entropy in all scientific approaches seems natural. It is also natural to think of entropy as a measure of dispersion that occurs in systems in nature. Low entropy, little dispersion. Fundamentally, entropy means the number of micro-configurations of a macro-state.

Figure 1: An overview of uncertainty from the perspective of entropy



Ebrahimi et al., 1999, stated that there is no universal relationship between entropy and variance. However, even if there is no formal relationship such a relationship can be verified either from a theoretical or practical point of view, as will be demonstrated. Figure 1 provides a brief overview.

Regarding Shewhart Control Charts, it should be pointed out that they are not tied to a normal distribution and that the ± 3σ limits were established when various distributions, those that occur most frequently in practice, were considered for analysis. In fact, the result is that all the distributions analyzed presented the highest number of results within these limits. This means that control charts are not based on models, and this gives them a universal character.

Some authors consider the Gaussian distribution of such variables as essential. However, this is not the basis on which control charts are built. We prefer to think that control charts do not depend on any distribution, especially because in 1929 countries were preparing for war. Since they were without computers, it would have been impossible to manually establish the process distribution in a timely manner. Thus, Shewhart's idea of generalizing the application of control charts to any distribution seems remarkable. The fact that the ± 3σ limits represent 99.73% of all possible outcomes considering a Gaussian distribution is a weak reason. It is worth highlighting that among the distributions analyzed, those that occur frequently in practice, is the normal distribution, and it is therefore natural to refer to Shewart's idea.

Still on the topic of control charts, it should be noted that there is a close association between these charts and hypothesis testing. Therefore, there is the necessary requirement to establish the parameters of the reference distribution (μ, σ^2) considered as reference estimators due to the lack of knowledge of the true distribution. These estimates can be made by:

- Substantial experience in the activity;
- Some well-adjusted model of the process;
- At the negotiating table between the buyer/seller.

In this paper, the entropy concept is treated from the perspective of information theory and statistical mechanics (Jaynes, 1957a, 1957b). It is simple and easy to show that for an isothermal, isobaric mixing process of gases, the mixing entropy is given by:

$$\Delta S = -nR\sum_i N_i \ln N_i \quad \text{or} \quad \frac{\Delta S}{nR} = -\sum_i N_i \ln N_i \tag{1}$$

where N_i denotes the mole fraction of each component. It is noted that the molar fraction has the properties of probability, being in general associated with the distribution of the probability of occurrence. Therefore, the following Equation can be expressed as the Shannon Entropy:

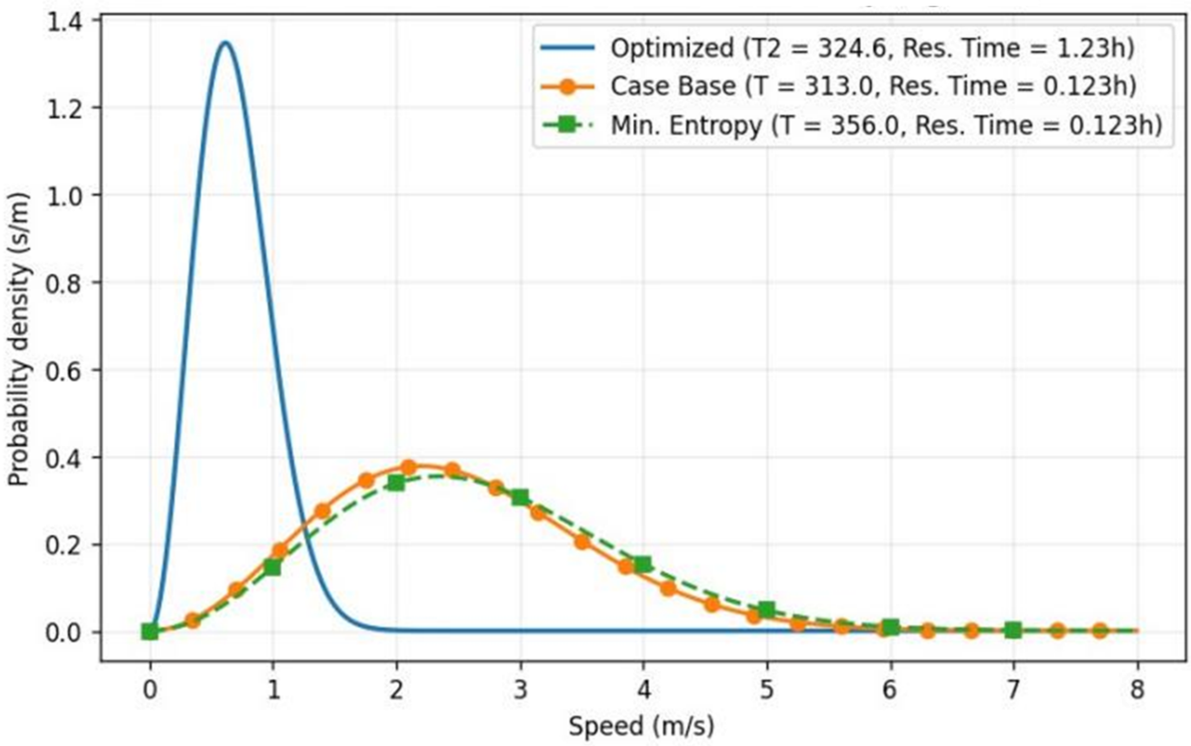
$$H(X) = H[p(x)] = -\sum_i p(x_i) \ln p(x_i) \tag{2}$$

