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THE VARIOGRAM AND ESTIMATION ERROR IN CONNECTION WITH THE ASSESSMENT OF CONTINUOUS STREAMS

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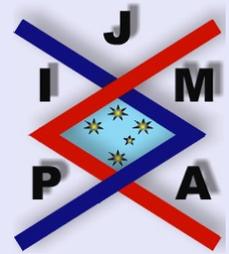
Abstract

The paper briefly reviews the concept of the variogram and the estimation error variance in connection with certain estimation problems. This is done in the context of their development in mineralogy. The results are then placed in the context of the assessment of flowing product streams that are continuous space, continuous time stochastic processes. The work in this area, to date, is then briefly reviewed and extended. The paper addresses both practical and theoretical issues, the latter being focused on bounding both the estimation error and the estimation error variance. For this, use is made of variations of Ostrowski's inequality and Holder-type variograms.

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Key words: Variograms, Estimation Error, Estimation Error Variance, Kriging, Hölder-type Variograms, Ostrowski's Inequality, Continuous Space, Continuous Time Stochastic Process.

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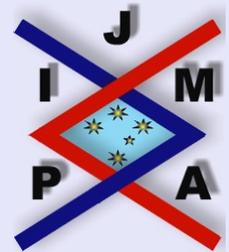
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1. The Concept of the Variogram

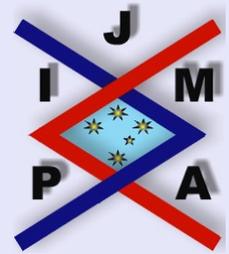
The variogram has a history that is associated with mining and mineralogy. It is a concept that is also extensively used in meteorology and ecology. In such applications it is largely concerned with spatial variability, for example, in geological core samples.

As is common with many statistical methods, an important issue in practical applications involving variograms is the fitting of a theoretical model to a set of collected data. In proceeding with this there are a few time honoured, empirically useful models that are fitted, governed mainly by particular characteristics of the collected data, through previous experience with handling data of a similar nature and, of course, by a desire for simplicity in the chosen model.

Suppose a mineral core sample of a particular strata is taken that returns n sample values collected a distance, d , apart, d is generally a consequence of the instrument being used to collect the core sample. The characteristic of focus for these samples is assessed and denoted by $x(x_i)$ where x_i is the displacement value of the i th sample from a given reference point. A measure of the variability of the characteristic across the data points is afforded by the sample variogram,

$$V(kd) = \frac{1}{2(n-k)} \sum_{i=1}^{n-k} [x(x_i) - x(x_{i+k})]^2.$$

This is the average of the variances of the data, $x(x_i)$ taken in pairs, when value



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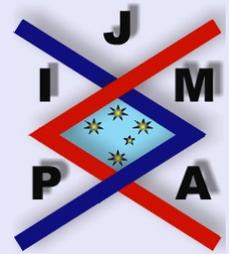
pairs are kd apart, $k = 1, 2, 3, \dots, n - 1$, i.e.

$$V(kd) = \frac{1}{n - k} \left(\left(x(x_1) - \frac{x(x_1) + x(x_{1+k})}{2} \right)^2 + \left(x(x_{1+k}) - \frac{x(x_1) + x(x_{1+k})}{2} \right)^2 + \dots + \left(x(x_{n-k}) - \frac{x(x_{n-k}) + x(x_n)}{2} \right)^2 + \left(x(x_n) - \frac{x(x_{n-k}) + x(x_n)}{2} \right)^2 \right).$$

The estimation problem that then remains, in order to obtain a more complete picture of the mineral deposit, is to assess the value of the characteristic at points for which there are no sample data. Often data are collected from different directions so as to better obtain an appreciation of the deposit over its three dimensions. Once the data collection is complete one or more sample variograms can be plotted for values of $k = 1, 2, \dots, n - 1$ to assist in fitting a suitable theoretical model, from which estimates of the characteristic at points where data is unavailable may be obtained. Any particular variogram model fitted to a single dimension is assumed to comprehensively describe the deposit variability,

$$V(u) = \frac{1}{2} E [X(s + u) - X(s)]^2,$$

where $E(\cdot)$ denotes the usual statistical expectation.



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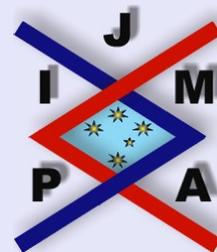
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Writing it in this fashion implies a degree of stationarity in the model in that the variogram value is assumed to depend only on the distance of points apart and not on their specific locations. It is also possible to consider fitting different models for different directions / dimensions.

Fitting a particular model to the data, of course, requires not only a suitable choice of model but also estimation of any model parameters. Only when this is complete can it be used for estimation of $x(\cdot)$ at unobserved points.

The standard method of estimation of $x(\cdot)$ is termed Kriging after the South African mining engineer, D. G. Krige and it is a method that was developed fully by Matheron [10] in the nineteen fifties. Kriging is essentially interpolation and the most common, ordinary Kriging, uses a weighted linear combination of the observed data of the characteristic of the sample to provide estimates. These weights are determined using the model variogram that has been fitted and so the appropriateness and fit of the model are critical. Ordinary Kriging, and there are numerous refinements, produces best linear unbiased estimators. Once estimation is made possible the quality of it is established by reference to an entity called the estimation error variance – the long term average of the squared deviation of the true value from its estimate.



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2. Common Variogram Models used in Mineralogy

The common variogram models used in mineralogy, the linear, exponential, spherical and the Gaussian models are defined as follows, (u is assumed positive):

The linear variogram (positive slope), $V(u) = A + Bu$.

The linear variogram (horizontal), $V(u) = A$.

The exponential variogram, $V(u) = A + B(1 - e^{-\frac{u}{C}})$.

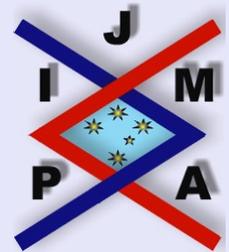
The spherical variogram,

$$\begin{aligned} V(u) &= A + B \left(1.5 \left(\frac{u}{C} \right) - 0.5 \left(\frac{u}{C} \right)^3 \right), & u < C \\ &= A + B, & u > C. \end{aligned}$$

The Gaussian variogram,

$$\begin{aligned} V(u) &= A + B \left(1 - e^{-\left(\frac{u}{C}\right)^2} \right), & u < C \\ &= A + B, & u > C. \end{aligned}$$

A key characteristic feature of the latter three models is the expectation that the variance will increase with distance apart of the values for a while and will then level off at a certain distance beyond which values tend to behave independently. In the geostatistical literature it is common to refer to the distance from the reference point at which the variance starts to level off as the ‘range’ and the level itself as the ‘sill’. Whilst the variance at distance zero apart is unobservable, if the back fitted model does not pass through $(0, V(0))$ the non-zero value is referred to as the ‘nugget effect’.



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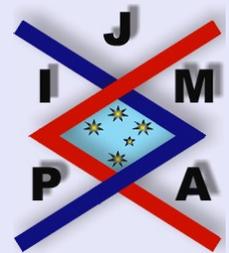
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Besides applications in mineralogy, meteorology and ecology the variogram as a concept has been used in connection with time series analysis where effectively the spatial variable u in, $V(u) = \frac{1}{2}E [X(s+u) - X(s)]^2$ is perceived, instead, as a time variable and it is in this context that it is used here. It should be noted that for applications of the type previously mentioned, we are essentially assuming that $V(u)$ is a continuous function of the continuous spatial variable u . We will also, in the context of u being time, consider a process that varies in a continuous manner over continuous time. (Use of the variogram is not, of course, restricted to this case).

Gy [9] made extensive use of the variogram in dealing with problems associated with the sampling of particulate materials. For his purposes he perceived the variogram as consisting of a number of additive components each having its own particular characteristics. In this context he discussed both periodic and non-periodic features in the variograms of these components, noting also the frequent usefulness of the parabolic variogram. Claiming a broad spectrum of practical experience, he commented (which additionally provides us with a defence for our pre-occupation with stationary variograms), “...For a given material under routine conditions, the variability expressed by one or several variograms may be regarded as a relatively time stable characteristic.”

In [6] Box and Jenkins introduced and analysed a number of discrete time stochastic models including among these, the stationary autoregressive and the non-stationary autoregressive integrated moving average models. Examination of the variograms of these, albeit in discrete time, show them to resemble the shape of one or other of the models commonly used in mineralogy and listed



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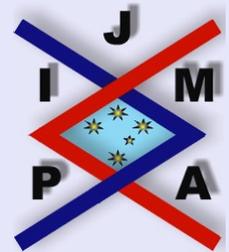
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earlier. If we talk in terms of stationary and non-stationary processes it is observed that a stationary process will typically be one that has a variogram with a sill effect and a non-stationary process one with a continually increasing variogram.



