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ACCURATE CALCULATION OF BLOCK-SAMPLE COVARIANCES USING GAUSS QUADRATURE

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by

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ABSTRACT

The usual method for calculating the covariance between a block and a sample point is by discretizing the block into regularly spaced grid points, calculating the covariance between the sample point and each of the grid points, and then averaging the covariances. This thesis demonstrates that a calculation can be made with superior accuracy by using Gauss quadrature to approximate the areal or volumetric integral for block-sample covariance. The experiment shows that four Gauss points is optimal for the calculation.

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Chapter I

Introduction

The classical method for the estimation of covariances between a sample point and a block is to discretize the block into regularly spaced grid points, calculate the covariance between the sample and each grid point, and then average the covariance values. An alternate method which yields more accurate results is Gauss quadrature. The Gauss quadrature method uses grid points which are symmetrically spaced about its center, rather than regularly spaced grid points, in order to minimize the error in the calculations.

Block-sample covariance can be calculated using an areal block or a volumetric block. For an areal block of size (xmax-xmin) by (ymax-ymin), the covariance between the sample and the block is defined:

$$COV_{oi} = \frac{1}{AREA} \int_{xmin}^{xmax} \int_{ymin}^{ymax} COV(h_{xy}, i)\,dydx$$

where o represents the block, and i represents the sample point. For a volumetric block of size (xmax-xmin) by (ymax-ymin) by (zmax-zmin), the covariance between the sample and the block is defined as

$$COV_{oi,VOL} = \frac{1}{VOL} \int_{zmin}^{zmax} \int_{xmin}^{xmax} \int_{ymin}^{ymax} COV(h_{xyz}, i)\,dydxdz$$

The classical method is to approximate the integrals for block-sample covariance (for the areal case) as the summation

$$COV_{oi} = \sum_{j=1}^{P} \sum_{k=1}^{M} W_j W_k COV(h_{i,jk})$$

where $h_{i,jk}$ is the distance between the sample location and each grid point within the block. For a block discretized into P rows and M columns, $W_j = 1/P$ and $W_k = 1/M$ (David, 1977). The area of the block, A, is equal to PM and the summation becomes

$$COV_{oi} = \frac{1}{PM} \sum_{j=1}^{P} \sum_{k=1}^{M} COV(h_{i,jk})$$

For the case of a volumetric block, the covariance integrals can be approximated by the following triple summation:

$$COV_{oi,VOL} = \sum_{j=1}^{P} \sum_{k=1}^{M} \sum_{m=1}^{O} W_j W_k W_m COV(h_{i,jkm})$$

where P, M, and O are the discretized dimensions of the block. The coefficients W_j, W_k, and W_m then become $W_j = 1/P$, $W_k = 1/M$, and $W_m = 1/O$. The volume of the block is then PMO and the triple summation then becomes:

$$COV_{oi,VOL} = \frac{1}{PMO} \sum_{j=1}^{P} \sum_{k=1}^{M} \sum_{m=1}^{O} COV(h_{i,jkm})$$

The coefficients W_j, W_k, and W_m are equal to the regularly spaced grid spacing of the block. P, Q, and O are equal for the case of a cubic block, and the coefficients then become equal to each other.

Another method for evaluating the integrals is to use variable coefficients that are weighted to minimize the error of the approximation. This is the approach that is used in the Gauss quadrature method. Gauss quadrature uses a variable grid spacing which is dependent on the weighted coefficients, unlike the regularly spaced grid used with the classical method. The grid points used in Gauss quadrature correspond to Gauss points which are used in dividing the integration interval.

The Gauss quadrature method to approximate the integrals for the covariance between the sample and the block is with the following summation (for the areal case):

$$COV_{0i} = \frac{1}{AREA}\sum_{j=1}^{N}\sum_{k=1}^{N} W_j W_k COV(h_{i,jk})$$

and for the volumetric case, the integrals can be approximated by the following:

$$COV_{0i,VOL} = \frac{1}{VOL}\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{m=1}^{N} W_j W_k W_m COV(h_{i,jkm})$$

where N is the number of Gauss points per spatial direction, W_j, W_k, and W_m are the weighted coefficients, or weights.

An experiment can be done to determine the number of Gauss points that are optimal for the Gauss quadrature method. Calculations can be made for both Gauss quadrature and the classical method for comparison. For the classical method, the number of grid points can be varied in the experiments. For the Gauss quadrature method, the number of Gauss points can be varied to compare with the classical results. The block-sample covariances can be compared between the two methods to determine the most accurate method.

Different geometries can be tested to find differences between the two methods. The position of the sample point can be varied relative to the block. The different positions to be tested are close to the block, far from the block, mid-distance from the block and a location that is oblique to the block.

The method with the best accuracy for a given number of grid points is the superior method. This thesis shows that Gauss quadrature is superior to the classical method currently used (David 1977). A comparison of the number of grid points needed in the classical method to achieve the accuracy of Gauss quadrature will be made. The optimal number of Gauss points needed will be determined from the experiment.

Chapter II

Kriging and Block Kriging

Geostatistics is the application of statistics to the analysis and estimation of spatial data. Spatial data is data collected at arbitrary locations on an areal or volumetric collection site. This data can be used to determine values of unknown samples within the region if the region has a certain degree of continuity. If the region has a high degree of continuity then the range or distance that the estimation can be made is high. If the continuity is not high then the estimation range will be very small.

The value of an unknown sample in an area or volume can be estimated by the method of kriging. The unknown sample, or regionalized variable (Matheron, 1963), is a spatially distributed random variable. Kriging takes into account both the structured and random components of the regionalized variable. Kriging is based on minimizing the variance of the error. It is named after D.G. Krige, a South African mining engineer, and developed by Georges Matheron who first translated it to english in 1963.

The concept of regionalized variables takes into account the position of the unknown sample as well as the magnitude of the sample. This has many applications including the mineral industry for which the use of kriging was developed. The range or area of influence of a sample can be determined using these techniques. A measure of the continuity and anisotropy of the region surrounding the sample can also be made.

The most important use of geostatistics is to make an estimate of the unknown sample and to make an estimate of the error of the estimate. This error will need to be minimized for kriging to be effective.

The continuity of the sample values in a region can be highly variable. Some regions show a high correlation between the sample magnitude and the sample location while other regions show very little correlation. The regions with high correlation have samples which are related to nearby samples. Regions with low correlation have a random component which is independent of the location and nearby samples. Such regions are associated with semi-variograms (to be explained momentarily) which have a sizeable nugget effect.

It is desirable to minimize the nugget effect in order to reduce the variance between adjacent samples and a sample and the regional area or volume. One way of doing this is to take large size regions. Larger regions have the tendency to have lower nugget effects (David, 1977), because larger regions contain higher numbers of equal size grains, for example, in a rock mass. This will reduce the error of the estimate for the unknown regionalized variable. In application, the regional size may be restricted to the method and tools used to obtain the samples and the total size of the region.

In a continuous region, the closer two samples are to each other, the more alike they likely are. As the distance between samples is increased, the more dissimilar they likely become. The variation between sample values at different distances can be plotted on a graph which is called a semi-variogram. This is the variance between sample point values and is a measure of the spatial correlation of the region containing the sample points. Kriging uses the semi-variogram to model the spatial phenomena between the sample points.

The variance between the sample points in a region is determined by squaring the difference between the sample values at different distances and averaging the values. The variance, or semi-variogram function, can be written as the spatial correlation function:

$$\gamma(h)=\frac{1}{2N}\sum_{i=1}^{N}[z(x_i)-z(x_i+h)]^2$$

where

h = a separation distance (lag) between sample points

N = the total number of pairs separated by h

$z(x_i)$ = the data value at the location x_i

$z(x_i+h)$ = a different data value located at a distance h from x_i

The semi-variogram function depends only on the distance between sample points, h, and not on the spatial position of the sample point. This is known as the intrinsic hypothesis.

A semi-variogram is a graph of the semi-variogram function plotted as a function of the distance, h. A typical semi-variogram is shown in Figure II.1. The semi-variogram function increases with increasing values of distance until it reaches a constant value. The constant value is labeled on Figure II.1 as the sill. The range

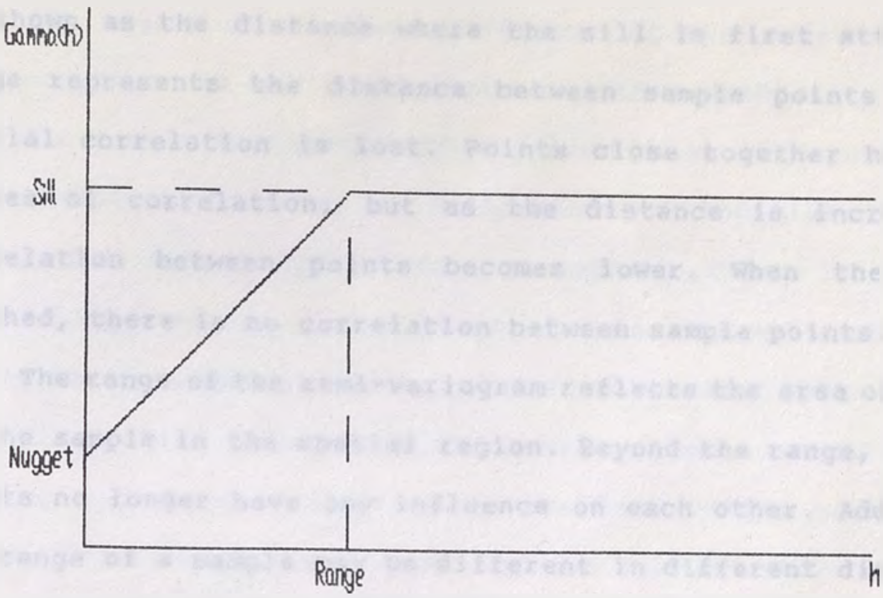


Figure II.1. A typical semi-variogram.

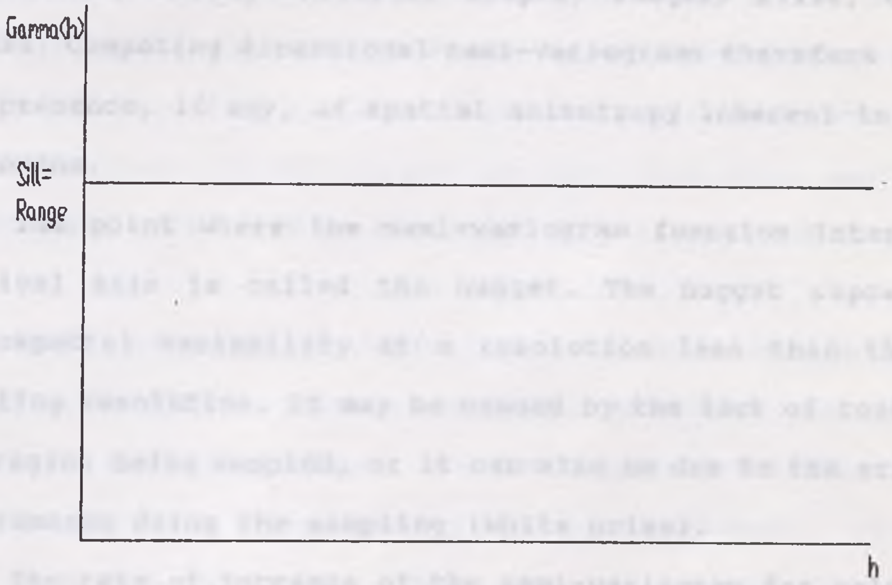


Figure II.2. A nugget effect semi-variogram.

is shown as the distance where the sill is first attained. The range represents the distance between sample points where the spatial correlation is lost. Points close together have a high degree of correlation, but as the distance is increased, the correlation between points becomes lower. When the range is reached, there is no correlation between sample points.

The range of the semi-variogram reflects the area of influence of the sample in the spatial region. Beyond the range, the sample points no longer have any influence on each other. Additionally, the range of a sample may be different in different directions in an anisotropic region. This will result in several ranges for a sample, which can be determined by calculating the semi-variogram in several directions. These semi-variograms will be different from each other, having different shapes, ranges, sills, and nugget values. Computing directional semi-variograms therefore identifies the presence, if any, of spatial anisotropy inherent to a spatial phenomena.

The point where the semi-variogram function intercepts the vertical axis is called the nugget. The nugget represents the microspatial variability at a resolution less than the minimum sampling resolution. It may be caused by the lack of continuity of the region being sampled, or it can also be due to the error in the instruments doing the sampling (white noise).

The rate of increase of the semi-variogram for values of the distance, h, less than the range shows the amount of continuity of the spatial region. If the rate of increase is smooth and steady, then the region is highly continuous. If the rate of growth is erratic, then the spatial region has little continuity.