Since the distribution parameters (μ, σ^2) have been defined beforehand, it is not difficult to show that the maximum entropy distribution, for such fixed parameters, has a normal distribution. The essentially aim of this paper is to reach the requirements of those who use such procedures in factories, then the text needs to be clear and simple, in order to provide a complete understanding. For these reasons, the use of complex mathematical formulations has been minimized.

2 Theoretical Background

First, we present some results of minimizing the entropy production rate of producing propylene glycol and its effects on the Maxwell-Boltzmann distribution of energy (Bispo et al., 2013). The corresponding behavior is illustrated in Figure 2, shown below, that presents the Maxwell-Boltzmann distribution before and after minimizing the entropy generation rate. As can be seen after minimization, the normal curve is tighter, exhibiting a reduced variance, i.e., the consequence of lower entropy is a reduction in variance. Thus, from a practical point of view, there is indeed a relationship between entropy and variance.

Figure 2: Maxwell-Boltzmann Energy Distribution before and after the Entropy Minimization Procedure



Consider a continuous, real, centered random variable X with a probability density function $f(x)$. Then, Entropy (Shannon Entropy) can be defined as:

$$H(X) = -E\{\ln[f_X(x)]\} = -\int_{-\infty}^{+\infty} f_X(x)\ln[f_X(x)]\,dx \tag{3}$$

Since entropy is a random variable it must be well-defined and represented by its probability distribution. Therefore, the question now is to determine which distribution or distributions maximize entropy, since our interest is in maximizing entropy.

To answer this question, the following classical problem must be posed: Maximize $H(x)$ over all distributions $f_X(x)$ that satisfy the following conditions

- $f_X(x) \geq 0$ - where the equality is valid only outside the support S of the random variable;
- $\int f_X(x)\,dx = 1$ - over the support S, (property of probability distribution);
- $\int f_X(x) f_i(x)\,dx = k_i$, for $1 \leq i \leq k$, where k_i is the i-th centered moment and $f_i(x)$ is a function that forces $f_X(x)$ to respect the constraints.

This problem can be solved with the classical use of Lagrange multipliers. Let us consider two cases to be dealt with: those in which the expected value and variance are fixed and those with fixed support. First case or constraint 1, the one in which the expected value and the variance are fixed. The Lagrangian function, L, that uses the aforementioned constraints can be written as:

$$L(f_X(x)) = -\int f_X(x)\ln[f_X(x)]\,dx + \beta_0\left(\int f_X(x)\,dx - 1\right) + \sum_{i=1}^{k}\beta_i\left(\int\int f_X(x)dx f_i(x)\,dx = k_i\right) \tag{4}$$

where $\beta_0, \ldots, \beta_i$ are Lagrange multipliers.

Within the scope of our interest, it is not difficult to deduce the following equation:

$$f_X(x) = \exp\left[\beta_0 + \beta_1 x + \beta_2 x^2 - 1\right] \tag{5}$$

This generates a system of equations that is established based on the expected value, variance, and properties of the distribution, and the solution of which will determine the values of the Lagrange multipliers. By substituting these Lagrange multiplier values into the function $f_X(x)$, the following result can be obtained:

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-k_1}{\sigma}\right)^2\right] \tag{6}$$

Clearly a normal distribution. Therefore, considering the fixed expected value and variance, the probability distribution that maximizes entropy is the normal distribution.