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3. Kriging

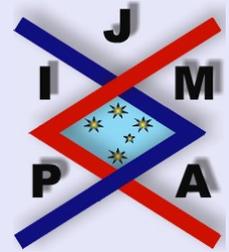
As mentioned previously, Kriging is a method for estimation of the value of a spatial variable at a particular location using observations of the spatial variable at a number of other locations. The result depends on the ‘distance’ of the points of observation from the point in question and on the variogram of the spatial variable.

Rather than consider, for example, a variable space of two or more physical dimensions we here adapt the method so that the ‘distance’ variable represents time and use it for estimation and in the general study of the behaviour of a single dimension continuous space stochastic variable in continuous time. We can then contemplate estimation of the variable at points unobserved using observed values at particular times. We can do this retrospectively in time or as a method of forecasting.

The method of Kriging has numerous variations, we, however, consider the simplest, sometimes referred to as, ‘ordinary Kriging’. In the following, results are obtained for a univariate stochastic process.

Let $X(t)$ be a continuous space stochastic process in continuous time for which we have observations at n discrete instants, $X(t_1), X(t_2), \dots, X(t_n)$. We wish to estimate the variable value at a time, t_0 which is unobserved, we designate this estimate by, $\hat{X}(t_0)$. The estimation is performed by using a linear combination of the observed values, $\hat{X}(t_0) = \sum_{i=1}^n \lambda_i X(t_i)$ and stipulating estimation criteria that determine each λ_i uniquely. These are,

- (i) that the estimation of $X(t_0)$ by $\hat{X}(t_0)$ is unbiased (i.e. $E(\hat{X}(t_0)) = X(t_0)$) and



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- (ii) that the estimation error variance, $EEV, E[(\hat{X}(t_0) - X(t_0))^2]$ is minimized. (We subsequently focus attention on the estimation error variance in a broader sense in relation to studying the behaviour of a continuous product stream.)

Condition (i) is guaranteed provided that $\sum_{i=1}^n \lambda_i = 1$.

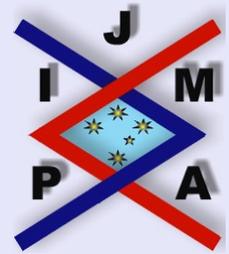
Now,

$$\begin{aligned} EEV &= E[(\hat{X}(t_0) - X(t_0))^2] \\ &= E \left[\left(\sum_{i=1}^n \lambda_i X(t_i) - X(t_0) \right)^2 \right] \\ &= E[(\lambda_1(X(t_1) - X(t_0)) + \lambda_2(X(t_2) - X(t_0)) + \dots \\ &\quad + \lambda_n(X(t_n) - X(t_0)))^2] \\ &= E \left[\sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j (X(t_i) - X(t_0))(X(t_j) - X(t_0)) \right]. \end{aligned}$$

This can further be expressed as,

$$\begin{aligned} \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n E[\lambda_i \lambda_j \{ -(X(t_i) - X(t_j))^2 + (X(t_i) - X(t_0))^2 \\ + (X(t_0) - X(t_j))^2 - (X(t_0) - X(t_0))^2 \}] \end{aligned}$$

which can be written in terms of the process variogram, $V(h) = \frac{1}{2}E[(X(t) - X(t+h))^2]$ as,



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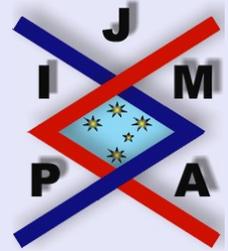


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$$EEV = -V(t_0 - t_0) - \sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j V(t_i - t_j) + 2 \sum_{i=1}^n \lambda_i V(t_i - t_0)$$

on which we now need to perform a minimization. Expressing this in matrix vector form and denoting the vector, $(X(t_1), X(t_2), \dots, X(t_n))$ by X^T and $(\lambda_1, \lambda_2, \dots, \lambda_n)$ by λ^T we have $X(t_0) = \lambda^T X$. The requirement for the sum of the lambdas to be 1 is captured by the vector equation $\lambda^T \mathbf{1} = 1$, $\mathbf{1}$ being a column vector of n ones. It is now possible to express the EEV in matrix vector form as,

$$EEV = -V(0) - \lambda^T V \lambda + 2 \lambda^T V_0$$

where V is the n by n matrix,

$$V = \begin{pmatrix} V(t_1 - t_1) & V(t_1 - t_2) & \cdots & V(t_1 - t_n) \\ V(t_2 - t_1) & V(t_2 - t_2) & \cdots & V(t_2 - t_n) \\ \vdots & \vdots & \vdots & \vdots \\ V(t_n - t_1) & V(t_n - t_2) & \cdots & V(t_n - t_n) \end{pmatrix}$$

and

$$V_0 = \begin{pmatrix} V(t_1 - t_0) \\ V(t_2 - t_0) \\ \vdots \\ V(t_n - t_0) \end{pmatrix}.$$

We need then to find the vector, λ^T that minimizes $EEV = -V(0) - \lambda^T V \lambda + 2\lambda^T V_0$ subject to the constraint, $\lambda^T \mathbf{1} = 1$. Using a Lagrange multiplier this constrained minimization problem can be converted into the unconstrained problem of minimizing,

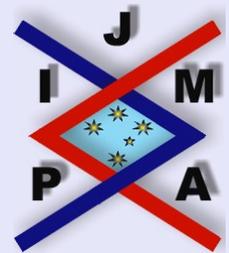
$$E = -V(0) - \lambda^T V \lambda + 2\lambda^T V_0 - 2l(\lambda^T \mathbf{1} - 1)$$

Differentiating, setting the derivatives to 0 and solving the equations gives,

$$l = \frac{\mathbf{1}^T V^{-1} V_0 - 1}{\mathbf{1}^T V^{-1} \mathbf{1}} \quad \text{and} \quad \lambda = V^{-1}(V_0 - l\mathbf{1}).$$

As $V(0) = 0$ we have that the $EEV = -\lambda^T V \lambda + 2\lambda^T V_0$ which returns a minimum value of $\lambda^T(V_0 + l\mathbf{1})$ since the equation, $\lambda = V^{-1}(V_0 - l\mathbf{1})$ implies $V\lambda = V_0 - l\mathbf{1}$.

We note the fact that both the values of the constants in the linear combination and the expression for the estimation error variance itself are functions of the variogram.



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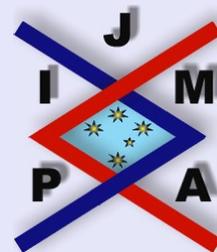
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4. The Estimation Error and Industrial Processes

Efforts to monitor and control manufacturing processes, with the ultimate aim of ensuring the quality of manufactured product, frequently focus on information obtained from regular product samples. From this data, decisions need to be made on whether or not process adjustments are warranted. For processes producing discrete product items the notion of control frequently revolves around the assumption that data from successive samples are uncorrelated and that process stability is the norm from which control decisions can sensibly be made. In such discrete manufacturing environments, individual items are of significance and statistical tools to aid in control frequently appear in simple graphical form. Various so-called capability indices are regularly used to connect process behaviour with product requirements and even to help assess the overall quality of batches of final manufactured product.

There are, however, many industrial processes, manufacturing and otherwise, that do not model so simply, particularly is this the case for products that appear as continuous flows as for example in the chemical manufacture of liquids, gases and granular materials. Data from successive samples are frequently correlated and processes seldom meet the stable norm assumption of discrete manufacturing. Furthermore, in such environments the quality of product has no 'individual' meaning in the sense that it does for discrete manufactured items. These and other differences are demanding of a different approach to monitoring, control and product assessment. For these there is considerable potential for use of the process variogram in the context of the industrial operation being a continuous space, continuous time stochastic process. The need for continual product assessment over time in the form of quality estimation from



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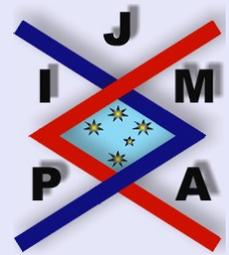
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sample data means that the estimation error variance (EEV) assumes considerable importance. As has been illustrated in a 'micro' sense in the technique of Kriging, it is true also in a more 'macro' sense that the process variogram and the estimation error variance are integrally linked. We will see this in connection with the estimation of the product flow mean using a single sample value or, more commonly, using the mean of a number of sample values.



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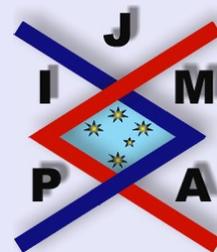
5. Continuous Flow Streams

In [11], Saunders, Robinson et al introduced a method for assessing the quality of a product that is delivered by means of a continuous, constant flow stream. The technique involves estimating the flow variogram for 'short' time intervals and then estimating the flow mean of a particular product characteristic over a given time using the average of a number of collected sample values. They obtained an expression for the estimation error variance of this procedure in terms of the short lag process variogram, making special note of the case where the short lag variogram is linear.