For a semi-variogram with the form shown in Figure II.2, the semi-variogram function is independent of location, h. This is called the nugget effect semi-variogram. There is no spatial correlation over the entire range of data. The values of the data points are completely random and are independent of each other.

The spatial behavior of the semi-variogram can be modeled by fitting a continuous function to the data values of the spatial region. The function which describes the spatial behavior is called the intrinsic function. To be able to use the intrinsic function to describe the spatial behavior, the intrinsic hypothesis and data stationarity must be assumed. The intrinsic hypothesis means that the semi-variogram depends only on the distance, h, and not the location within the spatial region. Data stationarity means that the local average of the data values in one area is the same as in all other areas. If this is not the case, then there may be a trend in the data values and an intrinsic function may not be able to be applied.

There are many intrinsic functions which can be applied to describe the spatial behavior of a region. Four types of intrinsic functions will be reviewed for this paper. The four intrinsic functions are the linear model, the spherical model, the Gaussian model, and the exponential model. They are graphically illustrated in Figure II.3. The graphs in Figure II.3 do not show a nugget value, however they may have one in many actual applied cases.

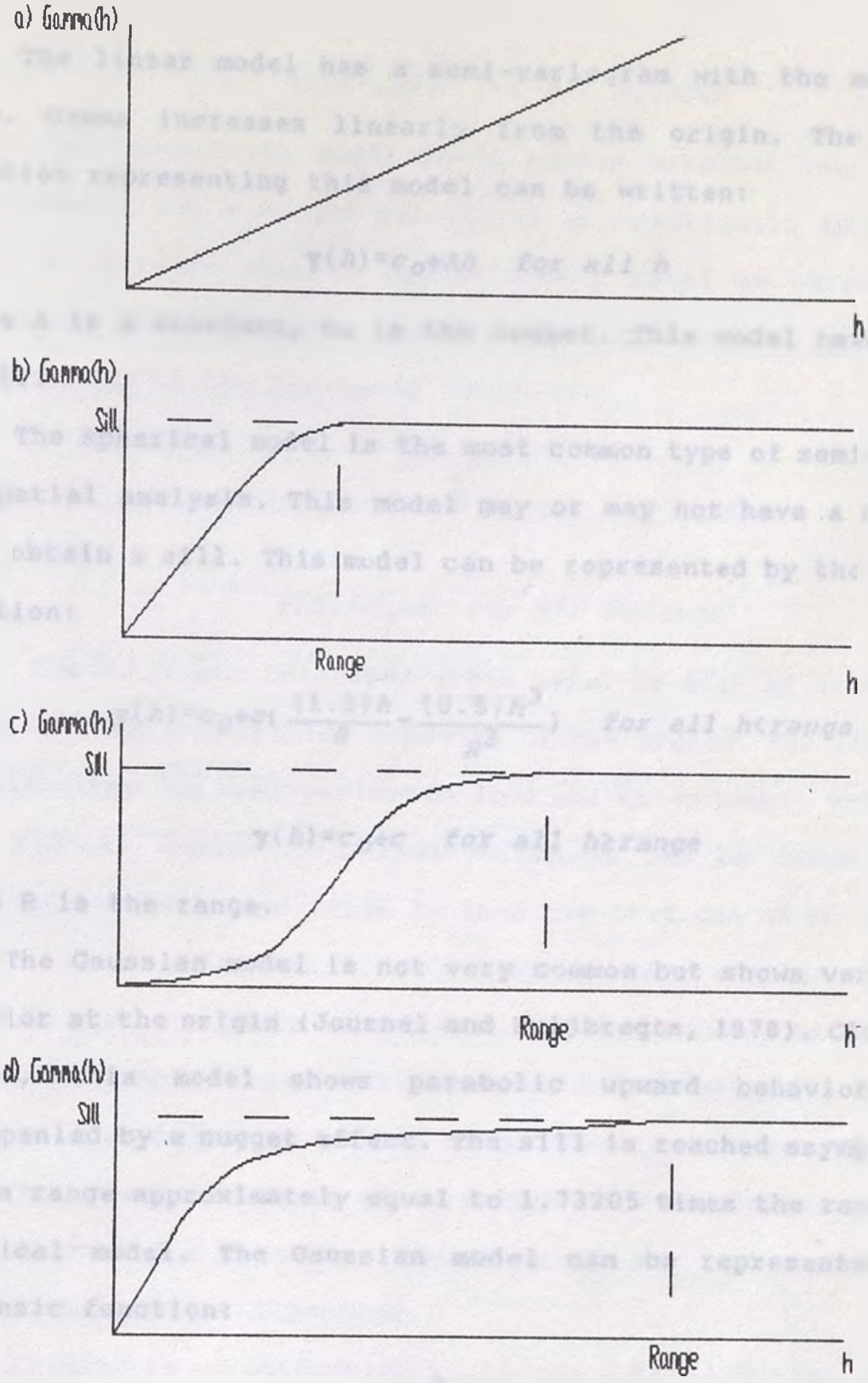


Figure II.3. Semi-variogram models: a) linear model b) spherical model c) Gaussian model d) exponential model.

The linear model has a semi-variogram with the most simple form. Gamma increases linearly from the origin. The intrinsic function representing this model can be written:

$$\gamma(h)=c_o+Ah \quad for\ all\ h$$

where A is a constant, c_o is the nugget. This model never attains a sill.

The spherical model is the most common type of semi-variogram in spatial analysis. This model may or may not have a nugget and will obtain a sill. This model can be represented by the intrinsic function:

$$\gamma(h)=c_o+c\left(\frac{(1.5)h}{R}-\frac{(0.5)h^3}{R^3}\right) \quad for\ all\ h<range$$

$$\gamma(h)=c_o+c \quad for\ all\ h\geq range$$

where R is the range.

The Gaussian model is not very common but shows very regular behavior at the origin (Journel and Huijbregts, 1978). Close to the origin, this model shows parabolic upward behavior usually accompanied by a nugget effect. The sill is reached asymptotically with a range approximately equal to 1.73205 times the range of the spherical model. The Gaussian model can be represented by the intrinsic function:

$$\gamma(h)=c_o+c\left(1-e^{\frac{-h^2}{R^2}}\right) \quad for\ all\ h<range$$

$$\gamma(h)=c_0+c \quad \text{for all } h \geq range$$

The exponential model has a linear behavior near the origin and usually has a nugget effect. It asymptotically approaches the sill at a range that is approximately equal to three times the range of the spherical model. The exponential model can be represented by the intrinsic function:

$$\gamma(h)=c_0+c(1-e^{\frac{-h}{R}}) \quad \text{for all } h<range$$

$$\gamma(h)=c_0+c \quad \text{for all } h \geq range$$

The intrinsic functions given here, as well as others, can be used to model the spatial behavior of the region. The first step is to calculate the semi-variogram from the known sample points within the spatial region. The semi-variogram can be compared to the various intrinsic functions to find one that can be an approximate model. If an intrinsic function has a shape similar to the data then it may be useable as a model. The semi-variogram data may not have a sill or a nugget effect but the models may still be useable. Once an appropriate model has been determined, then estimates can be made. Several methods of estimation are available, for example inverse-distance weighting and kriging. For this paper, kriging will be the method discussed.

Kriging is an estimation technique applied for the estimation of regionalized variables and is based on the notion to minimize the variance of the error. Kriging is a linearly weighted averaging estimator which uses the values of its nearest neighboring samples.

Kriging takes the form:

$$Z^*(x_0)=\sum_{i=1}^{N}\lambda_i Z(x_i)$$

where

x_0 = the location of the sample being estimated

$Z^*(x_0)$ = the estimate of the unknown sample at x_0

x_i = the locations of the known samples

$Z(x_i)$ = the values of known samples at x_i

λ_i = *the weight applied for sample* i

The kriging weights are determined by the estimation variance. Kriging is considered to be a best linear unbiased estimator. This non-biased condition assumes that the mean of Z remains unchanged during the estimation. This is a constraint that means that the sum of the weights must equal one:

$$\sum_{i=1}^{N}\lambda_i=1$$

Kriging is a technique which will find a set of weights that will minimize the estimation variance. It utilizes the geometry of the spatial region by taking into account the position of the samples relative to each other. The weights are calculated as a function of the semi-variogram.

There are two conditions that are imposed on the unknown sample estimation, Z^*, and the weights. The first is that Z^* must be an unbiased estimator such that $E[Z(x_0)-Z^*(x_0)] = 0$, where E is the expected value of the difference between the actual value of the unknown sample and the estimated value of the same sample. This expected value has the highest probability of being optimal, such that the variance of the kriging error is a minimum. This is the second condition. Both of these conditions must be met in order for kriging to be used to find a set of weights using the constraint that the sum of the weights equal one.

The variance of the kriging error must be minimized with respect to the weights. The Kriging error, q, can be expressed:

$$q = E[Z(x_o)-Z^*(x_o)]^2$$

The highest probability of the kriging error is zero. This implies that the error is normally distributed about the mean. The local expected value of the estimate is equal to the local mean value of Z at location x_o. Expanding this equation will give:

$$q = E[Z(x_o)-Z^*(x_o)][Z(x_o)-Z^*(x_o)]$$

$$q = E[Z(x_o)]^2 - 2E[Z(x_o)Z^*(x_o)] + E[Z^*(x_o)]^2$$

substituting the kriging equation in gives:

$$q=E[Z(x_o)]^2-2E[\sum_{i=1}^{N}\lambda_i Z(x_o)Z(x_i)]+E[\sum_{i=1}^{N}\lambda_i Z(x_i)]^2$$

The expected values in this equation can be replaced by using the notion of variances, covariances, and autocovariances. Variance can be defined as:

$$var(Z) = E[Z]^2 - m_z^2$$

where m_z is the mean value of Z. Covariance is a measure of the linear correlation between two variables Z and Z^* and is defined as:

$$cov(Z,Z^*) = E[Z,Z^*] - m_z m_{z^*}$$

Autocovariance is the covariance between a variable and itself. For this example, the autocovariance is defined:

$$\mathrm{cov}(Z,Z) = E[Z^2] - m_z^2$$

The kriging error can be further expanded:

$$q=E[Z(x_0)]^2-2\sum_{i=1}^{N}\lambda_i E[Z(x_0)Z(x_i)]+\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j E[Z(x_i)Z(x_j)]$$

Now the substitutions can be made to eliminate the expected values. This gives the following equation for the kriging error:

$$q=var[Z_R]+m_Z^2-2\sum_{i=1}^{N}\lambda_i(cov[Z_R,Z(x_i)]+m_Z^2)$$

$$+\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j[cov(Z(x_i),Z(x_j))+m_Z^2]$$

where m_z is the mean value of Z, and Z_R is the average value of the samples within the region R. The mean value terms will drop out of the equation after doing the addition. After doing this, the equation for kriging variance becomes:

$$q=var[Z_R]-2\sum_{i=1}^{N}\lambda_i(cov[Z_R,Z(x_i)])$$

$$+\sum_{i=1}^{N}\sum_{j=1}^{N}\lambda_i\lambda_j[cov(Z(x_i),Z(x_j))]$$

This equation is the fundamental formula representing the estimation variance of an estimate of an unknown sample within a spatial region. The value of the estimation variance is dependent on the magnitudes and positions of the neighboring samples.

The equation for the estimation variance is composed of three terms. The first term is the variance of the sample values within the spatial region R. The variance of the region depends on the average differences in the values between any two samples within the region. The value of this term can be determined by using the average semi-variogram.

The second term in the equation for the estimation variance is the covariance between the spatial region, R, and all of the known samples within the spatial region. This is the average variance between any point in the region and the region itself.

The third term in the equation for the estimation variance represents the covariance between the values of any two samples within the spatial region. This term can be found by using data from the semi-variogram.

Kriging is used to find the set of weights which minimizes the estimation variance under the condition that the expected value of the difference between the estimate of the unknown sample value and the actual value of the unknown sample. This leads to the constraint that the sum of the weights equal one. This leads to the use of a Lagrangian function of equating to zero the derivatives of:

$$Q=q-2\mu\left[\sum_{i=1}^{N}\lambda_i-1\right]$$

where μ is the Lagrangian multiplier, and Q is the optimized estimation variance plus the Lagrangian constraint. Taking the derivatives of this equation and setting equal to zero, will give the minimum value for the estimation variance. The derivatives must be taken with respect to the weights and the Lagrangian multiplier, μ.