Second case or constraint 2, the one dealing with fixed support ($S = [a, b]$).
Taking the derivative of the Lagrangian function with respect to $f_X(x)$ and setting it equal to zero,

$$\frac{\partial L}{\partial f_X(x)} = 0 \tag{7}$$

where the parameters are chosen to satisfy the constraints, the following equation can be obtained:

$$\ln\left[f_X(x)\right] = \beta_0 - 1 \quad \text{or} \quad f_X(x) = e^{\beta_0 - 1} \tag{8}$$

Therefore, taking into account constraint 2, the result for $f_X(x)$ is:

$$f_X(x) = \frac{1}{b-a}, \quad a \le x \le b \tag{9}$$

From this, it can be concluded that, under the constraint of the fixed support, the distribution of maximum entropy is a uniform distribution.

Both results can be obtained by using the MaxEnt principle as an optimization problem. On the other hand, even taking into account that control charts are not based on a normal distribution, but also considering that the normal distribution is an integral part of Shewhart's strategy for choosing the ± 3σ limits, then from the point of view of control charts, given their properties, the use of the normal distribution can therefore be considered natural. Since the expected value and variance of true distributions are usually unknown, the fundamental step lies in determining the estimated values for these parameters, which should be unbiased. The control charts are well established and operate well, although some controversies and contradictions may exist. However, despite this, authors have shown that these charts generally work well, and when applied in practice, they have been shown to be of great value (MacGregor, 1988; Wheeler, 1995; Wu et al., 2019).

All analytical strategies based on Shewhart's ideas are well established and reported in the literature, whether using classic Shewhart control charts or more specific control charts such as the Exponentially Weighted Moving Average (EWMA) or the Cumulative Sum (Das & Zhou, 2015; MacGregor, 1988; Wheeler, 1995; Wu et al., 2019).

3 Results and Discussion

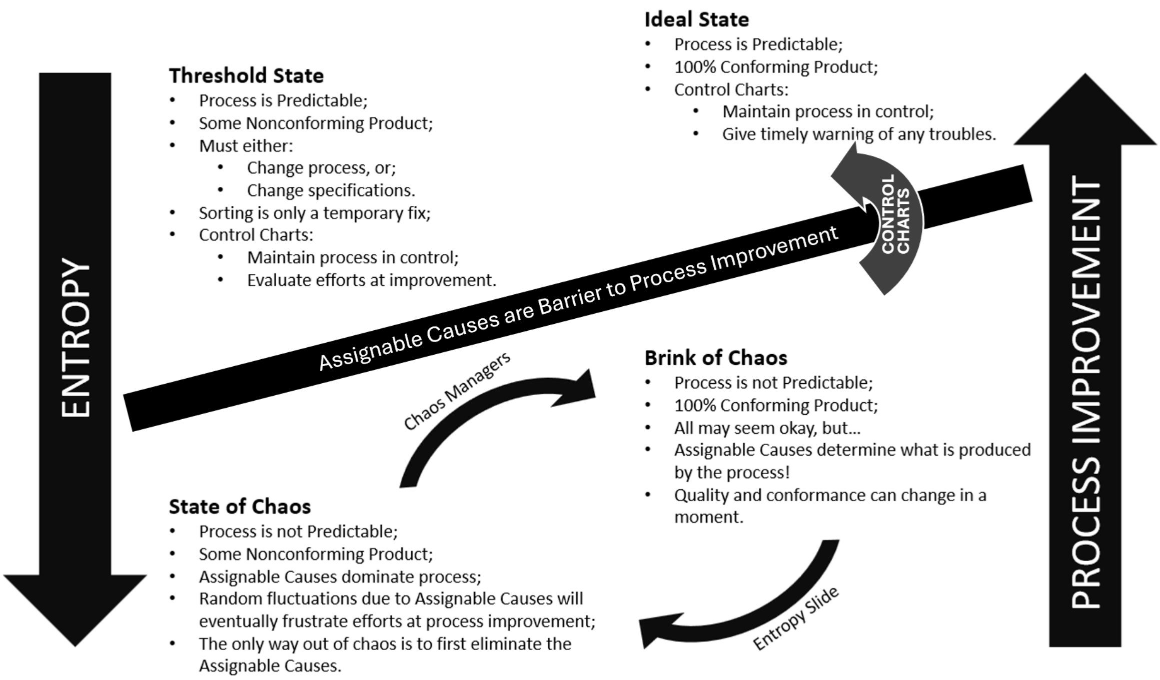
First, let us differentiate between chaotic and entropic processes: a chaotic process is a deterministic and non-linear system, highly sensitive to initial conditions, and as such, it leads to unpredictable and extremely different results, even if it is due to, for example, a very small difference in the initial conditions (the "butterfly effect"), i.e., it is a dynamic system with an unpredictable evolution.