Barnett et al, in [4], considered calculation of the estimation error variance under circumstances where the stream flow rate varies and where the variogram is either linear or negative exponential in form. The objective of their paper was to focus on the most appropriate location at which to sample within an interval of pre-determined length, so as to minimize the estimation error variance. The authors also placed the results of their paper in the context of a manufacturing environment. Subsequent papers by Barnett and Dragomir et al [2], [1], [3], [5] examined inequalities associated with the estimation error and the estimation error variance. This current paper brings these and a number of other results together.

The paper by Saunders, Robinson et al [11] was set in the context of assessment, the authors did not deal with the issues of monitoring and control, which are additional requirements in the manufacturing environment. Once their technique and variations of it are considered in the context of manufacturing, however, the issue of monitoring and control naturally arises.

There are many situations where a continuous stream is the mode of product



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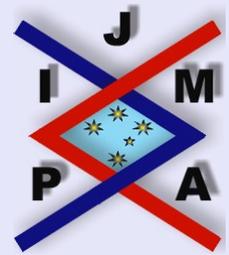
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delivery and where stream assessment alone is required. The example of ore delivery, cited in [11], is a case in point. There are, however, other situations of delivery where, in addition to assessment, there is also the opportunity to exert a limited degree of control on the stream, for example, by varying the flow rate or re-directing flows. In this respect the extension to consideration of non-constant flows, introduced by Barnett et al in [4] is relevant. Further still, there is the manufacturing environment where on-going assessment, monitoring and control are all required and, at the same time, there are a number of control opportunities available.

Continuous production streams are generally flows of product consisting of liquids, gases or fine granular material. Such streams are found commonly in the chemical processing industries where a range of chemicals and materials undergo a chain of manufacturing stages before becoming important additives in other manufactured products.

An essential characteristic of a continuous stream is that the ‘quality’ or general status of the product being conveyed is determined, not in an individual way, but in bulk sense.

In the chemical processing environment, typically, ultimate product status (quality or key characteristic) is established in batch mode (e.g in a tanker, truck or silo) dependent upon the manner in which the product is being stored or transported. In the absence of continuous monitoring, this status is generally estimated on the basis of periodic grab samples of product taken either during the final stages of production and/or when it is decanted from large containers into smaller ones for the purpose of transportation and delivery. There are many practical issues that surround the collection and analysis of this data and these all impinge on the reliability of the declared status of the product to the



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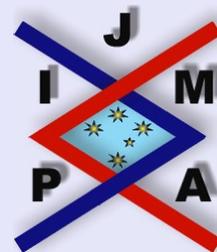
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customer.

Whilst it is sample characteristics that are used to assess the product status, there is a distinction here that needs to be made between assessing production of discrete items as opposed to assessing product that is processed, manufactured or conveyed in a continuous stream. For the former, it is rarely appropriate that the product be assessed in an average sense but rather assessment focuses on individual manufactured items. For continuous streams, however, there is no clearly identifiable 'item', so the norm is to evaluate and assess product on the basis of an average of sample values.



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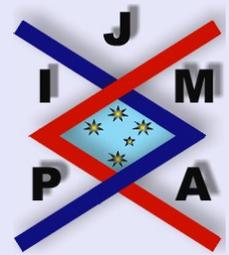
6. Assessment, Compensation and Control

There is a difference between sampling for the quality assessment of a production batch and sampling for process control purposes.

In quality assessment, we use data in a historic context in order to summarize a batch of final product. For monitoring and control purposes we use the sampled data, as it becomes available, to make process adjustments, as necessary, in an attempt to preserve the stipulated status level of the batch of which the sample is a part. We can reason that this could also be done on the basis of a forecast provided we can develop a reliable forecasting method.

If we talk in the context of a manufacturing environment, the issue of control stems from individual characteristics of the process as well as from occasional events that we aim to avoid in the future if possible. Many processes are partially and some even completely, computer controlled (engineering control). Under these circumstances a range of automatic controllers regulate various parameters of the process using well established algorithms that attempt to ‘force’ the product to be manufactured as required. Inherent in the operation of such controllers is the notion of taking compensatory action as a consequence of the critical characteristic variable not being precisely the intended value at its most recent observation. To do this effectively we need to know the general pattern of behaviour of the characteristic in question and to know the nature of any delays in changes to it caused by changes to production parameters.

In an attempt to stabilize a process or make it stationary with respect to one or more critical characteristics, deficiencies in the values of input variables are frequently compensated for using automatic controllers. Some of these variables may be dependent on one another and so to provide a stationary process



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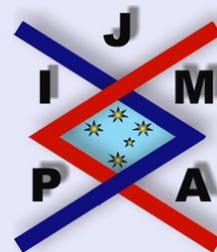
their interdependence needs to be understood.

Statistical process control, on the other hand, is geared to keep in harmony with an existing stable state and to adjust only when this stability appears to have been lost. Inherent in this approach is the assumption that stability is a viable norm but, unfortunately, this is not always the case. Compensatory control, on the other hand, is involved with constantly adjusting process inputs in order to achieve its objective.

In the absence of a completely computer controlled environment, data has to be deliberately and continually sought in order to facilitate manual judgments on how to further adjust the process in order to achieve desired goals. This may well be done on the basis of conformance to a particular statistical model, this is only of merit, however, if such conformance is consistent with delivering the specifications that have been imposed on the product.

Whilst it is now standard procedure to control many basic process variables by computer controllers, it is not unusual to find that other process factors prevent the achievement of stability, even with these computer controllers operable and correctly tuned. Hence, even under computer control we are frequently faced with a non-stationary process through which an ‘orderly’ product has to be manufactured.

Whilst computer controllers can be easily used to regulate such things as temperatures and flow rates, they can seldom, for example, deal with issues related directly to the ‘quality’ of raw materials unless the precise consequences of a drop in raw material quality is known. Many industries use as their basic raw materials, substances that are the by-products of other industries, which are materials that other industries do not want and consequently do not control. In many instances, such by-products are lacking in consistency or uni-



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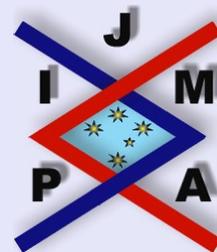
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formity, which makes their further processing in a predictable manner, at best difficult. It is, therefore, not uncommon for there to be computer control yet non-stationarity in the 'controlled' process. Add to this the fact that many industrial processes are essentially chemical reactions and whilst there is generally a considerable body of knowledge about the reaction itself and what makes it function, a full knowledge of 'what makes the process tick', is often lacking. As one industrial chemist put it, there is an element of 'witchcraft' in most processes. These are aspects of the process that are not fully understood and frequently interfere with predictability. Under such circumstances the challenge is to effectively further adjust the process in order to deliver an acceptable product.

It should also be noted that in certain non-manufacturing environments the need for stream monitoring occurs in situations where there is absolutely no way of controlling the input variables. It has become common for sewage treatment facilities, for example, to exploit the treatment process to collect methane gas and to use this to generate power to off-set the costs of treating the raw sewage further. Controlling the production of methane gas requires knowledge of incoming loadings and certain characteristics of the effluent. Few sewage treatment facilities, however, can control the volumes or the nature of their inputs.

The reality is that there is the need for stream assessment in situations where there is total computer control, partial computer control or where no computer control exists or is even possible. There is also the need for 'control' of products that are delivered by a process that is still non-stationary despite a certain degree of compensatory action having been taken.