Once the derivatives have been taken, then a systems of equations can be formed which can be used to model the data on the semi-variograms. These equations can be represented by the matrix system of the form:

$$[COV_{ij}]\begin{vmatrix}\lambda_i\\ \mu\end{vmatrix}=\begin{vmatrix}COV_{oi}\end{vmatrix}$$

This system of equations can be solved for the various values of the weights and for the Lagrangian multiplier, μ. Once this is done, the estimate can be made for the unknown sample. This can be done for any location within the spatial region.

Up to this point, the punctual form of kriging has been discussed to estimate the value of an unknown sample at a specific point in space. The specific case of block kriging will now be discussed.

Block kriging

Block kriging is a method of calculating the covariance between a sample point and an areal or volumetric block. The sample point can be located either within the block or on the outside of the block. One method of calculating the covariance between the sample point and the block, for the two dimensional case of an areal block, is given by the general equation:

$$[COV_{0i}] = \frac{1}{AREA}\iint_{AREA} COV_{0i}\ dxdy$$

where AREA is the area of the block. Using the semi-variogram, the covariance between the sample point and the block is the sill minus the value of the intrinsic function which describes the behavior between the sample and the block. Making this substitution with the sill equal to c_0+c, the equation becomes:

$$[COV_{0i}] = \frac{1}{AREA}\iint_{AREA}[c_0+c-\gamma(h_{0i})]\ dxdy$$

where h_{0i} is the distance between the sample point and the block. This equation can be put in the following form by making the assumption that the nugget effect and the sill is a constant:

$$[COV_{0i}] = \frac{1}{AREA}\iint_{AREA}c_0\ dxdy+\frac{1}{AREA}\iint_{AREA}c\ dxdy$$

$$-\frac{1}{AREA}\iint_{AREA}\gamma(h_{0i})\ dxdy$$

$$[COV_{oi}] = \frac{c_o}{AREA}\iint_{AREA} dxdy + \frac{c}{AREA}\iint_{AREA} dxdy$$

$$- \frac{1}{AREA}\iint_{AREA}\gamma(h_{oi})\ dxdy$$

$$[COV_{oi}] = c_o + c - \frac{1}{AREA}\iint_{AREA}\gamma(h_{oi})dxdy$$

The classical approach to block kriging is to discretize the block into a series of discrete points within the block. The points which form the mesh are regularly spaced. This method of computing covariances between the block and the sample point are shown in Figure II.4. The mesh points in the discretized block can be divided into an i,j coordinate system to identify each individual point. In this method, the value of $h_{o,i}$ becomes $h_{o,ij}$ and is the distance between the sample point and each of the mesh points within the block. Figure II.4 shows the sample point, labeled S, and a block divided into a sixteen mesh grid labeled i,j. Each mesh point is a node which can be labeled n_{ij}, where i and j vary from 1 to 4. The total area of the block is dxdy. The distances $h_{o,ij}$ are the sixteen distances between the sample point and each of the points in the mesh. After the block has been discretized into mesh points, the general equation for the covariance between the sample point and the block becomes (David, 1977):

$$[COV_{oi}] = c_o + c - \frac{1}{AREA}\iint_{AREA}\gamma(h_{o,ij})dxdy$$

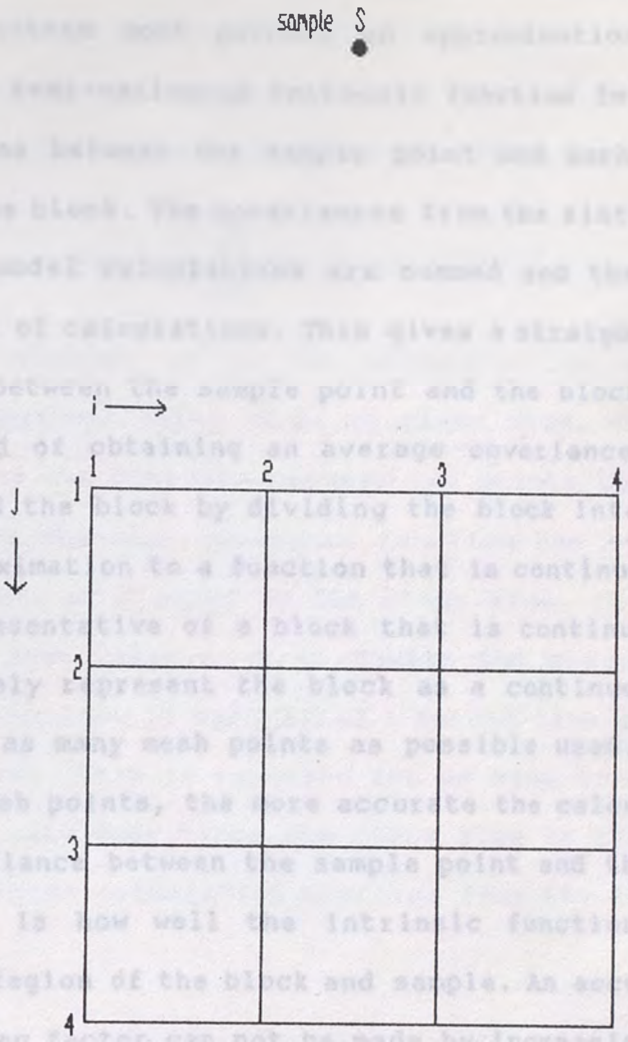


Figure II.4. The method of block kriging to calculate the covariance between a sample point, S, and a discretized block.

where $h_{o,ij} = [(X_{i,j}-X_o)^2 + (Y_{i,j}-Y_o)^2]^{1/2}$.

To evaluate the integral given above, for the case of a block divided into sixteen mesh points, an approximation is made by calculating the semi-variogram intrinsic function for each of the sixteen distances between the sample point and each of the mesh points within the block. The covariances from the sixteen different semi-variogram model calculations are summed and then divided by the total number of calculations. This gives a straight average for the covariance between the sample point and the block.

This method of obtaining an average covariance between the sample point and the block by dividing the block into mesh points is only an approximation to a function that is continuous. The mesh points are representative of a block that is continuous. For the mesh to adequately represent the block as a continuous function, there should be as many mesh points as possible used. The greater the number of mesh points, the more accurate the calculations will be for the covariance between the sample point and the block. The limiting factor is how well the intrinsic function models the behavior of the region of the block and sample. An accuracy greater than this limiting factor can not be made by increasing the number of mesh points. It is possible that sixteen, or even four mesh points can be adequate for the covariance calculation.

The method of block kriging can be used in three dimensions by using a three dimensional volumetric block with a three dimensional grid in an ijk coordinate system. The procedure is the same as in the two dimensional case.

Examples

1. Use the data values on the grid in Figure II.5 to plot a semi-variogram. Do calculations only in the east-west direction.

Solution:

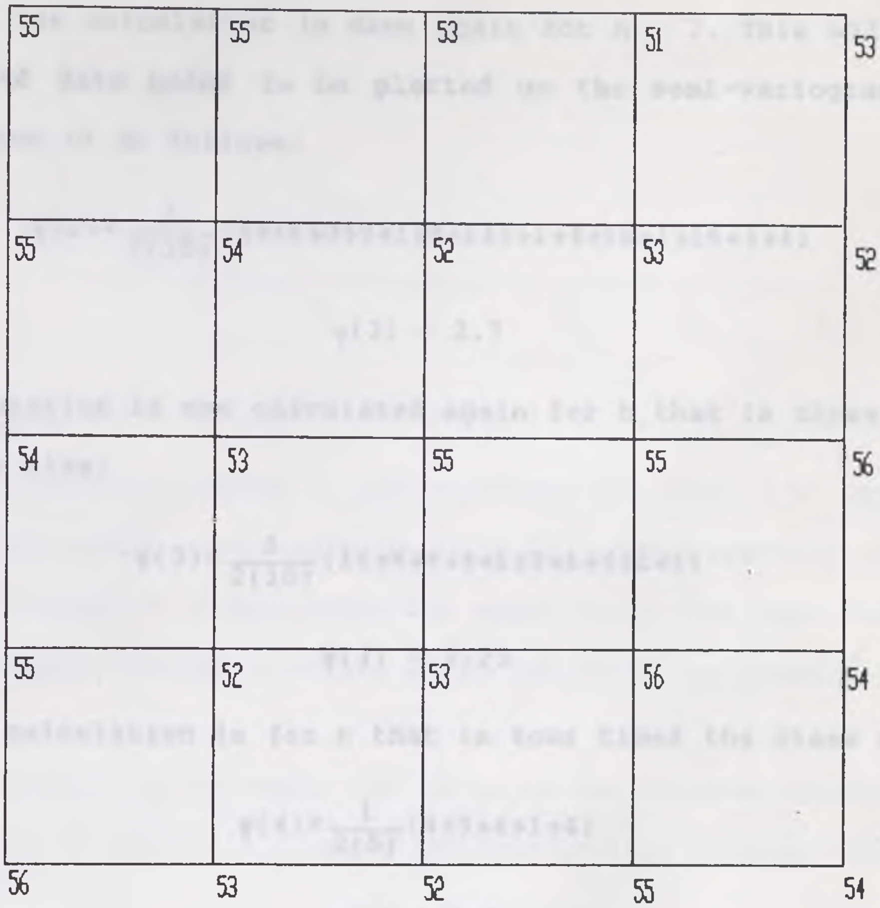
The semi-variogram is a graph of the function:

$$\gamma(h)=\frac{1}{2N}\sum_{i=1}^{N}[z(x_i)-z(x_i+h)]^2$$

plotted as a function of h. To calculate the semi-variogram function, the smallest value of h, or class size, should be used. The class size is the distance between two points that are next to each other. Once the semi-variogram function has been calculated for all the points of h equal to the class size, it is graphed as one point. The next value of h is double the class size and the semi-variogram function is calculated a second time giving a second data point to plot. This is repeated for as many times as the data allows, in this case four times the class size is the maximum. The first semi-variogram calculation starting from the top left corner is:

$$\gamma(1)=\frac{1}{2(20)}(0+4+4+4+1+4+1+1+1+4+0+1+9+1+9+4+9+1+9+1)$$

$$\gamma(1) = 1.7$$



55	55	53	51	53
55	54	52	53	52
54	53	55	55	56
55	52	53	56	54
56	53	52	55	54

Figure II.5. The data grid which is used for example 1 to calculate a semi-variogram.

This data value is the first point to be calculated on the semi-variogram. This value is plotted at h = 1 since h is equal to the class size. The value of h is now incremented to twice the class size and the calculation is done again for h = 2. This will give the second data point to be plotted on the semi-variogram. The calculation is as follows:

$$\gamma(2)=\frac{1}{2(15)}(4+16+0+9+1+0+1+4+1+4+16+1+16+4+4)$$

$$\gamma(2) = 2.7$$

The calculation is now calculated again for h that is three times the class size:

$$\gamma(3)=\frac{1}{2(10)}(16+4+4+4+1+9+1+4+1+1)$$

$$\gamma(3) = 2.25$$

The last calculation is for h that is four times the class size:

$$\gamma(4)=\frac{1}{2(5)}(4+9+4+1+4)$$

$$\gamma(4) = 2.2$$

This will give a fourth data point to plot on the semi-variogram. The semi-variogram is graphed in Figure II.6.

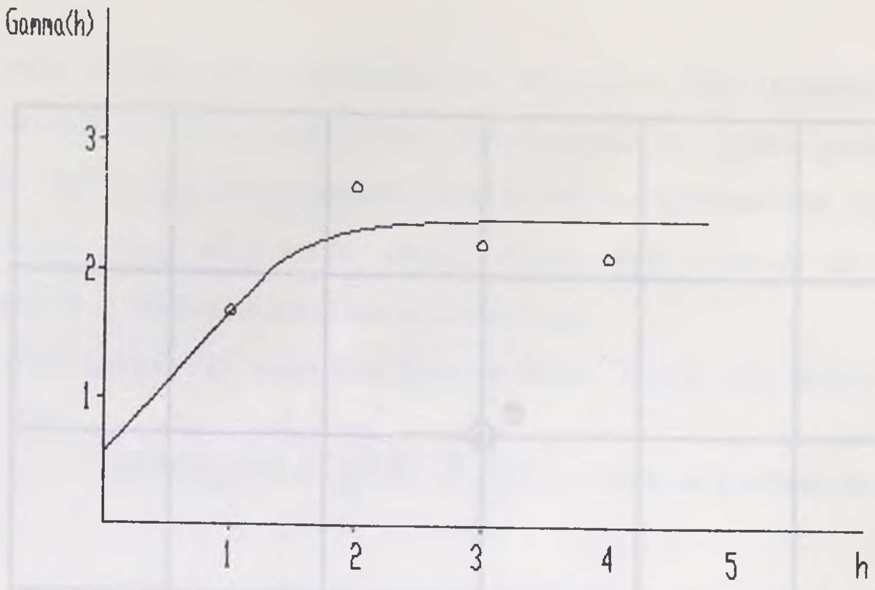


Figure II.6

The semi-variogram shows a nugget effect of about 0.5. The semi-variogram function increases up to a sill approximately equal to 2.3 at a range of h approximately equal to 2. The semi-variogram remains approximately constant after the range is reached.