While an entropic process is a random process which moves the system from ordered to disordered states (from a common point of view) and which measures the static, disordered state. Entropy deals with the micro-configurations of a macro-state. Although chaotic processes are technically deterministic, being unpredictable, entropic processes are unpredictable on a microscopic scale, but predictable on a macroscopic level and this proves to be fundamental in identifying and removing assignable causes from the system. In those chaotic processes, as Shewhart said, it is a waste of time to try to identify them, because there is no dominant cause-and-effect relationship.

Entropy, as previously mentioned, is always continuously present to disrupt the system, and therefore every process will move towards the state of maximum perturbation. To overcome the effects of entropy, the process needs to be continuously and systematically monitoring the system. In the previous section, it was shown that, depending on the constraints, the maximum entropy distribution can be a Gaussian distribution or a Uniform distribution. For some systems, restriction 1 mentioned earlier is a better fit, while, for others, restriction 2 is more appropriate. It is important to note that, in systems where restriction 2 is valid, the maximum entropy is distributed according to a uniform distribution, and since there are no driving forces (gradients) between the system and the environment or potential differences, no energy can be extracted, thus reaching the dead state. Hence, remembering that nature is driven by differences in potentials, this consideration may explain the death of living systems.

Therefore, our interest falls on those where restriction 1 is applied. Since the distribution of maximum entropy for the fixed condition of expected value and variance is a Gaussian distribution, then such a process can be included in the analysis established by Shewhart for control charts, for which the $\pm 3\sigma$ limits play a fundamental role, aggregated with the sensitization rules. It is important to emphasize that, when designing a control chart, the so-called characteristic operating curves of the process in question must be developed to establish the strategies involved in operating the chart; otherwise, the operation will be done blindly. So, the effects of entropy and the role of control charts are outlined in the figure below.

Figure 3: The effects of entropy and the role of the control chart (Wheeler, 1995 - Advanced Topics in Statistical Process Control)



4 Conclusions

The basic characteristics and properties of entropy and its influence on systems in general were presented, explored and discussed, demonstrating that, for fixed expected values and variance, it exhibits a Gaussian distribution for maximum values. A brief discussion of chaotic and entropic processes was also presented to delineate the space for discussion. Two cases in which the distribution of maximum entropy was considered in the discussion, that resulting in the Gaussian distribution and that resulting in the Uniform distribution. The case of interest for the analysis in this article falls under that of the Gaussian distribution. Several important characteristics of control charts were also mentioned, such as the origin of the control limits at $\pm 3\sigma$, which proves to be independent of any distribution. Nevertheless, since the Gaussian distribution was part of the analysis for choosing the control limits, its use is natural when necessary to determine some parameters. Furthermore, results on the Maxwell-Boltzmann energy distribution were presented before and after the entropic minimization procedure, clearly showing a correlation between entropy and variance. Based on the results presented, the conclusion that can be drawn for process monitoring and analysis is that, in principle, given that both strategies are supported by the Gaussian distribution, the procedure that uses the entropic concepts generates equivalent results to those obtained by control charts. However, the control chart is easier to understand, operate, and analyze, is sufficiently robust, and has a low operating cost, which makes it a suitable strategy for process monitoring and analysis.

Referências

Bispo, H., Silva, N., Brito, R., & Manzi, J. (2013). On the equivalence between the minimum entropy generation rate and the maximum conversion rate for a reactive system. *Energy Conversion and Management*, *76*, 26–31.

Das, D., & Zhou, S. (2015). Statistical process monitoring based on maximum entropy density approximation and level set principle. *IIE Transactions*, *47*, 215–229.

Ebrahimi, N., Maasoumi, E., & Soofi, E. (1999). Ordering univariate distributions by entropy and variance. *Journal of Econometrics*, *90*, 317–336.

Jaynes, E. T. (1957a). Information theory and statistical mechanics. *Physical Review*, *106*, 620–630.

Jaynes, E. T. (1957b). Information theory and statistical mechanics ii. *Physical Review*, *108*, 171–190.

MacGregor, J. F. (1988). On-line statistical process control [October]. *Chemical Engineering Progress*, 21–31.

Wheeler, D. J. (1995). *Advanced topics in statistical process control: The power of shewhart's charts*. SPC Press.

Wu, P., Guo, L., Duan, Y., Zhou, W., & He, G. (2019). Control loop performance monitoring based on weighted permutation entropy and control charts. *The Canadian Journal of Chemical Engineering*, *97*, 1488–1495.