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7. The Basic Model

In what follows, both from the perspective of assessment and control, we assume that the status of a continuous production stream at a time, t , after commencement, is denoted by $X(t)$. This status will generally refer to some critical characteristic of the product that directly affects its utility and consequently its quality. Grab samples of the product are required and are taken at times, t_1, t_2, \dots, t_n and, following testing or measurement, provide data values, $X(t_1), X(t_2), X(t_3), \dots, X(t_n)$. If we now suppose that the actual mean status of the stream over a time interval $[0, T]$, assuming a constant flow rate, is our focus, then it is denoted by,

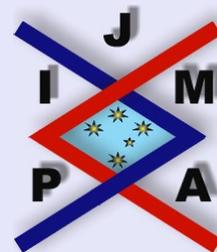
$$\bar{X} = \frac{1}{T} \int_{t=0}^T X(t) dt.$$

Further, if we seek to estimate this by using the sample values collected, then it is logical to perform this estimation using the sample mean,

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X(t_i).$$

We here assume that there is no reason to give precedence to particular sample values and so they are assumed to be of equal ‘weight’. How good the estimation is, is wrapped up in the estimation error, $|\bar{X} - \bar{X}_n|$. A reasonable statistical measure of how well this estimation does the job, is the estimation error variance (*EEV*), defined as,

$$EEV = E((\bar{X} - \bar{X}_n)^2) = E\left(\left(\frac{1}{T} \int_{t=0}^T X(t) dt - \frac{1}{n} \sum_{i=1}^n X(t_i)\right)^2\right).$$



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If we now contemplate obtaining a numerical value for this, it is clear that its value depends not only on the process values collected at, t_1, t_2, \dots, t_n but on the stochastic behaviour of the process, $X(t)$, itself. Whilst the sampling times may well be at our discretion or choosing, the nature of $X(t)$ is not, although its nature is likely the result of what we have set up or the end result of our attempts to regulate the process. $X(t)$ is then frequently the manifested process after the effects of certain control actions have occurred. The *EEV* can be expressed in terms of the process variogram as,

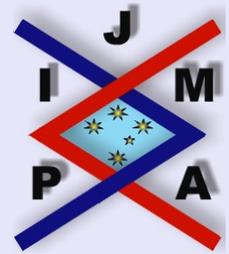
$$EEV = -\frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n V(t_i - t_j) - \frac{1}{T^2} \int_0^T \int_0^T V(u - v) dudv + \frac{2}{nT} \int_0^T \sum_{i=1}^n V(u - t_i) du.$$

As Saunders et al [11] point out, in principle this can be evaluated numerically once $V(\cdot)$ has been estimated but the expression is inherently unstable which is likely to give accuracy problems. In any event, seeking a more analytical approach is likely more interesting with the potential to tell us far more about the general structure of the problem and its solution.

Having defined the stationary variogram of the process $X(t)$ as,

$$V(u) = \frac{1}{2} E [(X(s+u) - X(s))^2],$$

we further stipulate that $V(0) = 0$ and $V(-u) = V(u)$. This means that from a purely mathematical perspective a model for $V(u)$ is likely to have a jump



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discontinuity at the origin. If not a discontinuity then almost certainly the origin will be a point of non-differentiability.

Focusing on the case where the variogram is indeed stationary we expect, for the practical application area under consideration here that, $V(u)$ will be strictly increasing on $u > 0$. The actual variogram in any instance will generally be unknown and so will need to be estimated from sample data. Such sample variograms may have non increasing features due to sample fluctuations or, commonly, as a result of insufficient data values being available to provide reliable estimates of the variogram for large time lags.

It is important to realize that assuming that $V(u)$ is stationary is not equivalent to assuming that the process, $X(t)$ itself is stationary. The former is a less stringent condition and means that assuming merely that the variogram is stationary enables us to include in our consideration some processes that are, in fact, non-stationary. Of course, if $X(t)$ is stationary then so too is $V(u)$.

In order to conceptualize further just what the variogram actually represents with regard to the process in continuous time, consider the situation when $X(t)$ is indeed stationary. In this case, $E[X(t)] = E[X(t + u)]$, $E[X^2(t)] = E[X^2(t + u)]$ and $Cov[X(t), X(t + u)]$ is a function of u only, designated by $\gamma(u)$. It follows then, by simplification, that,

$$V(u) = \sigma^2 - \gamma(u),$$

where σ^2 is the stable process variance and $\gamma(u)$ is the process autocovariance of lag u . In this case, the variogram is the difference between the stationary variance and the autocovariance function. A more general descriptor of the variogram is given by Saunders et al in [11], as the average smoothness of the process. For a manufacturing process that is stationary the expectation is that $\gamma(u)$



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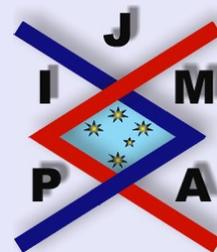
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will diminish with increasing u . These features lead us to expect a functional representation for the variogram, $V(u)$, of a stationary process to eventually level off. Non-stationary processes that have a stationary variogram are typified by having the variance at points lag u apart steadily increasing as u increases rather than tailing off as for the stationary case.

Generally speaking, the variogram can be conceptualized as representing, in the case of a chemical reaction for example, the actual stochastic dynamics of the reaction itself under basic control and this would not be expected to vary appreciably over a reasonable range of process adjustments, if process adjustments are indeed called for. If there is any doubt over this assumed robustness of the variogram to process adjustments, as the process is sampled for process monitoring purposes, and if necessarily adjusted, we can also plot the sample variogram in order to glean possible evidence of any change.

We focus here, however, primarily on the issue of product assessment on the basis of product samples. If we consider a single product sample taken at time, t_i , then for constant flow streams Barnett et al [4], have shown that on the basis of minimizing the EEV , this sample best represents the product flow over an interval with t_i as its mid-point, irrespective of the exact functional form of the process variogram, other than it being stationary. If \bar{X} denotes the mean characteristic of the flow over the interval, assumed, without loss of generality, to be $(0, d)$, then the error variance of estimating the mean characteristic by the single observation $X(t)$ at time t is given by,

$$E[(\bar{X} - X(t))^2] \\ = E \left[\left(\frac{1}{d} \int_0^d X(u) du - X(t) \right)^2 \right]$$



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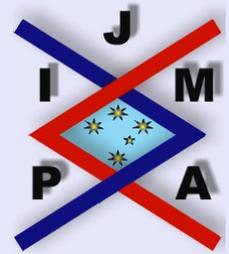
$$\begin{aligned}
&= \frac{1}{d^2} E \left[\int_0^d \int_0^d (X(u) - X(t))(X(v) - X(t)) dudv \right] \\
&= -\frac{1}{d^2} \int_0^d \int_0^d V(v - u) dudv + \frac{2}{d} \left\{ \int_0^t V(u) du + \int_0^{d-t} V(u) du \right\}.
\end{aligned}$$

To confirm the assertion with respect to this being minimal when the sample is taken at the mid-point of the interval $(0, d)$, we have only to differentiate this expression with respect to t and place it equal to zero in order to obtain, $V(t) = V(d - t)$. From the assumed monotonicity of $V(t)$ it follows that the optimal sampling location is at $t = \frac{d}{2}$, irrespective of the specific form of the process variogram.

The importance of the EEV is evident since it impacts on the reliability of our estimation of product quality.

It should be noted at this juncture that the issue of estimating the mean flow characteristic by a single sample value is essentially the mathematical problem of estimation of the mean of a continuous function over a finite interval by a single value lying in the interval. Attempts to put a bound on this difference is the substance of Ostrowski's inequality which has been the subject of much generalization over recent years, see for example [8] and the many references given there.

It can be seen from the foregoing that the EEV is a function of the variogram alone which in practical terms means that knowledge of the variogram over $(0, d)$ is sufficient information about the process to determine the EEV .



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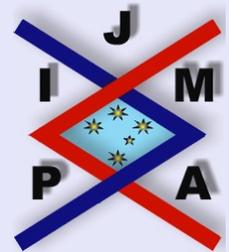
When $t = \frac{d}{2}$ this gives,

$$E \left[\left(\bar{X} - X \left(\frac{d}{2} \right) \right)^2 \right] = -\frac{1}{d^2} \int_0^d \int_0^d V(v-u) dudv + \frac{4}{d} \int_0^{\frac{d}{2}} V(u) du,$$

and this, for the linear variogram, $V(u) = A + Bu$, simplifies to give:-

$$(7.1) \quad EEV = A + \frac{Bd}{6}.$$

From practical considerations then, we need to be able to be confident of both the functional form and the value of the parameters of the process variogram and then we can find the error variance of estimating the flow mean over a given period by using a single value taken centrally from it. Generally, we will be estimating the mean characteristic of the flow over a given time period, not by a single sample value, but by the average of a number of sample values. This is dealt with in the next section.



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8. Stream Assessment on the Basis of the Sample Mean-Some Exact Results

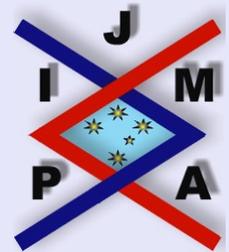
It is frequently the case that the mean characteristic of a continuous stream over a period, $[0, T]$ is assessed by reference to the mean of a number of samples taken from the stream over the same period. In other words $\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X(t_i)$ is used to estimate $\bar{X} = \frac{1}{T} \int_{t=0}^T X(t)dt$. The reliability of so doing is gauged by the estimation error variance,

$$EEV = E((\bar{X} - \bar{X}_n)^2) = E \left(\left(\frac{1}{T} \int_{t=0}^T X(t)dt - \frac{1}{n} \sum_{i=1}^n X(t_i) \right)^2 \right).$$

In order to develop a procedure for evaluating this we need to proceed in a manner similar to that presented in [11]. We suppose that the interval, $[0, T]$ is divided into n individual time intervals, $[(i-1)d, id]$, $i = 1, 2, \dots, n$. We assume that by design, or for simplicity, T is exactly divisible by d and so $d = \frac{T}{n}$. If we now let $t_1, t_2, t_3, \dots, t_n$ be n sampling times where $t_i \in ((i-1)d, id)$ then we can show [11] that:-

$$EEV = -\frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n V(t_i - t_j) - \frac{1}{T^2} \int_{u=0}^T \int_{v=0}^T V(u-v)dudv + \frac{2}{nT} \int_{u=0}^T \sum_{i=1}^n V(u-t_i)du.$$

The number of samples (collected at a constant interval apart) is taken to define a sub-interval of length, $d = \frac{T}{n}$ and the ‘best’ sampling times are at, $t_1 = \frac{d}{2}$,



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$t_2 = \frac{3d}{2}, t_3 = \frac{5d}{2}, \dots, t_n = \frac{(2n-1)d}{2}$. Throughout, ‘best’ is used in the context of providing the smallest *EEV* amongst all possible sampling point options once the time between the start of taking successive samples has been decided.