2. Use kriging to estimate the value of the unknown sample point labeled S_o in Figure II.7 using the surrounding samples with known values.

Solution:

The value of the unknown sample can be estimated by using the matrix equation given previously:

$$[COV_{ij}]\begin{vmatrix}\lambda_i\\ \mu\end{vmatrix}=\begin{vmatrix}COV_{oi}\end{vmatrix}$$

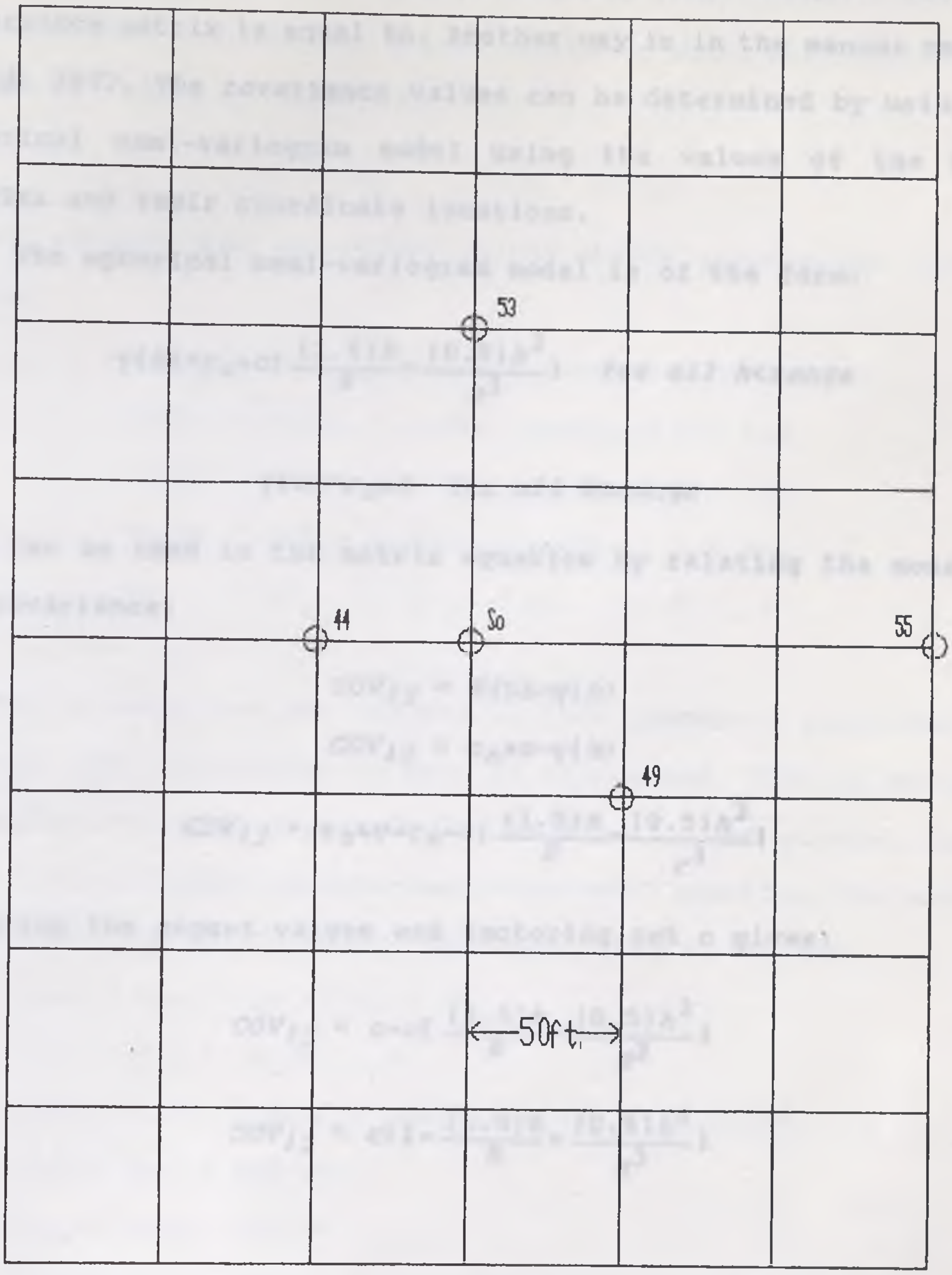


Figure II.7. Grid used in example 2 to estimate an unknown sample, So, by using the four surrounding known samples with labeled values.

One way to make the estimate is to solve the integral that the covariance matrix is equal to. Another way is in the manner used in David, 1977. The covariance values can be determined by using the spherical semi-variogram model using the values of the known samples and their coordinate locations.

The spherical semi-variogram model is of the form:

$$\gamma(h)=c_o+c\left(\frac{(1.5)h}{R}-\frac{(0.5)h^3}{R^3}\right) \quad \textit{for all } h<\textit{range}$$

$$\gamma(h)=c_o+c \quad \textit{for all } h\geq \textit{range}$$

This can be used in the matrix equation by relating the model to the covariance:

$$COV_{ij} = SILL-\gamma(h)$$

$$COV_{ij} = c_o+c-\gamma(h)$$

$$COV_{ij} = c_o+c-c_o-c\left[\frac{(1.5)h}{R}-\frac{(0.5)h^3}{r^3}\right]$$

Canceling the nugget values and factoring out c gives:

$$COV_{ij} = c-c\left[\frac{(1.5)h}{R}-\frac{(0.5)h^3}{R^3}\right]$$

$$COV_{ij} = c\left[1-\frac{(1.5)h}{R}+\frac{(0.5)h^3}{R^3}\right]$$

The matrix equation can written as a set of simultaneous equations which can be solved for the values of the weights. For simplicity, making the change of variables:

$$a_i = \lambda_i \qquad \sigma_{ij} = COV_{ij}$$

The set of equations equivalent to the matrix equation can now be written:

$$\begin{array}{l}
a_1\sigma_{11} + a_2\sigma_{12} + a_3\sigma_{13} + a_4\sigma_{14} + \mu = \sigma_{01} \\
a_1\sigma_{21} + a_2\sigma_{22} + a_3\sigma_{23} + a_4\sigma_{24} + \mu = \sigma_{02} \\
a_1\sigma_{31} + a_2\sigma_{32} + a_3\sigma_{33} + a_4\sigma_{34} + \mu = \sigma_{03} \\
a_1\sigma_{41} + a_2\sigma_{42} + a_3\sigma_{43} + a_4\sigma_{44} + \mu = \sigma_{04} \\
a_1 \quad + a_2 \quad + a_3 \quad + a_4 \quad + 0 = 1
\end{array}$$

In order to solve for the weights in this system of equations, a value for the covariance, σ, must be calculated. This is done by calculating all of the values of distance, h, and placing these values into the spherical semi-variogram model equation. The values of h between the sample points are calculated as follows:

$h_{11} = h_{22} = h_{33} = h_{44} = 0$

$h_{01} = h_{10} = 50$ ft.

$h_{02} = h_{20} = [(50)^2 + (50)^2]^{1/2}$ ft. = 70.71 ft.

$h_{03} = h_{30} = 100$ ft.

$h_{04} = h_{40} = 150$ ft.

$h_{12} = h_{21} = [(50)^2 + (100)^2]^{1/2}$ ft. = 111.80 ft.

$h_{13} = h_{31} = [(50)^2 + (100)^2]^{1/2}$ ft. = 111.80 ft.

$h_{14} = h_{41} = 200$ ft.

$h_{23} = h_{32} = [(50)^2 + (150)^2]^{1/2}$ ft. = 158.11 ft.

$$h_{24} = h_{42} = [(50)^2 + (100)^2]^{1/2} \text{ ft.} = 111.80 \text{ ft.}$$

$$h_{34} = h_{43} = [(100)^2 + (150)^2]^{1/2} \text{ ft.} = 180.28 \text{ ft.}$$

The values of h can now be put into the spherical semi-variogram model equation:

$$\sigma_{ij} = c[1 - \frac{(1.5)h}{R} + \frac{(0.5)h^3}{R^3}]$$

Using, for example, the values c_o = 5ft., c = 50ft., and R = 250ft. will give the following values for the covariances:

$$\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_{44} = 50.00$$

$$\sigma_{01} = \sigma_{10} = 35.20$$

$$\sigma_{02} = \sigma_{20} = 29.35$$

$$\sigma_{03} = \sigma_{30} = 21.60$$

$$\sigma_{04} = \sigma_{40} = 10.40$$

$$\sigma_{12} = \sigma_{21} = 18.50$$

$$\sigma_{13} = \sigma_{31} = 18.70$$

$$\sigma_{14} = \sigma_{41} = 2.80$$

$$\sigma_{23} = \sigma_{32} = 8.89$$

$$\sigma_{24} = \sigma_{42} = 18.70$$

$$\sigma_{34} = \sigma_{43} = 5.29$$

These values for the covariance can now be substituted into the set of equations for the matrix:

$$a_1(50.00) + a_2(18.70) + a_3(18.70) + a_4(2.80) + \mu = 35.20$$

$$a_1(18.70) + a_2(50.00) + a_3(8.89) + a_4(18.70) + \mu = 29.35$$

$$a_1(18.70) + a_2(8.89) + a_3(50.00) + a_4(5.290) + \mu = 21.60$$

$$a_1(2.80) + a_2(18.70) + a_3(5.29) + a_4(50.00) + \mu = 10.40$$

$$a_1 + a_2 + a_3 + a_4 + 0 = 1.00$$

There are five equations and five unknowns, consisting of the four weights and μ. These five unknowns can be found by many solving techniques available, for example Gaussian elimination. The solution to the set of equations are:

$$a_1 = 0.4866$$

$$a_2 = 0.3465$$

$$a_3 = 0.1602$$

$$a_4 = 0.006697$$

$$\mu = 1.3755$$

To make the final estimate for the unknown sample point, the values of the weights are needed. The unknown sample can be found by multiplying the known sample points with their corresponding weight and adding. The estimate of the unknown sample point is calculated as follows:

$$S_o = (0.4866)(44) + (0.3465)(49) + (0.1602)(53) + (0.006697)(55)$$

$$S_o = 47.25$$

In summary, the unknown value has been estimated using the known sample points and their locations. This involved kriging which uses the semi-variogram and an intrinsic function, the spherical semi-variogram model. These were used to calculate the weights to make the final calculation for the estimate.

Chapter III

Gauss Quadrature

Definite integrals can be evaluated in several ways, including the trapezoidal rule, Simpson's method, Weddle's method, and various types of Gaussian quadrature. The accuracy of these methods vary and the choice of the method to use may depend on the accuracy needed for any individual application. The method of integration of a function f(x) is approximated by all of these methods by evaluating the function for specific values of x and then multiplying this value by the width of the interval. This is an approximation for the area under the curve between the limits of the interval. This calculation for the area becomes exact when the function is linear and the curve becomes a straight line. The arguments, x, in all but Gauss quadrature are equally spaced about the midpoint of the integration interval. In Gauss quadrature, the argument is chosen at specific points in order to maximize the accuracy of the computation.

In order to achieve the best accuracy, the error of approximation must be minimized. The trapezoid rule, Simpson's method, and Weddle's method uses equally spaced points around the midpoint of the integration interval for the argument x. Gauss developed his quadrature methods to obtain better accuracy than the previous methods. He used points that are unequally spaced about the midpoint of the integration interval and are chosen to give a minimum of error.

In Gauss quadrature, as well as the other methods, the points used are symmetric about the integration midpoint. The sampling points, or Gauss points, are paired on each side of the midpoint. In contrast to the other methods, Gauss quadrature uses a variable spacing between each pair of selected points. The distance between pairs of Gauss points decreases as the location of the Gauss points increases from the midpoint (see Figure III.1). The spacing between pairs of Gauss points can be determined by using calculus techniques for minimizing the error.

Figure III.1 shows the location of Gauss points for functions using two, three, and four points. In the figure, M is the midpoint of the integration interval from a to b. The midpoint of the interval is (a+b)/2. Gauss points are located at a distance of t from the midpoint. For two Gauss points, The locations of the points are a distance of +t and -t away from the midpoint. For three points, there is a point located at the midpoint of the interval, labeled t_1. Two other points are symmetrically located at a distance $+t_2$ and $-t_2$ from the midpoints. For four Gauss points, the pairs of points are located $+/-t_1$ and $+/-t_2$ from the midpoint. The function is evaluated at each of the Gauss points and are shown as f(t) along the curve. Each Gauss point has an interval of width, W. The widths are symmetrically spaced due to the symmetric spacing of the Gauss points.