Clearly,

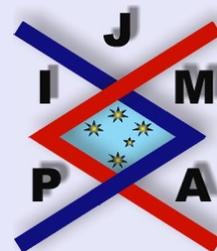
$$\bar{X} = \frac{1}{n} \sum_{i=1}^n \frac{1}{d} \int_{u=(i-1)d}^{id} X(u) du = \frac{1}{n} \sum_{i=1}^n \bar{X}(i),$$

and so the *EEV* can be written alternatively [11] as:-

$$EEV = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \left(-\frac{1}{d^2} \int_{u=(i-1)d}^{id} \int_{v=(j-1)d}^{jd} V(u-v) dudv \right. \\ \left. + \frac{1}{d} \int_{u=(i-1)d}^{id} V(u-t_j) du + \frac{1}{d} \int_{v=(j-1)d}^{jd} V(t_i-v) dv - V(t_i-t_j) \right)$$

with $t_i = \frac{(2i-1)d}{2}$ and $t_j = \frac{(2j-1)d}{2}$. Now the terms of the *EEV* corresponding to $i \neq j$, for the situation when the variogram is linear, can be shown to be equal to 0. This can be done by specific direct evaluation, by a general Taylor series expansion of $V(u)$ or by obtaining an upper bound for individual terms of the *EEV* for $i \neq j$ in terms of the second derivative of the variogram using the following two-dimensional Ostrowski type inequality obtained by Barnett and Dragomir in [2].

Let $f : [a, b] \times [c, d] \rightarrow \mathbb{R}$ so that $f(\cdot, \cdot)$ is integrable on $[a, b] \times [c, d]$, $f(x, \cdot)$ is integrable on $[c, d]$ for any $x \in [a, b]$ and $f(\cdot, y)$ is integrable on $[a, b]$ for any $y \in [c, d]$, $f''_{x,y} = \frac{\partial^2 f}{\partial x \partial y}$ exists on $(a, b) \times (c, d)$ and is bounded i.e., $\|f''_{s,t}\|_{\infty} :=$



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$\sup_{(x,y) \in (a,b) \times (c,d)} \left| \frac{\partial^2 f(x,y)}{\partial x \partial y} \right| < \infty$, then we have the inequality:-

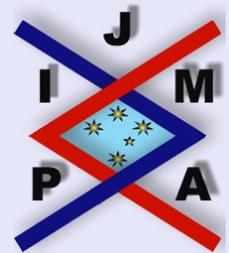
$$\begin{aligned} & \left| \int_a^b \int_c^d f(s,t) ds dt - [(b-a) \int_c^d f(x,t) dt \right. \\ & \quad \left. + (d-c) \int_a^b f(s,y) ds - (d-c)(b-a)f(x,y)] \right| \\ & \leq \left[\frac{1}{4}(b-a)^2 + \left(x - \frac{a+b}{2}\right)^2 \right] \left[\frac{1}{4}(d-c)^2 + \left(y - \frac{c+d}{2}\right)^2 \right] \|f''\|_{\infty}, \end{aligned}$$

for all $(x, y) \in [a, b] \times [c, d]$.

If we now apply this inequality for $f(u, v) = V(v - u)$ and with 'a' = $(i - 1)d$, 'b' = id , 'c' = $(j - 1)d$, 'd' = jd we get, under the assumption that V is twice differentiable and with the second derivative bounded,

$$\begin{aligned} & \left| \int_{(i-1)d}^{id} \int_{(j-1)d}^{jd} V(v-u) dudv \right. \\ & \quad \left. - \left[d \int_{(j-1)d}^{jd} V(v-x) dv + d \int_{(i-1)d}^{id} V(y-u) du - d^2 V(y-x) \right] \right| \\ & \leq \left[\frac{1}{4}d^2 + \left(x - \frac{d(2i-1)}{2}\right)^2 \right] \left[\frac{1}{4}d^2 + \left(y - \frac{d(2j-1)}{2}\right)^2 \right] \|V''\|_{\infty}, \end{aligned}$$

and for $V(\cdot)$ being linear the LHS must be 0.



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Hence,

$$EEV = \frac{1}{n^2} \sum_{i=1}^n \sum_{i=1}^n \left(-\frac{1}{d^2} \int_{u=(i-1)d}^{id} \int_{v=(i-1)d}^{id} V(u-v) dudv \right. \\ \left. + \frac{2}{d} \int_{u=(i-1)d}^{id} V\left(u - \frac{d}{2}(2i-1)\right) du \right)$$

which further simplifies to:-

$$EEV = \frac{1}{n^2} \sum_{i=1}^n \sum_{i=1}^n \left(-\frac{1}{d^2} \int_{u=0}^d \int_{v=0}^d V(u-v) dudv + \frac{2}{d} \int_{u=0}^d V\left(u - \frac{d}{2}\right) du \right),$$

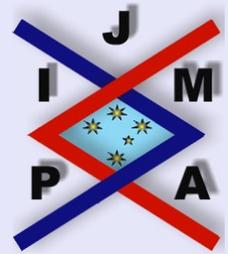
where the argument of the summation can be shown to be [11]:-

$$\int_0^d w(u)V(u)du, \quad \text{where } w(u) = \begin{cases} \frac{2}{d^2}(u+d), & 0 \leq u < \frac{d}{2} \\ \frac{2}{d^2}(u-d), & \frac{d}{2} \leq u < d \end{cases}$$

For $V(u) = A + Bu$ in this interval, the result is easily seen to be:- $EEV = \frac{1}{n} (A + \frac{1}{6}Bd)$, where $T = nd$, giving $EEV = \frac{1}{n} (A + \frac{BT}{6n})$, and (7.1) as a special case when $n = 1$.

When a Taylor expansion of $V(u)$ is made for the case where $i \neq j$ (for the general case where there is no assumption regarding the form of $V(u)$) the lowest order derivative of V that appears in the terms of the EEV is 4 [11]. This means that not only if the short lag process variogram is linear does,

$$EEV = E(\bar{X}_n - \bar{X})^2 = \frac{1}{n} \sum_{i=1}^n E(X(t_i) - \bar{X}(i))^2,$$



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but also when the short lag process variogram is quadratic or cubic. When the process variogram is $V(u) = A + Bu + Cu^2$ it can be shown again, that,

$$EEV = \frac{1}{n} \left(A + \frac{1}{6}Bd \right).$$

When the process variogram is $V(u) = A + Bu + Cu^2 + Du^3$ it can be shown that,

$$EEV = \frac{1}{n} \left(A + \frac{Bd}{6} - \frac{3Dd^2}{80} \right).$$



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9. Generally Bounding the Estimation Error

The estimation error itself of estimating \bar{X} by \bar{X}_n is given by $|\bar{X} - \bar{X}_n|$ and theoretical bounds for this can be obtained by using another variation of Ostrowski's inequality. In [8] the authors obtain the following inequality for differentiable functions, $f(x)$,

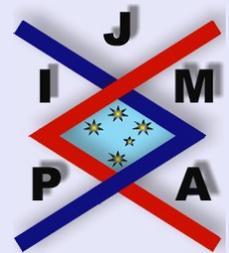
$$\left| \int_a^b f(x)dx - \sum_{i=0}^{n-1} f(\xi_i)h_i \right| \leq \|f'\|_\infty \sum_{i=0}^{n-1} \left[\frac{h_i^2}{4} + \left(\xi_i - \frac{x_i + x_{i+1}}{2} \right)^2 \right] \\ \leq \frac{\|f'\|_\infty}{2} \sum_{i=0}^{n-1} h_i^2,$$

where $\|f'\|_\infty$ is $\sup_{t \in (a,b)} |f'(t)| < \infty$, $a = x_0 < x_1 < \dots < x_{n-1} < x_n = b$ is an arbitrary partition of $[a, b]$ and $h_i = x_{i+1} - x_i$, $\xi_i \in [x_i, x_{i+1}]$, $i = 0, 1, 2, \dots, n - 1$.

If $f(t)$ is chosen to be the stochastic process, $X(t)$, (assumed differentiable) then clearly $\bar{X} = \frac{1}{T} \int_0^T X(t)dt$ and $\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$. Taking $b = T$, $a = 0$, $\xi_i = \frac{x_i + x_{i+1}}{2}$ and $x_i = i\frac{T}{n}$, T being the time duration over which the process is being assessed, we have,

$$|\bar{X} - \bar{X}_n| = \left| \frac{1}{T} \int_0^T X(t)dt - \frac{1}{n} \sum_{i=1}^n X_i \right| \leq \frac{\|X'(t)\|_\infty T}{2n},$$

which provides an upper bound for the estimation error for a particular class of process.



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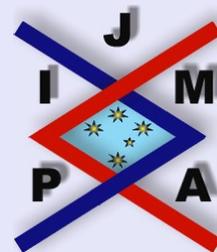
Sampling is generally considered to be an instantaneous operation which in practical terms means that the time to collect a process sample is negligible compared with the time between commencing successive samplings. The author has, however, met situations where the sampling time is appreciable in this sense.

When sampling is not instantaneous, the estimation error can be considered to be $|\bar{X}(T) - \bar{X}(p)|$ where $\bar{X}(T)$ is merely \bar{X} and $\bar{X}(p) = \frac{1}{p} \int_s^{s+p} X(t)dt$, s being the time at which sampling commences and $s + p$ the time at which it is completed. To obtain a bound for the estimation error, in this case, we can use another variation of Ostrowski's inequality given by Barnett and Dragomir [5], that is,

If $f : [a, b] \rightarrow \mathbb{R}$ is an absolutely continuous mapping on $[a, b]$, $[c, d] \subseteq [a, b]$ and $\|f'\|_\infty$ is $\sup_{t \in (a,b)} |f'(T)| < \infty$, then,

$$\left| \frac{1}{b-a} \int_a^b f(t)dt - \frac{1}{d-c} \int_c^d f(s)ds \right| \leq \left(\frac{1}{4}(b-a) + \frac{(d-c)}{2} + \frac{1}{b-a} \left[\left| \frac{c+d}{2} - \frac{a+b}{2} \right| - \frac{d-c}{2} \right]^2 \right) \|f'\|_\infty.$$

For application of this result to estimation of the mean flow quality we take $a = 0$, $b = T$ and $c = s$, $d = s + p$ with $s + p < T$. With respect to the time, s , at which sampling commences it is interesting to note that with reference to the mid-point of the time period over which it is desired to estimate \bar{X} , $(0, T)$, if sampling commences at the mid-point then the bound is, $\left(\frac{s+p}{2}\right) \|X'(t)\|_\infty$. If sampling concludes at the mid-point, however, the bound for the estimation



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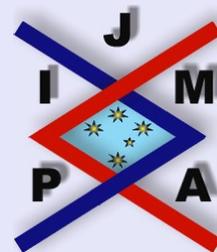
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error variance is, $\left(\frac{2s+3p}{4}\right) \|X'(t)\|_\infty$ a proportional change of $\frac{p}{2(s+p)}$. The tightest bound is provided when sampling is symmetrical about the mid-point of the interval, i.e. when $\frac{T}{2} = \frac{2s+p}{2}$ in which case the bound is:-

$$|\bar{X}(t) - \bar{X}(p)| \leq \left(\frac{T+p}{4}\right) \|X'(t)\|_\infty.$$

Whilst this result points to the most appropriate sampling regime, it is, together with the previous result for bounding the estimation error when sampling is instantaneous, largely of theoretical interest since neither $\bar{X}(t)$ nor $X'(t)$ will, in general be known. The desire for more practical results leads us to consider the estimation error *variance*, rather than the estimation error itself.



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10. Bounding the Estimation Error Variance - Single Value Estimation

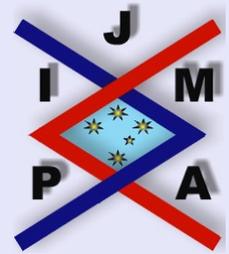
Considering first the situation of a single value used to estimate the flow mean characteristic, we have:-

$$\begin{aligned}
 & E[(\bar{X} - X(t))^2] \\
 &= E \left[\left(\frac{1}{d} \int_0^d X(u) du - X(t) \right)^2 \right] \\
 &= \frac{1}{d^2} E \left[\int_0^d \int_0^d (X(u) - X(t))(X(v) - X(t)) dudv \right] \\
 &= -\frac{1}{d^2} \int_0^d \int_0^d V(v-u) dudv + \frac{2}{d} \left\{ \int_0^t V(u) du + \int_0^{d-t} V(u) du \right\}.
 \end{aligned}$$

In order to obtain bounds for this expression when we make no specific assumption about the form of the variogram, we can again appeal to the bivariate generalization of Ostrowski's inequality [2], used previously.

If we use it for $f(u, v) = V(v - u)$ and with $a = c = 0, b = d$, we get, under the assumption that V is twice differentiable and with the second derivative bounded on that interval,

$$\begin{aligned}
 & \left| \int_0^d \int_0^d V(v-u) dudv \right. \\
 & \quad \left. - \left[d \int_0^d V(v-x) dv + d \int_0^d V(y-u) du - d^2 V(y-x) \right] \right|
 \end{aligned}$$



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$$\leq \left[\frac{1}{4}d^2 + \left(x - \frac{d}{2}\right)^2 \right] \left[\frac{1}{4}d^2 + \left(y - \frac{d}{2}\right)^2 \right] \|V''\|_\infty,$$

for all $x, y \in [0, d]$.

If we now let $x = y = t$, we get,

$$\left| \int_0^d \int_0^d V(v-u) dudv - \left[d \int_0^d V(v-t) dv + d \int_0^d V(t-u) du \right] \right| \leq \left[\frac{1}{4}d^2 + \left(t - \frac{d}{2}\right)^2 \right]^2 \|V''\|_\infty.$$

Further simplification gives,

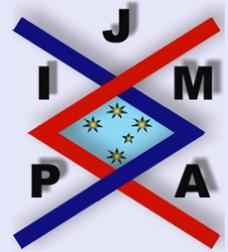
$$\left| \frac{1}{d^2} \int_0^d \int_0^d V(v-u) dudv - \frac{2}{d} \left[\int_0^t V(v) dv + \int_0^{d-t} V(v) dv \right] \right| \leq \left[\frac{1}{4} + \frac{\left(t - \frac{d}{2}\right)^2}{d^2} \right]^2 d^2 \|V''\|_\infty.$$

From this,

$$E \left[(\bar{X} - X(t))^2 \right] \leq \left[\frac{1}{4} + \frac{\left(t - \frac{d}{2}\right)^2}{d^2} \right]^2 d^2 \|V''\|_\infty.$$

The best inequality that we can get is that for which $t = \frac{d}{2}$ giving the bound,

$$E \left[\left(\bar{X} - X \left(\frac{d}{2} \right) \right)^2 \right] \leq \frac{d^2}{16} \|V''\|_\infty.$$



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It should be noted that this result requires double differentiability of V in $(-d, d)$ and that this condition will frequently not hold, for example, for the case of a linear variogram.

The following results, however, do not require this differentiability restriction and they include commonly used variogram models as special cases.

A mapping $f : [a, b] \subset \mathbb{R} \rightarrow \mathbb{R}$ is said to be of the r -Hölder type with $r \in (0, 1]$ if $|f(x) - f(y)| \leq H|x - y|^r$ for all $x, y \in [a, b]$ with a certain $H > 0$. If $r = 1$ then the mapping is said to be Lipschitzian. Also, any differentiable mapping $f : [a, b] \rightarrow \mathbb{R}$ having its derivative bounded in (a, b) is Lipschitzian on (a, b) . Should the variogram be of the r -Hölder type then we are able to use this property to obtain a bound for the *EEV*.