The accuracy of the computation depends on the number of Gauss points selected. If too few Gauss points are chosen then an inaccurate result will be obtained. The number of Gauss points

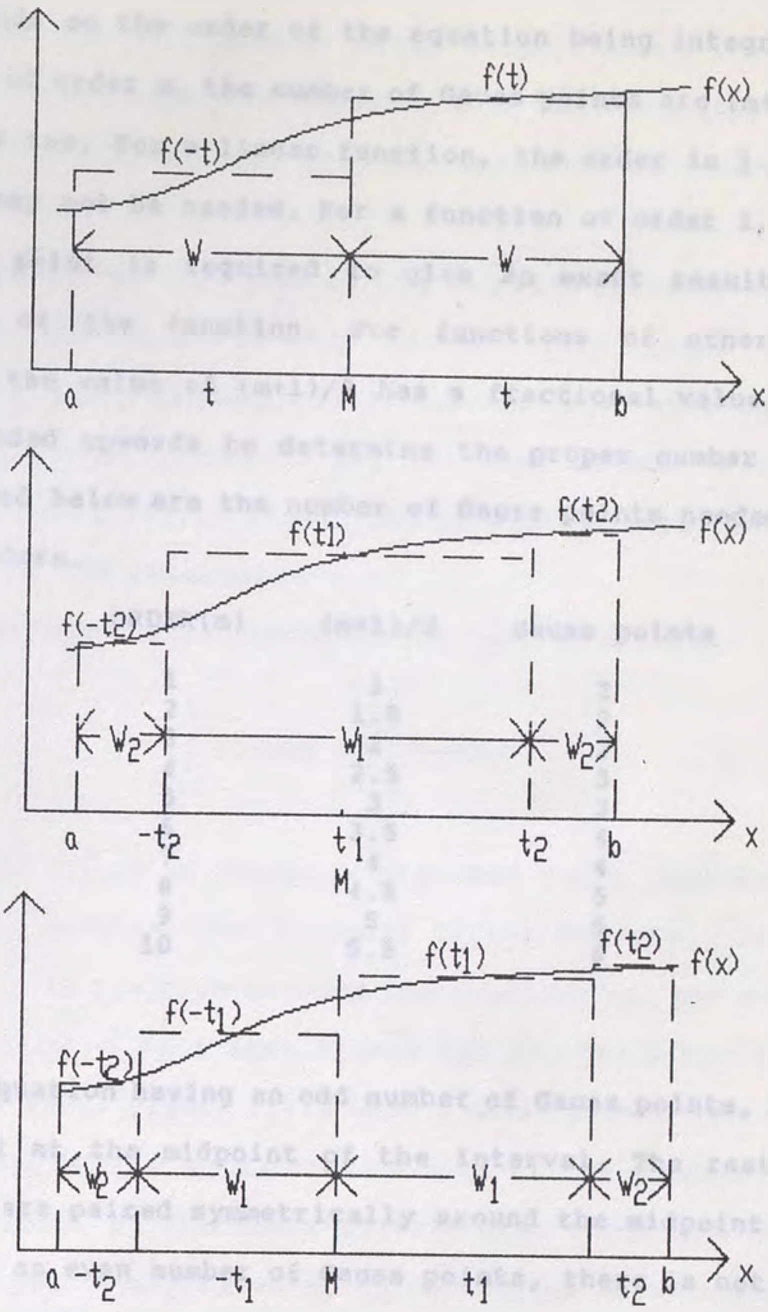


Figure III.1. A graphical representation for Gauss quadrature for two, three, and four Gauss points for a function f(x). The Gauss points are located at points t, W is the width of the rectangles, and M is the midpoint of the integration interval.

needed depends on the order of the equation being integrated. For an equation of order m, the number of Gauss points are (m+1)/2 with a minimum of two. For a linear function, the order is 1 and Gauss quadrature may not be needed. For a function of order 1, only one integration point is required to give an exact result for the integration of the function. For functions of other orders, moreover if the value of (m+1)/2 has a fractional value, then it must be rounded upwards to determine the proper number of Gauss points. Listed below are the number of Gauss points needed for the first ten orders.

ORDER(m)	(m+1)/2	Gauss points
1	1	2
2	1.5	2
3	2	2
4	2.5	3
5	3	3
6	3.5	4
7	4	4
8	4.5	5
9	5	5
10	5.5	6

For an equation having an odd number of Gauss points, there is a Gauss point at the midpoint of the interval. The rest of the Gauss points are paired symmetrically around the midpoint. For an equation with an even number of Gauss points, there is not a point located at the midpoint of the integration interval. There are only equally spaced pairs of points around the midpoint.

Each interval between Gauss points is weighted proportional to the width of the interval. The intervals closer to the midpoint will be larger and will have a larger weight. Since the width of the intervals decreases with distance from the midpoint, then the weight for each interval will also decrease with distance from the midpoint.

The intervals on each side of the midpoint correspond to Gauss points which are symmetrically paired. This means that the intervals are also symmetrically paired. The weights of the symmetrically paired intervals are the same on each side of the midpoint. In Figure III.1, the weight of each interval is equal to W, the width of the interval.

The Gauss quadrature approximation can be written:

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} W_i f(x)$$

where n is the number of Gauss points used for a function, f(x), and W_i are the weights. The integral of the function, f(x), with limits -1 to 1, is the area between the function and the x-axis for the interval from -1 to 1 (see Figure III.2). The midpoint of the interval is at zero. Figure III.2 uses 2 Gauss points labeled t and -t. The weights, W, are equal on each side of the midpoint and are equal to the width of the interval. The area under the curve for each interval can be approximated by rectangles whose widths are W and heights are the value of the function at the Gauss points. This is also the approximation for the evaluation of the definite integral. For increased accuracy, a higher number of intervals and Gauss points can be used. Then the areas of each interval can be

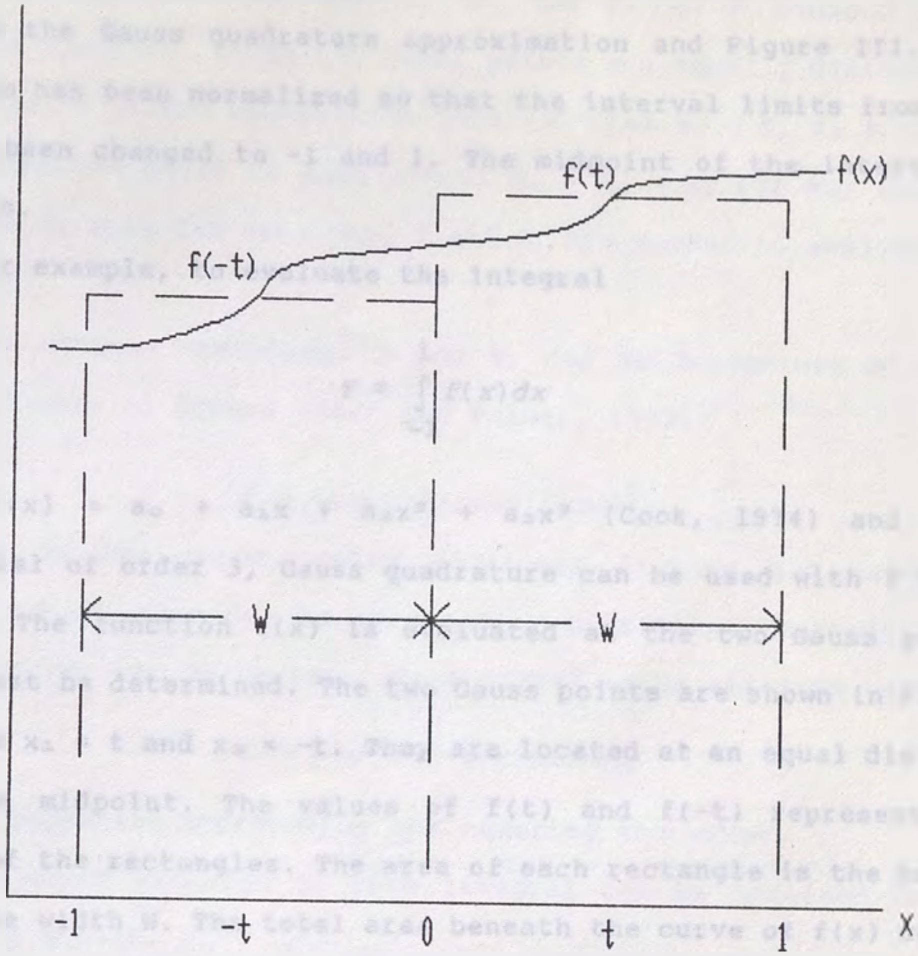


Figure III.2. A graphical representation of Gauss quadrature for two Gauss points for a function f(x). The Gauss points are located at x=-t and x=+t relative to the midpoint of the integration interval. The integration interval is from x=-1 to x=+1 and the midpoint is located at x=0.

summed giving the total area.

In the Gauss quadrature approximation and Figure III.2 the function has been normalized so that the interval limits from a to b have been changed to -1 and 1. The midpoint of the interval is now zero.

For example, to evaluate the integral

$$Y = \int_{-1}^{1} f(x)\,dx$$

where $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$ (Cook, 1974) and is a polynomial of order 3, Gauss quadrature can be used with 2 Gauss points. The function f(x) is evaluated at the two Gauss points which must be determined. The two Gauss points are shown in Figure III.2 as $x_1 = t$ and $x_2 = -t$. They are located at an equal distance from the midpoint. The values of f(t) and f(-t) represent the height of the rectangles. The area of each rectangle is the height times the width W. The total area beneath the curve of f(x) can be approximated by the sum of the rectangular areas, W(f(x)). In this case, the width of each rectangle is the same. For a larger number of Gauss points the widths vary.

The approximation using Gauss quadrature can be written

$$Y = \int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{2} W_i f(x_i)$$

where the four unknowns, x_1, x_2, W_1, and W_2 can be reduced to two by using symmetry. Since the Gauss points are equally distant from the midpoint of the integration interval then $x_1 = t$, $x_2 = -t$, and the widths are equal to each other, $W_1 = W_2 = W$. For any function of order 3, only two unknowns, t and W, are needed to evaluate the integral.

The unknown variables, t and W, can be determined by using Gauss' Theory of Errors (Carr and Palmer, 1993):

$$\epsilon \propto [\mathit{actual}\text{-}\mathit{predicted}]^2$$

where ϵ is the error, using difficult algebra and calculus. However, a solution can be obtained by more simple methods where the error, ϵ, can be written (Cook, 1974) as an absolute value:

$$\epsilon \propto \left|[\mathit{actual}\text{-}\mathit{predicted}]\right|$$

using a Laplacian approach by not squaring the error.

The exact solution to this integral can be obtained in the following manner.

$$Y = \int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} (a_0 + a_1x + a_2x^2 + a_3x^3)\,dx$$

$$Y = a_0x + \frac{1}{2}a_1x^2 + \frac{1}{3}a_2x^3 + \frac{1}{4}a_3x^4 \Big|_{-1}^{1}$$

$$Y = 2(a_0) + \frac{2}{3}(a_2)$$

The predicted solution to the integration using Gauss quadrature is found by

$$Y \approx Wf(x_1) + Wf(x_2) = W[f(x_1)+f(x_2)]$$

$$Y \approx W[f(t)+f(-t)]$$

where

$$f(t) = a_0 + a_1t + a_2t^2 + a_3t^3$$

$$f(-t) = a_0 - a_1t + a_2t^2 - a_3t^3$$

Adding f(t) and f(-t) and multiplying by W gives the approximate value of the integral

$$Y \approx W[2a_0 + 2a_2t^2] = 2Wa_0 + 2Wa_2t^2$$

The error can be found as the difference between the actual and the predicted solutions

$$\epsilon = \mathit{actual\text{-}predicted}$$

$$\epsilon = 2a_0+\frac{2}{3}a_2-2Wa_0-2Wa_2t^2$$

The values of the variables W and t can be found by minimizing the error for any values of a_0 and a_2. This is done by taking the derivative of the error with respect to a_0 and a_2 and then setting them equal to zero. Then W and t can be solved for. This is done in the following

$$\frac{\partial\epsilon}{\partial a_0} = 2-2W = 0$$

$$\frac{\partial \epsilon}{\partial a_2} = \frac{2}{3} - 2Wt^2 = 0$$

The first equation can be solved for W giving W = 1. The second equation can be solved for t by substituting in 1 for W. The result for +t and -t becomes

$$\pm t = \pm \frac{1}{\sqrt{3}}$$

The solutions for W and t are for the specific case of the integration limits of -1 and 1. For an integration interval of a to b, then the general case for two point Gauss quadrature integration approximation is

$$W = \frac{b-a}{2}; \quad \pm t = \frac{b+a}{2} \pm \frac{b-a}{2\sqrt{3}}$$

These values of W and t are sufficient to evaluate the integral of a function of order three or less.