We have, in the foregoing, seen that,

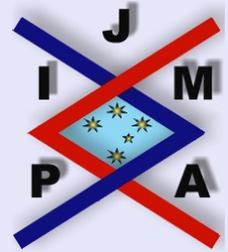
$$0 \leq E[(\bar{X} - X(t))^2] = \frac{1}{d^2} \int_0^d \int_0^d [V(v - t) + V(t - u) - V(v - u)] dv du.$$

If $V(u)$ is of the r -Hölder type then,

$$|V(v - t) - V(v - u)| \leq H|v - t - v + u|^r = H|u - t|^r, \text{ for all } u, v, t \in [0, d].$$

Also,

$$|V(t - u)| = |V(t - u) - V(0)| \leq H|t - u|^r, \text{ for all } t, x \in [0, d].$$



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We have, therefore,

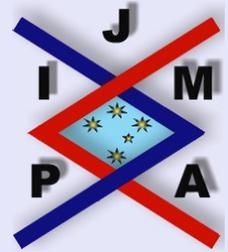
$$\begin{aligned}
 E \left[(\bar{X} - X(t))^2 \right] &= \left| \frac{1}{d^2} \int_0^d \int_0^d [V(v-t) + V(t-u) - V(v-u)] dv du \right| \\
 &\leq \frac{1}{d^2} \int_0^d \int_0^d |V(v-t) - V(v-u) + V(t-u)| dv du \\
 &\leq \frac{1}{d^2} \int_0^d \int_0^d |V(v-t) - V(v-u)| + |V(t-u)| dv du \\
 &\leq \frac{1}{d^2} \int_0^d \int_0^d [H |t-u| + H |t-u|^r] dv du \\
 &= \frac{2H}{d} \int_0^d |t-u|^r du \\
 &= \frac{2H}{d} \left[\int_0^t (t-u)^r du + \int_t^d (u-t)^r du \right] \\
 &= \frac{2H}{d} \left[\frac{t^{r+1} + (d-t)^{r+1}}{r+1} \right].
 \end{aligned}$$

We have thus shown that for a variogram of the r -Hölder type on $[-d, d]$ with $H > 0$,

$$EEV = E \left[(\bar{X} - X(t))^2 \right] \leq \frac{2H}{d} \left[\frac{t^{r+1} + (d-t)^{r+1}}{r+1} \right] \leq \frac{2Hd}{r+1}.$$

If V is Lipschitzian with $L > 0$ then this becomes (with $r = 1$),

$$EEV = E \left[(\bar{X} - X(t))^2 \right] \leq \left[\frac{1}{4} + \frac{(t - \frac{d}{2})^2}{d^2} \right] Ld.$$



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Representing $t^{r+1} + (d - t)^{r+1}$ by $g(t)$ it is easy to see that the mapping $g : [0, d] \rightarrow \mathbb{R}$ is such that,

$$\inf_{t \in [0, d]} g(t) = g\left(\frac{d}{2}\right) = \frac{d^{r+1}}{2^r} \quad \text{and} \quad \sup_{t \in [0, d]} g(t) = g(0) = g(d) = d^{r+1}.$$

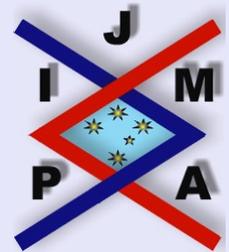
From these we can again deduce that the bound is at its smallest when $t = \frac{d}{2}$, we then have:-

$$E \left[\left(\bar{X} - X \left(\frac{d}{2} \right) \right)^2 \right] \leq \frac{2^{1-r} H d^r}{r + 1}.$$

For the Lipschitzian case,

$$E \left[\left(\bar{X} - X \left(\frac{d}{2} \right) \right)^2 \right] \leq \frac{1}{2} L d.$$

If the variogram is in fact of the r -Hölder type then the *EEV* itself can be shown to also be of the r -Hölder type with constant $2H$ rather than the H that is the constant for the variogram [3].



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11. The Convexity of the EEV

If the variogram is monotonic non-decreasing on $[0, d]$ then the EEV of estimating the mean flow in $[0, d]$ by a single value in the interval, $E[(\bar{X} - X(t))^2]$, is convex on $[0, d]$.

Since the

$$EEV = E_v(t) = -\frac{1}{d^2} \int_0^d \int_0^d V(v-u) dudv + \frac{2}{d} \left\{ \int_0^t V(u) du + \int_0^{d-t} V(u) du \right\},$$

$$\text{then } E'_v(t) = \frac{2}{d}[V(t) - V(d-t)].$$

If $t_1, t_2 \in [0, d]$ and $t_2 > t_1$ then,

$$E_v(t_2) - E_v(t_1) - (t_2 - t_1)E'_v(t_1) = \frac{2}{d} \left(\int_{t_1}^{t_2} V(u) du - \int_{d-t_2}^{d-t_1} V(u) du + (t_2 - t_1)V(t_1) + (t_2 - t_1)V(d-t_1) \right).$$

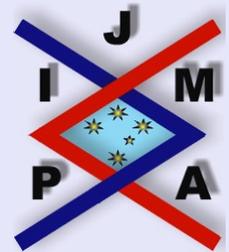
Since V is non-decreasing on the interval $[0, d]$ we have,

$$\int_{t_1}^{t_2} V(u) du \geq (t_2 - t_1)V(t_1) \quad \text{and} \quad \int_{d-t_2}^{d-t_1} V(u) du \geq (t_2 - t_1)V(d-t_1)$$

and these imply that

$$E_v(t_2) - E_v(t_1) \geq (t_2 - t_1)E'_v(t_1) \quad \text{for all } t_2 > t_1 \in [0, d],$$

showing that $E_v(\cdot)$ is convex on $[0, d]$.



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12. Bounding the EEV when using a Sample Mean

We now consider the case where we have an average of sample values available to us to estimate the flow mean characteristic in an interval $[0, T]$ where we have a fixed sampling interval of d with $nd = T$. The results follow similarly to the previous simpler case where $n = 1$.

We have previously seen that we can write,

$$\begin{aligned}
 E(\bar{X} - \bar{X}_n)^2 &= \frac{1}{n^2 d^2} \sum_{i=1}^n \sum_{j=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} \{-V(u-v) + V(u-t_j) \\
 &\quad + V(t_i-v) - V(t_i-t_j)\} dudv.
 \end{aligned}$$

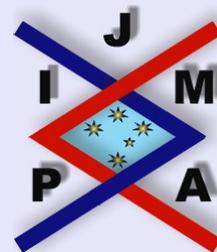
Applying the Hölder property to the integrand,

$$\{V(u-t_j) - V(u-v)\} + \{V(t_i-v) - V(t_i-t_j)\}$$

we have,

$$\begin{aligned}
 |V(u-t_j) - V(u-v)| &\leq H |v-t_j|^r \quad \text{and} \\
 |V(t_i-v) - V(t_i-t_j)| &\leq H |t_j-v|^r
 \end{aligned}$$

with v and $t_j \in [(j-1)d, jd] \subset [0, T]$.



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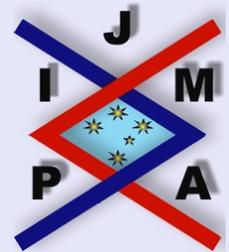
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Therefore,

$$\begin{aligned}
 & |E(\bar{X} - \bar{X}_n)^2| \\
 &= \frac{1}{n^2 d^2} \left| \sum_{i=1}^n \sum_{j=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} \{-V(u-v) + V(u-t_j) \right. \\
 &\quad \left. + V(t_i-v) - V(t_i-t_j)\} dudv \right| \\
 &\leq \frac{1}{n^2 d^2} \sum_{i=1}^n \sum_{j=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} \{|V(u-t_j) - V(u-v)| \\
 &\quad + |V(t_i-v) - V(t_i-t_j)|\} dudv \\
 &\leq \frac{1}{n^2 d^2} \sum_{i=1}^n \sum_{j=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} \{H|v-t_j|^r + H|t_j-v|^r\} dudv \\
 &= \frac{2H}{nd} \sum_{j=1}^n \left[+ \int_{v=(j-1)d}^{t_j} (t_j-v)^r dv + \int_{t_j}^{jd} (v-t_j)^r dv \right] \\
 &= \frac{Hd^r}{2^{r-1}(r+1)} = \frac{2H}{r+1} \left(\frac{T}{2n} \right)^r
 \end{aligned}$$

which for the Lipschitzian case gives the bound as $\frac{HT}{2n}$.



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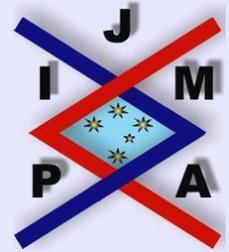
13. Bounding the *EEV* when the Flow Rate Varies

We suppose that the stream flow rate at time t is given by $Y(t)$ and that the stream is sampled at times $t_1, t_2, t_3, \dots, t_n$, distance d apart, at which the flow rate is also recorded, affording two values at every sample, $X(t_i)$, the flow characteristic at t_i and $Y(t_i)$, the flow rate at time t_i . The mean characteristic of the flow over $[0, T]$ is then estimated by the mean of the sample characteristic values weighted by their flow rate, giving the *EEV* as,

$$E \left[\frac{\int_0^T Y(t)X(t)dt}{\int_0^T Y(t)dt} - \frac{\sum_{i=1}^n Y(t_i)X(t_i)}{\sum_{i=1}^n Y(t_i)} \right]^2.$$

It should be noted that for the following analysis to make sense the flow rate function is assumed deterministic for all $t \in [0, T]$ meaning that it is not subject to a probability distribution but is rather an entirely controlled and known function. There are, of course, many other practical circumstances that can arise, these include the situation where the flow rate is kept constant for a period of time and is then deliberately ramped up or down and maintained at this new constant flow level for an assigned period of time when it is likely changed in a similar manner again. Provided the appropriate practical set of circumstances exist, then it may be possible, in this case, to view the total behaviour of the flow over $[0, T]$ as simply a number of separate constant flow rate periods - for all intents and purposes the flow rate change being assumed instantaneous.