The unknown variables, t and W, can also be found for the general case of using the integration limits from a to b. To evaluate the integral

$$Y = \int_a^b f(x)\,dx$$

where $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$, the same method can be used. The exact solution to this integral is obtained by integrating:

$$Y = \int_a^b (a_0+a_1x+a_2x^2+a_3x^3)\,dx$$

$$Y = a_0x+\frac{1}{2}a_1x^2+\frac{1}{3}a_2x^3+\frac{1}{4}a_3x^4 \Big|_a^b$$

$$Y = a_0b+\frac{1}{2}a_1b^2+\frac{1}{3}a_2b^3+\frac{1}{4}a_3b^4-a_0a-\frac{1}{2}a_1a^2-\frac{1}{3}a_2a^3-\frac{1}{4}a_3a^4$$

$$Y = a_0(b-a)+\frac{1}{2}a_1(b^2-a^2)+\frac{1}{3}a_2(b^3-a^3)+\frac{1}{4}a_3(b^4-a^4)$$

The solution using Gauss quadrature is:

$$Y = W[f(x_1)+f(x_2)] = W[f(-t)+f(t)]$$

$$Y = W[a_0+a_1(-t)+(-t)^2+a_3(-t)^3+a_0+a_1t+a_2t^2+a_3t^3]$$

$$Y = W[2a_0+2a_2t^2] = 2Wa_0+2Wa_2t^2$$

The error can be found as the difference between the actual and the predicted solutions

$$\epsilon = actual-predicted$$

$$\epsilon = a_0(b-a)+\frac{1}{2}a_1(b^2-a^2)+\frac{1}{3}a_2(b^3-a^3)+\frac{1}{4}a_3(b^4-a^4)-2Wa_0-2Wa_2t^2$$

The values of the variables W and t can be found by minimizing the error for any values of a_0 and a_2. This is done by taking the derivative of the error with respect to a_0 and a_2 and then setting them equal to zero. Then W and t can be solved for. This is done in the following

$$\frac{\partial \epsilon}{\partial a_0} = (b-a)-2W = 0$$

$$\frac{\partial \epsilon}{\partial a_2} = \frac{1}{3}(b^3-a^3)-2Wt^2 = 0$$

The first equation can be solved for W giving W = (b-a)/2. The second equation can be solved for t by substituting in W. The result for +t and -t becomes

$$\pm t = \pm\sqrt{\frac{1}{3}\,\frac{(b^3-a^3)}{b-a}}$$

For symmetric spacing, a = -b and t then becomes

$$\pm t = \pm\sqrt{\frac{1}{3}\left(\frac{2b^3}{b-a}\right)}$$

In the case of higher order functions, more Gauss points are required for an accurate approximation of definite integrals. A function of order four or order five can be accurately approximated using three Gauss points. For this case, there is a Gauss point located at the midpoint of the integration interval. For an interval from x = -1 to x = 1, the midpoint of the interval lies at x = 0. This is shown in Figure III.3, with the Gauss point labeled as t_1. The other two Gauss points are located at a distance of $+t_2$ and $-t_2$ from the midpoint as shown in Figure III.3.

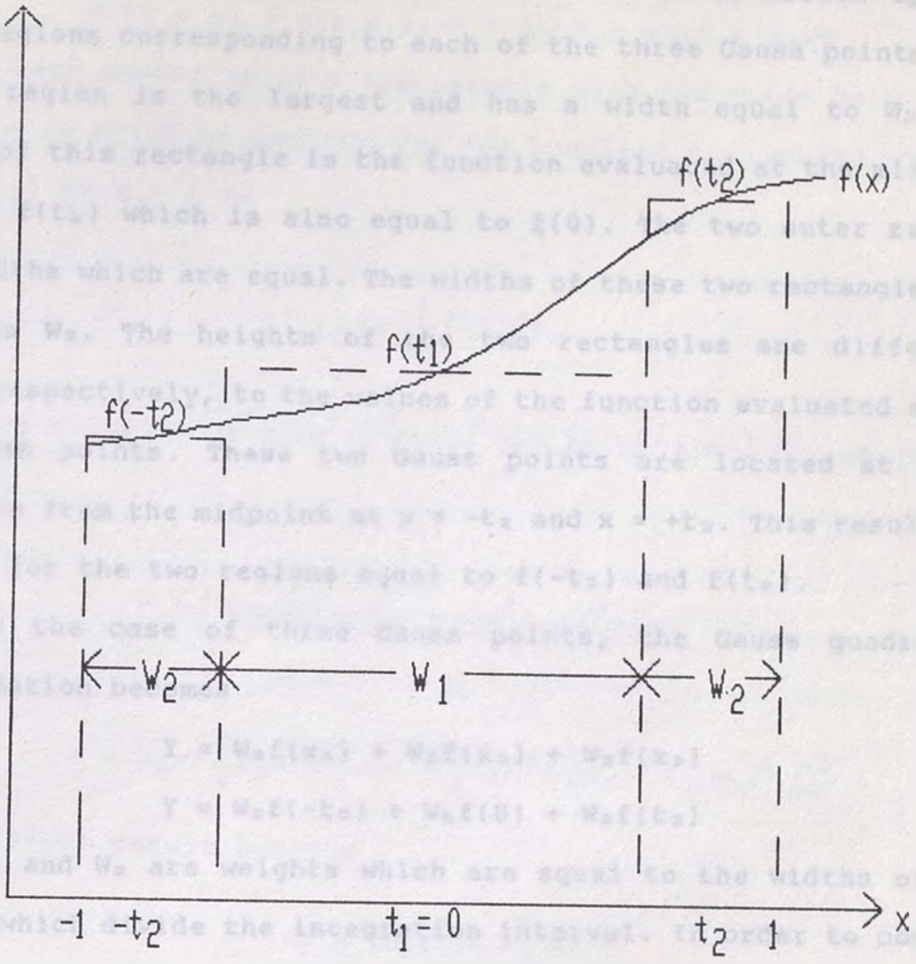


Figure III.3. A graphical representation of Gauss quadrature using three Gauss points for a function f(x). One Gauss point is located at the midpoint, x=0, and the other two are located at $x=-t_2$ and $x=+t_2$. The widths of the rectangles are labeled W_1 and W_2.

In Figure III.3, the integration interval is broken up into three regions corresponding to each of the three Gauss points. The center region is the largest and has a width equal to W_1. The height of this rectangle is the function evaluated at the midpoint labeled $f(t_1)$ which is also equal to $f(0)$. The two outer regions have widths which are equal. The widths of these two rectangles are shown as W_2. The heights of the two rectangles are different, equal, respectively, to the values of the function evaluated at the two Gauss points. These two Gauss points are located at equal distances from the midpoint at $x = -t_2$ and $x = +t_2$. This results in heights for the two regions equal to $f(-t_2)$ and $f(t_2)$.

For the case of three Gauss points, the Gauss quadrature approximation becomes

$$Y \approx W_2 f(x_1) + W_1 f(x_2) + W_2 f(x_3)$$

$$Y \approx W_2 f(-t_2) + W_1 f(0) + W_2 f(t_2)$$

where W_1 and W_2 are weights which are equal to the widths of the regions which divide the integration interval. In order to compute this approximation, the three unknown variables; t_2, W_1, and W_2 must be determined.

The unknown variables needed for the Gauss quadrature approximation can be determined in the same way as the previous example using two Gauss points. The error is the difference between the exact solution and the predicted solution obtained by Gauss quadrature. By minimizing the error, three equations can be formed in which to solve for the three unknown variables.

A function which has an order of five can be written as the following polynomial.

$$f(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5$$

In the same manner as with the example with two Gauss points, the integral in which to evaluate for the specific case of the interval of x = -1 to x = 1 is

$$Y = \int_{-1}^{1} f(x)\,dx$$

The exact solution of this integral can be obtained by integrating directly

$$Y = \int_{-1}^{1} (a_0+a_1x+a_2x^2+a_3x^3+a_4x^4+a_5x^5)\,dx$$

$$Y = a_0x+\frac{1}{2}a_1x^2+\frac{1}{3}a_2x^3+\frac{1}{4}a_3x^4+\frac{1}{5}a_4x^5+\frac{1}{6}a_5x^6 \Big|_{-1}^{1}$$

and the final result becomes

$$Y = 2a_0+\frac{2}{3}a_2+\frac{2}{5}a_4$$

The Gauss quadrature approximation to this integral will give the predicted solution which is

$$Y \approx W_2f(-t_2) + W_1f(0) + W_2f(t_2)$$

where

$$f(-t_2) = a_0 - a_1t_2 + a_2t_2^2 - a_3t_2^3 + a_4t_2^4 - a_5t_2^5$$

$$f(0) = a_0$$

$$f(t_2) = a_0 + a_1t_2 + a_2t_2^2 + a_3t_2^3 + a_4t_2^4 + a_5t_2^5$$

By placing these values of the function into the equation and canceling terms, the solution can be reduced to this form

$$Y \approx W_1 a_0 + 2W_2 a_0 + 2W_2 a_2 t^2 + 2W_2 a_4 t^4$$

$$Y \approx W_1 a_0 + 2W_2(a_0 + a_2 t^2 + a_4 t^4)$$

where t has been substituted in for t_2 since the value of t_1 is equal to zero.

The error can now be determined by subtracting the predicted Gauss quadrature approximation from the exact solution

$$\epsilon = 2a_0+\frac{2}{3}a_2+\frac{2}{5}a_4-W_1 a_0-2W_2(a_0+a_2 t^2+a_4 t^4)$$

The three unknowns; W_1, W_2, and t can be found by forming three equations by differentiating the equation for error with respect to a_0, a_2, and a_4. These equations are set equal to zero to allow a solution for W_1, W_2, and t that is a minimum for any values of a_0, a_2, and a_4. These three equations are

$$\frac{\partial\epsilon}{\partial a_0} = 2-W_1-2W_2 = 0$$

$$\frac{\partial\epsilon}{\partial a_2} = \frac{2}{3}-2W_2 t^2 = 0$$

$$\frac{\partial\epsilon}{\partial a_4} = \frac{2}{5}-2W_2 t^4 = 0$$

Solving the three equations for the unknown variables produces the results

$$W_2 = \frac{5}{9}; \quad W_1 = \frac{8}{9}; \quad \pm t = \pm\sqrt{\frac{3}{5}}$$

These values for W_1, W_2, and t are only valid for the specific integration interval between -1 and 1 with the midpoint at zero. More general solutions are available for the general case of any interval and any location of the midpoint. In general, for an integration interval between values a and b, the solutions for the case of three Gauss points (functions of orders four or five), are

$$W_1 = \frac{8}{9}\frac{(b-a)}{2} \; ; \quad t_1 = \frac{b+a}{2}$$

$$W_2 = \frac{5}{9}\frac{(b-a)}{2}$$

$$\pm t_2 = \frac{b+a}{2} \pm \left(\frac{b-a}{2}\right)\sqrt{\frac{3}{5}}$$

These equations are used in the approximation of the definite integral of a function of order four or five using Gauss quadrature and can be written

$$\int_a^b f(x)dx \approx W_1 f(t_1) + W_2(f(-t_2)+f(t_2))$$

The general form for Gauss quadrature can be written

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} W_i \cdot f(x_i)$$

where n is the number of Gauss points used. Table III.1. gives values of locations of Gauss points relative to the midpoint, t_i, and the weight of the interval over which the Gauss point is applied, W_i. Table III.1. shows data for a number of Gauss points ranging from two to six points. The data listed here are valid for the specific integration interval from -1 to 1 and the location of the midpoint at zero.

For the more general case of an integration interval from a to b, the weights and locations can be found in the following manner. The weights listed in Table III.1 must be multiplied by one-half of the integration interval. One-half of the integration interval is equal to (b-a)/2. Therefore, the new weights become

$$W_{i,new} = \frac{(b-a)}{2} W_i$$

The locations of the Gauss points are also changed when using the more general integration interval. The new location of the Gauss points are the old location multiplied by one-half of the integration interval, (b-a)/2. The new locations are now

$$t_{i,new} = \frac{(b-a)}{2} t_i$$

Table III.1. Gauss point locations and weights.