A similar yet different situation can arise when the only known flow rates are those observed at the time of sampling. Under these circumstances the individual flow rates can be used as assumed constant flow rates of the stream over the



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time period for which the individual sample values are being taken as estimates of the stream.

Assuming, however, that we have the first situation of completely known, deterministic flow, the integral over $[0, T]$ can be broken down into its component parts to give,

$$\begin{aligned}
 EEV = & \left(\frac{1}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 & \times E \left(\sum_{i=1}^n \sum_{j=i}^n Y(t_i) \int_{(j-1)d}^{jd} X(t)Y(t)dt \right. \\
 & \left. - \sum_{i=1}^n \sum_{j=1}^n X(t_i)Y(t_i) \int_{(j-1)d}^{jd} Y(t)dt \right)^2
 \end{aligned}$$

which gives further,

$$\begin{aligned}
 EEV = & \left(\frac{1}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 & \times E \left(\sum_{i=1}^n \sum_{j=i}^n \int_{(j-1)d}^{jd} (X(t)Y(t)Y(t_i) - X(t_i)Y(t_i)Y(t)dt) \right)^2 .
 \end{aligned}$$

Expressing the squared component within the expectation as a double sum and double integration and taking the expectation, noting that $Y(t)$ is assumed de-



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terministic, we have,

$$\begin{aligned}
 EEV &= \left(\frac{1}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 &\times \left(\sum_{i=1}^n \sum_{j=i}^n \sum_{k=1}^n \sum_{s=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} Y(t_s)Y(t_k)Y(u)Y(v) \right. \\
 &\quad \left. \times \{-V(u-v) + V(u-t_j) + V(t_i-v) - V(t_i-t_j)\} dudv \right)
 \end{aligned}$$

If we now consider the case for a linear flow rate function, $Y(t) = At$, the integrand / summand becomes,

$$A^4 t_i t_k u v \{-V(u-v) + V(u-t_j) + V(t_i-v) - V(t_i-t_j)\}.$$

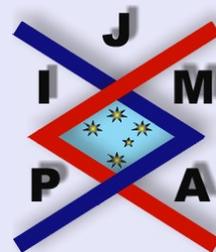
We now assume that the variogram is of the Hölder type. Applying the Hölder property to the integrand,

$$\{V(u-t_j) - V(u-v)\} + \{V(t_i-v) - V(t_i-t_j)\}$$

we get,

$$\begin{aligned}
 |V(u-t_j) - V(u-v)| &\leq H |v-t_j|^r \quad \text{and} \\
 |V(t_i-v) - V(t_i-t_j)| &\leq H |t_j-v|^r
 \end{aligned}$$

with v and $t_j \in [(j-1)d, jd] \subset [0, T]$.



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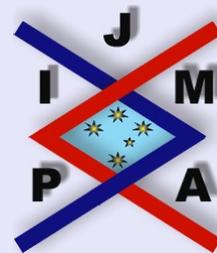
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We have, therefore,

$$\begin{aligned}
 EEV &\leq \left(\frac{A^2}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 &\times \left(\sum_{i=1}^n \sum_{j=i}^n \sum_{k=1}^n \sum_{s=1}^n \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} t_s t_k u v \{ |-V(u-v) + V(u-t_j)| \right. \\
 &\qquad \qquad \qquad \left. + |V(t_i-v) - V(t_i-t_j)| \} dudv \right),
 \end{aligned}$$

which gives further,

$$\begin{aligned}
 EEV &\leq \left(\frac{A^2}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 &\times \left(\sum_{i=1}^n \sum_{j=i}^n \sum_{k=1}^n \sum_{s=1}^n t_s t_k \int_{v=(j-1)d}^{jd} \int_{u=(i-1)d}^{id} Huv \{ |v-t_j|^r + |t_j-v|^r \} dudv \right) \\
 &= d^2 H \left(\frac{A^2}{\int_0^T Y(t)dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \\
 &\times \left(\sum_{i=1}^n \sum_{j=i}^n \sum_{k=1}^n \sum_{s=1}^n t_s t_k (2i-1) \int_{v=(j-1)d}^{jd} v |t_j-v|^r dv \right)
 \end{aligned}$$



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$$= d^2 H \left(\frac{A^2}{\int_0^T Y(t) dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \times \left(\sum_{s=1}^n \sum_{k=1}^n t_s t_k \sum_{i=1}^n (2i-1) \left(\sum_{j=1}^n \int_{v=t_j}^{jd} v(v-t_j)^r dv + \int_{v=(j-1)d}^{t_j} v(t_j-v)^r dv \right) \right).$$

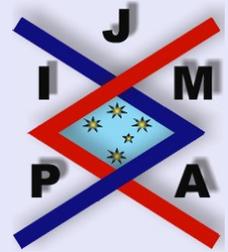
If we integrate by parts and once again assume that each sample represents an interval of length d symmetric about the time of sampling (central sampling), then we have:-

$$= d^2 H \left(\frac{A^2}{\int_0^T Y(t) dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \left(\sum_{s=1}^n \sum_{k=1}^n t_s t_k \sum_{i=1}^n (2i-1) \times \left(\sum_{j=1}^n \left(\frac{d^{r+2}}{2^{r+1}(r+1)} \left(j - \frac{1}{2(r+2)} \right) + \frac{d^{r+2}}{2^{r+1}(r+1)} \left(j-1 + \frac{1}{2(r+2)} \right) \right) \right) \right),$$

which reduces to,

$$d^2 H \left(\frac{A^2}{\int_0^T Y(t) dt \cdot \sum_{i=1}^n Y(t_i)} \right)^2 \left(\sum_{s=1}^n \sum_{k=1}^n t_s t_k \sum_{i=1}^n (2i-1) \frac{n^2 d^{r+2}}{(r+1)2^{r+1}} \right),$$

giving, finally, $\frac{Hd^r}{(r+1)2^{r-1}}$.



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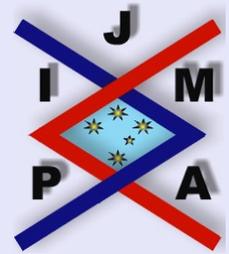
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If we once more take the case where $r = 1$ we again obtain the bound, $\frac{HT}{2n}$. It should be noted, however, that when the flow rate varies, central sampling is not the 'best' from the point of view of minimizing the *EEV*, whether this is sufficiently significant to warrant taking into account would need further investigation.



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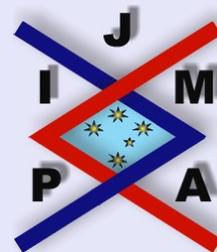
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14. Controlling a Continuous Flow Process – Concluding Remarks

In this paper we have directed attention to the estimation error and estimation error variance in connection with the assessment of continuous flows. In passing, mention has been made of the necessity, where such flows occur in the manufacturing environment, of also controlling such streams and this will invariably mean adjusting the generating process as the need arises, over and above routine control. One approach to such control is to proceed on the basis of a running mean of sample values. Whether this is a suitable approach or not will depend on the specific practical context and, in particular, on how the product is stored immediately following manufacture. Granted that these running means of the flow characteristic under focus are merely a surrogate for the actual continuous flow mean characteristic, we again face the issue of estimation error.

In all that has been presented the variogram has been assumed stationary. In particular, the final assessment of the product stream is dependent on this stability so we need to be confident that any additional process adjustments do not appreciably impact this. Saunders et al [11] discuss stream assessment when the variogram is non-stationary.

In proceeding on the basis of control that is focused on the value of the running mean, we can contemplate forecasting a next process value and use this to construct a forecast of the running mean. In so doing, we can consider using a technique that is similar to the method of Kriging. A detailed discussion of such control, however, is reserved for a subsequent paper.



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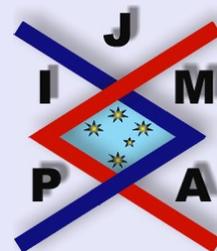
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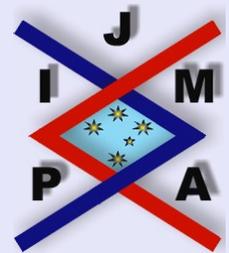
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