No. of Gauss Points	i	t_i	W_i
2	1	-0.5773502692	1.0000000000
	2	0.5773502692	1.0000000000
3	1	-0.7745966692	0.5555555556
	2	0.0000000000	0.8888888889
	3	0.7745966692	0.5555555556
4	1	-0.8611363116	0.3478548452
	2	-0.3399810436	0.6521451548
	3	0.3399810436	0.6521451548
	4	0.8611363116	0.3478548452
5	1	-0.9061798460	0.2369268850
	2	-0.5384693102	0.4786286704
	3	0.0000000000	0.5688888889
	4	0.5384693102	0.4786286704
	5	0.9061798460	0.2369268850
6	1	-0.9324695142	0.1713244924
	2	-0.6612093864	0.3607615730
	3	-0.2386191860	0.4679139346
	4	0.2386191860	0.4679139346
	5	0.6612093864	0.3607615730
	6	0.9324695142	0.1713244924

This new value for Gauss point locations must be added to the midpoint of the integration interval which may no longer be located at zero. The location of the midpoint of the interval is now

$$midpoint = \frac{(b+a)}{2}$$

The resulting locations of the Gauss points for the integration interval from a to b, with a midpoint of (b+a)/2, becomes

$$t_{i,new} = \frac{(b+a)}{2} \pm \frac{(b-a)}{2} \cdot t_i$$

As shown in Table III.1 all of the functions with an odd number of Gauss points have a Gauss point located at the center of the integration interval. All of the functions with an even number of Gauss points listed in Table III.1 have no Gauss point at the midpoint. As shown in Table III.1 the Gauss points are symmetrically spaced around the midpoint of the integration interval. Also, each pair of Gauss points are weighted equally on each side of the midpoint.

Examples

1. Approximate the following definite integral using Gauss quadrature:

$$\int_{1}^{10} (9x+5)\,dx$$

Solution:

The function in this example has an order of one, and therefore is a linear function. The minimum number of Gauss points required for this function is (1+1)/2 or one. Using two Gauss points, an accurate solution can be found. The following values for the Gauss quadrature approximation need to be calculated.

$$W = \frac{b-a}{2} = \frac{10-1}{2} = \frac{9}{2} = 4.5$$

$$-t = \frac{b+a}{2} - \frac{W}{\sqrt{3}} = \frac{10+1}{2} - \frac{4.5}{\sqrt{3}} = 2.901923789$$

$$+t = \frac{b+a}{2} + \frac{W}{\sqrt{3}} = \frac{10+1}{2} + \frac{4.5}{\sqrt{3}} = 8.098076211$$

$$f(-t) = 9(-t) + 5 = 9(2.901923789) + 5 = 31.11731410$$

$$f(+t) = 9(+t) + 5 = 9(8.098076211) + 5 = 77.88268590$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_{1}^{10} (9x+5)\,dx \approx W(f(-t)+f(+t))$$

$$\int_{1}^{10} (9x+5)\,dx \approx (4.5)(31.11731410+77.88268590) = 490.500000000$$

The precision that these equations are expressed is needed to closely approximate the exact value from direct integration. This will determine the accuracy of the Gauss quadrature approximation. The exact solution by integrating directly is

$$\int_1^{10}(9x+5)\,dx = \frac{9}{2}x^2+5x\Big|_1^{10} = \frac{9}{2}(10)^2+5(10)-\frac{9}{2}(1)^2-5(1) = 490.500000000$$

The difference between the exact solution and the Gauss quadrature solution is zero. For this example, the Gauss quadrature approximation is exact.

2. Approximate the following definite integral using Gauss quadrature:

$$\int_1^{10}(9x^2-7x+3)\,dx$$

Solution:

The function in this example has an order of two. The minimum number of Gauss points required in this function is (2+1)/2 or 3/2. This must be rounded upwards so that two Gauss points must be used to give an accurate solution. The following values must be calculated to use with the Gauss quadrature approximation.

$$W = \frac{b-a}{2} = \frac{10-1}{2} = \frac{9}{2} = 4.5$$

$$-t = \frac{b+a}{2} - \frac{W}{\sqrt{3}} = \frac{10+1}{2} - \frac{4.5}{\sqrt{3}} = 2.901923789$$

$$+t = \frac{b+a}{2} + \frac{W}{\sqrt{3}} = \frac{10+1}{2} + \frac{4.5}{\sqrt{3}} = 8.098076211$$

$$f(-t) = 9(-t)^2 - 7(-t) + 3 = 9(2.901923789)^2 - 7(2.901923789) + 3$$
$$= 58.47698857$$

$$f(+t) = 9(+t)^2 - 7(+t) + 3 = 9(8.098076211)^2 - 7(8.098076211) + 3$$
$$= 536.5230114$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_{1}^{10} (9x^2-7x+3)\,dx \approx W(f(-t)+f(+t))$$

$$\int_{1}^{10} (9x^2-7x+3)\,dx \approx (4.5)(58.47698857+536.5230114) = 2677.5000000000$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_{1}^{10} (9x^2-7x+3)\,dx = 3x^3-\frac{7}{2}x^2+3x\Big|_{1}^{10}$$

$$= 3(10)^3 - (3.5)(10)^2 + 3(10) - 3(1)^3 + (3.5)(1)^2 - 3(1)$$

$$= 2677.5000000000$$

The difference between the exact solution and the Gauss quadrature solution is zero. For this example, the Gauss quadrature approximation is exact.

3. Approximate the following definite integral using Gauss quadrature:

$$\int_{1}^{10} (x^3+3)\,dx$$

Solution:

The function in this example has an order of three. The minimum number of Gauss points required for this function is (3+1)/2 or two points. The following values must be calculated to use with the Gauss quadrature approximation.

$$W = \frac{b-a}{2} = \frac{10-1}{2} = \frac{9}{2} = 4.5$$

$$-t = \frac{b+a}{2} - \frac{W}{\sqrt{3}} = \frac{10+1}{2} - \frac{4.5}{\sqrt{3}} = 2.901923789$$

$$+t = \frac{b+a}{2} + \frac{W}{\sqrt{3}} = \frac{10+1}{2} + \frac{4.5}{\sqrt{3}} = 8.098076211$$

$$f(-t) = (-t)^3 + 3 = (2.901923789)^3 + 3$$

$$= 27.4375694000$$

$$f(+t) = (+t)^3 + 3 = (8.098076211)^3 + 3$$

$$= 534.0624305000$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_1^{10} (x^3+3)\,dx \approx W(f(-t)+f(+t))$$

which gives the approximate solution

$$\int_1^{10} (x^3+3)\,dx \approx (4.5)(27.43756940+534.0624305)$$

$$= 2526.7500000000$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_{1}^{10} (x^3+3)\,dx = \left.\frac{1}{4}x^4+3x\right|_{1}^{10}$$

$$= (0.25)(10)^4 + 3(10) - (0.25)(1)^4 - 3(1)$$

$$= 2526.7500000000$$

The difference between the exact solution and the Gauss quadrature solution is zero. For this example, the Gauss quadrature approximation is exact.

4. Approximate the following definite integral using Gauss quadrature:

$$\int_{2}^{7} (x^4)\,dx$$

Solution:

The function in this example has an order of four. The minimum number of Gauss points required for this function is (4+1)/2 or 2.5 points. This must be rounded upwards so that three Gauss points must be used to give an accurate solution.

For a function which uses three Gauss points, there are two weights which need to be calculated and the three locations for the Gauss points. The first Gauss point location is at the midpoint of the integration interval.

$$t_1 = \frac{b+a}{2} = \frac{7+2}{2} = 4.5$$

The other two Gauss point locations are

$$-t_2 = \frac{b+a}{2}-(\frac{b-a}{2})(0.7745966692) = \frac{7+2}{2}-(\frac{7-2}{2})(0.7745966692)$$

$$-t_2 = 2.563508327$$

$$+t_2 = \frac{b+a}{2}+(\frac{b-a}{2})(0.7745966692) = \frac{7+2}{2}+(\frac{7-2}{2})(0.7745966692)$$

$$+t_2 = 6.436491673$$

$$W_1 = \frac{b-a}{2}(0.8888888889) = (\frac{7-2}{2})(0.8888888889) = 2.2222222223$$

$$W_2 = \frac{b-a}{2}(0.5555555556) = (\frac{7-2}{2})(0.5555555556) = 1.3888888889$$

$$f(t_1) = (4.5)^4 = 410.062500$$

$$f(-t_2) = (2.563508327)^4 = 43.18559723$$

$$f(+t_2) = (6.436491673)^4 = 1716.314403$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_2^7 x^4 dx \approx W_1 f(t_1)+W_2 f(-t_2)+W_2 f(+t_2)$$

which gives the approximate solution

$$\int_2^7 x^4 dx \approx (2.2222222223)(410.062500)$$

$$+ (1.3888888889)(43.18559723)$$

$$+ (1.3888888889)(1716.314403)$$

$$= 3355.000$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_2^7 x^4 dx = \frac{1}{5}x^5\Big|_2^7$$

$$= (0.2)(7)^5 - (0.2)(2)^5 = 3361.400 - 6.400$$

$$= 3355.000$$

The difference between the exact solution and the Gauss quadrature solution is zero. For this example, the Gauss quadrature approximation is exact.

5. Approximate the following definite integral using Gauss quadrature:

$$\int_1^{10} (x^5+3x^2-2)dx$$

Solution:

The function in this example has an order of five. The minimum number of Gauss points required for this function is (5+1)/2 or three points which must be used to give an accurate solution.

For a function which uses three Gauss points, there are two weights which need to be calculated and the three locations for the Gauss points. The first Gauss point location is at the midpoint of the integration interval.

$$t_1 = \frac{b+a}{2} = \frac{10+1}{2} = 5.5$$

The other two Gauss point locations are

$$-t_2 = \frac{b+a}{2}-(\frac{b-a}{2})(0.7745966692) = \frac{10+1}{2}-(\frac{10-1}{2})(0.7745966692)$$

$$-t_2 = 2.014301489$$

$$+t_2 = \frac{b+a}{2}+(\frac{b-a}{2})(0.7745966692) = \frac{10+1}{2}+(\frac{10-1}{2})(0.7745966692)$$

$$+t_2 = 8.985698511$$

$$w_1 = \frac{b-a}{2}(0.8888888889) = (\frac{10-1}{2})(0.8888888889) = 4.000000$$

$$w_2 = \frac{b-a}{2}(0.5555555556) = (\frac{10-1}{2})(0.5555555556) = 2.500000$$

$$f(t_1) = (5.5)^5 + 3(5.5)^2 - 2$$

$$= 5121.593750$$

$$f(-t_2) = (2.014301489)^5 + 3(2.014301489)^2 - 2$$

$$= 43.18559723$$

$$f(+t_2) = (8.985698511)^5 + 3(8.985698511)^2 - 2$$

$$= 58821.556666$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_1^{10} (x^5+3x^2-2)\,dx \approx W_1 f(t_1) + W_2 f(-t_2) + W_2 f(+t_2)$$

which gives the approximate solution

$$\int_1^{10} (x^5+3x^2-2)\,dx \approx (4.000000)(5121.593750)$$

$$+ (2.500000)(43.33283062)$$

$$+ (2.500000)(58821.556666)$$

$$= 167648.5987$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_1^{10} (x^5+3x^2-2)\,dx = \frac{1}{6}x^6 + x^3 - 2x\Big|_1^{10}$$

$$= (1/6)(10)^{6} + (10)^{3} - 2(10)$$

$$- (1/6)(1)^{6} - (1)^{3} + 2(1)$$

$$= 167647.500000$$

The accuracy of the Gauss quadrature approximation can be found by calculating the relative difference between the exact solution and the approximate solution. This is done by

$$accuracy = \left|\frac{exact-approximate}{exact}\right| = \left|\frac{167747.500000-167648.5987}{167747.500000}\right|$$

$$= 6.553632(10)^{-6}$$

There is a 0.000655 percent difference between the Gauss quadrature approximation and the exact solution.

6. Approximate the following definite integral using Gauss quadrature:

$$\int_{1}^{10} \sqrt{x}\, dx$$

Solution:

The function in this example has an order of one-half. The minimum number of Gauss points required for this function is (0.5+1)/2 or 0.75. Using two Gauss points, an accurate solution can be found. The following values for the Gauss quadrature approximation need to be calculated.

$$W = \frac{b-a}{2} = \frac{10-1}{2} = \frac{9}{2} = 4.5$$

$$-t = \frac{b+a}{2} - \frac{W}{\sqrt{3}} = \frac{10+1}{2} - \frac{4.5}{\sqrt{3}} = 2.901923789$$

$$+t = \frac{b+a}{2} + \frac{W}{\sqrt{3}} = \frac{10+1}{2} + \frac{4.5}{\sqrt{3}} = 8.098076211$$

$$f(-t) = (-t)^{1/2} = (2.901923789)^{1/2} = 1.703503387$$

$$f(+t) = (+t)^{1/2} = (8.098076211)^{1/2} = 2.845711899$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_{1}^{10} \sqrt{x}\,dx \approx W(f(-t)+f(+t))$$

$$\int_{1}^{10} \sqrt{x}\,dx \approx (4.5)(1.703503387+2.845711899) = 20.47146879$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_{1}^{10} \sqrt{x}\,dx = \frac{2}{3}x^{\frac{3}{2}}\Big|_{1}^{10}$$

$$= (2/3)(10)^{3/2} - (2/3)(1)^{3/2}$$

$$= 20.41518440$$

The accuracy of the Gauss quadrature approximation can be found by calculating the relative difference between the exact solution and the approximate solution. This is done by

$$accuracy = \left|\frac{exact-approximate}{exact}\right| = \left|\frac{20.41518440-20.47146879}{20.41518440}\right|$$

$$= 2.7569866(10)^{-3}$$

There is a 0.276 percent difference between the Gauss quadrature approximation and the exact solution.

7. Approximate the following definite integral using Gauss quadrature:

$$\int_{1}^{10} (x^7+x-7)\,dx$$

Solution:

The function in this example has an order of seven. The minimum number of Gauss points required for this function is (7+1)/2 or four points which must be used to give an accurate solution.

For a function which uses four Gauss points, there are two weights which need to be calculated, W_1 and W_2. and the four locations for the Gauss points. The is no Gauss point located at the midpoint of the integration interval.

In Figure III.4, a graphical representation of Gauss

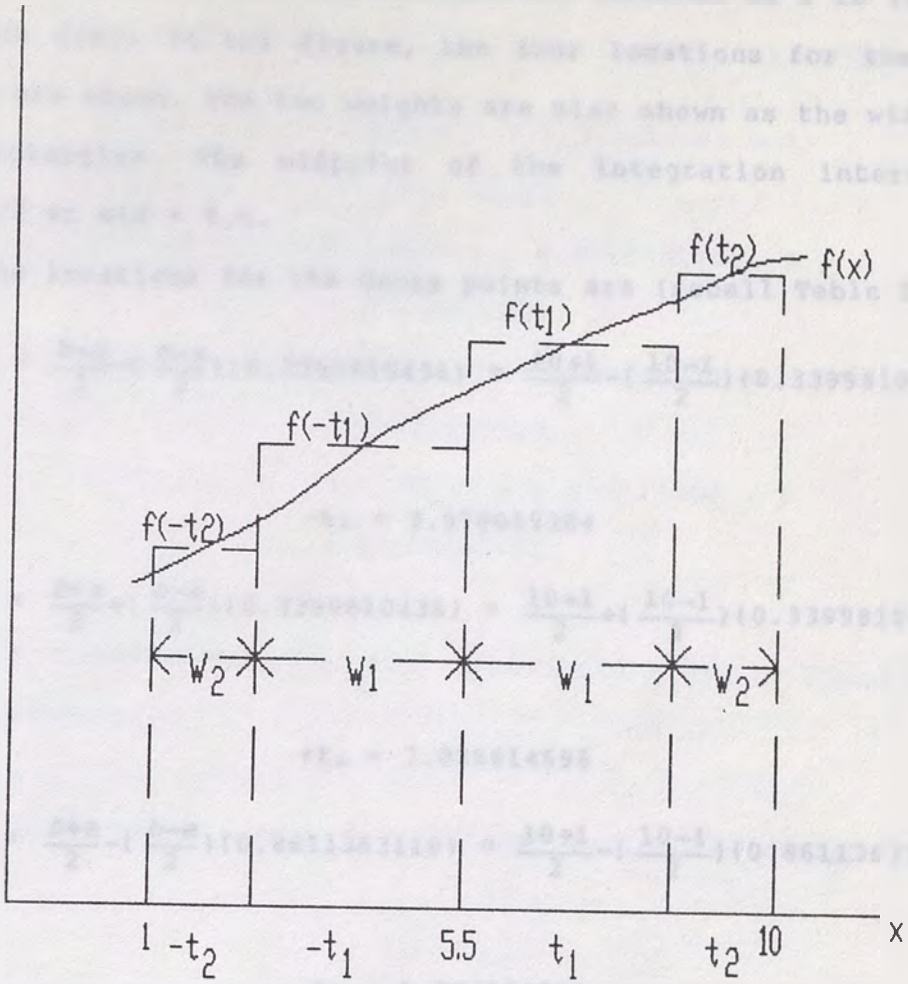


Figure III.4. This is a graphical representation of Gauss quadrature used in example 7. with an arbitrary function f(x). There are four Gauss points labeled $-t_1$, t_1, $-t_2$, t_2 and two weights labeled W_1 and W_2. The interval is in the range of one to ten, with the midpoint at 5.5.

quadrature is shown for the integration interval of 1 to 10 for a function f(x). In the figure, the four locations for the Gauss points are shown. The two weights are also shown as the widths of the rectangles. The midpoint of the integration interval is (10+1)/2 or mid = 5.5.

The locations for the Gauss points are (recall Table III.1):

$$-t_1 = \frac{b+a}{2}-\left(\frac{b-a}{2}\right)(0.3399810436) = \frac{10+1}{2}-\left(\frac{10-1}{2}\right)(0.3399810436)$$

$$-t_1 = 3.970085304$$

$$+t_1 = \frac{b+a}{2}+\left(\frac{b-a}{2}\right)(0.3399810436) = \frac{10+1}{2}+\left(\frac{10-1}{2}\right)(0.3399810436)$$

$$+t_1 = 7.029914696$$

$$-t_2 = \frac{b+a}{2}-\left(\frac{b-a}{2}\right)(0.8611363116) = \frac{10+1}{2}-\left(\frac{10-1}{2}\right)(0.8611363116)$$

$$-t_2 = 1.624886598$$

$$+t_2 = \frac{b+a}{2}+\left(\frac{b-a}{2}\right)(0.8611363116) = \frac{10+1}{2}+\left(\frac{10-1}{2}\right)(0.8611363116)$$

$$+t_2 = 9.375113402$$

The two weights are

$$W_1 = \frac{b-a}{2}(0.6521451548) = \left(\frac{10-1}{2}\right)(0.6521451548) = 2.934653197$$

$$W_2 = \frac{b-a}{2}(0.347854852) = (\frac{10-1}{2})(0.347854852) = 1.565346834$$

$$f(-t_1) = (3.970085304)^7 + 3.970085304 - 7$$

$$= 15542.26154$$

$$f(+t_1) = (7.029914696)^7 + 7.029914696 - 7$$

$$= 848497.1761$$

$$f(-t_2) = (1.624886598)^7 + 1.624886598 - 7$$

$$= 24.53109784$$

$$f(+t_2) = (9.375113402)^7 + 9.375113402 - 7$$

$$= 6365549.063$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_1^{10} (x^7+x-7)dx \approx W_1 f(-t_1)+W_1 f(+t_1)+W_2 f(-t_2)+W_2 f(+t_2)$$

which gives the approximate solution

$$\int_1^{10} (x^7+x-7)dx \approx (2.934653197)(15542.26154)$$

$$+ (2.934653197)(848497.1761)$$

$$+ (1.565346834)(24.53109784)$$

$$+ (1.565346834)(6365549.063)$$

$$= 12499986.570$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_{1}^{10} (x^7+x-7)\,dx = \frac{1}{8}x^8+\frac{1}{2}x^2-7x\Big|_{1}^{10}$$

$$= (1/8)(10)^8 + (1/2)(10)^2 - 7(10)$$

$$- (1/8)(1)^8 - (1/2)(1)^2 + 7(1)$$

$$= 12499986.380$$

The accuracy of the Gauss quadrature approximation can be found by calculating the relative difference between the exact solution and the approximate solution. This is done by

$$accuracy = \left|\frac{exact-approximate}{exact}\right| = \left|\frac{12499986.380-12499986.570}{12499986.380}\right|$$

$$= 1.520002(10)^{-8}$$

There is a 0.00000152 percent difference between the Gauss quadrature approximation and the exact solution.

8. Approximate the following definite integral using Gauss quadrature:

$$\int_{1}^{10} e^x dx$$

Solution:

The function in this example has an unknown order. Expanding this function into a Taylor's series expansion shows that the exponent will increase to infinity. Truncating the series will give an order equal to the highest exponent. This produces a truncation error which is the sum of all of the terms truncated. For an order of ten or eleven, six Gauss points are needed, and the truncation error is negligible (Carr and Palmer, 1993). For an order of eight or nine, five Gauss points are needed, the error is less than $1(10)^{-6}$.

For this example, four Gauss points will be used to determine the accuracy obtained by using the Gauss quadrature approximation. For a function which uses four Gauss points, there are two weights which need to be calculated, W_1 and W_2. and the four locations for the Gauss points. The is no Gauss point located at the midpoint of the integration interval. The four locations for the Gauss points are

$$-t_1 = \frac{b+a}{2}-(\frac{b-a}{2})(0.3399810436) = \frac{10+1}{2}-(\frac{10-1}{2})(0.3399810436)$$

$$-t_1 = 3.970085304$$

$$+t_1 = \frac{b+a}{2}+(\frac{b-a}{2})(0.3399810436) = \frac{10+1}{2}+(\frac{10-1}{2})(0.3399810436)$$

$$+t_1 = 7.029914696$$

$$-t_2 = \frac{b+a}{2}-(\frac{b-a}{2})(0.8611363116) = \frac{10+1}{2}-(\frac{10-1}{2})(0.8611363116)$$

$$-t_2 = 1.624886598$$

$$+t_2 = \frac{b+a}{2}+(\frac{b-a}{2})(0.8611363116) = \frac{10+1}{2}+(\frac{10-1}{2})(0.8611363116)$$

$$+t_2 = 9.375113402$$

The two weights are

$$W_1 = \frac{b-a}{2}(0.6521451548) = (\frac{10-1}{2})(0.6521451548) = 2.934653197$$

$$W_2 = \frac{b-a}{2}(0.347854852) = (\frac{10-1}{2})(0.347854852) = 1.565346834$$

$$f(-t_1) = e^{3.970085304} = 52.98905082$$

$$f(+t_1) = e^{7.029914696} = 1129.934218$$

$$f(-t_2) = e^{1.624886598} = 5.077843167$$

$$f(+t_2) = e^{9.375113402} = 11791.25462$$

Using these quantities, the approximation can be found using Gauss quadrature.

$$\int_1^{10} e^x dx \approx W_1 f(-t_1)+W_1 f(+t_1)+W_2 f(-t_2)+W_2 f(+t_2)$$

which gives the approximate solution

$$\int_{1}^{10} e^{x}dx \approx (2.934653197)(52.98905082)$$

$$+ (2.934653197)(1129.934218)$$

$$+ (1.565346834)(5.077843167)$$

$$+ (1.565346834)(5.077843167)$$

$$= 21936.82122$$

This solution will need to be compared to the exact solution from direct integration to determine the accuracy of the Gauss quadrature solution. The exact solution from integrating directly is

$$\int_{1}^{10} e^{x}dx = e^{x}\Big|_{1}^{10} = e^{10}-e^{1} = 22023.74751$$

The accuracy of the Gauss quadrature approximation can be found by calculating the relative difference between the exact solution and the approximate solution. This is done by

$$accuracy = \left|\frac{exact-approximate}{exact}\right| = \left|\frac{22023.74751-21936.82122}{22023.74751}\right|$$

$$= 3.94693455(10)^{-3}$$

There is a 0.394693455 percent difference between the Gauss quadrature approximation and the exact solution.

Chapter IV

An Experiment To Approximate Block-Sample Covariance

The covariance between a sample point and a block can be calculated by both kriging and Gauss quadrature. The classical method to do this is by discretizing the block into grid points, calculating the covariances between the sample point and each of the points in the block, and averaging. Another way to calculate covariances is by using Gauss quadrature to evaluate the block-sample covariance integrals. An experiment to compare the two different methods has been done on four covariance models. These models are the linear model, spherical model, exponential model, and the Gaussian model which have been previously discussed in chapter II.

The geometry of a sample point and the block which is used for the experiment is shown in Figure IV.1. The sample point is located at the position (9,3) and the block is 6x6 units which is centered at the position (3,3). The experiment will compute the covariance between the sample point and the block using both kriging and Gauss quadrature. The precision for both methods will then be compared to determine the best method.

The kriging method will discretize the block into five different grid sizes. The different grid sizes are 4 x 4, 50 x 50, 100 x 100, 150 x 150, and 200 x 200. The block covariance will be calculated for each grid size to compare with the Gauss quadrature results. The accuracy of the kriging calculations will improve as

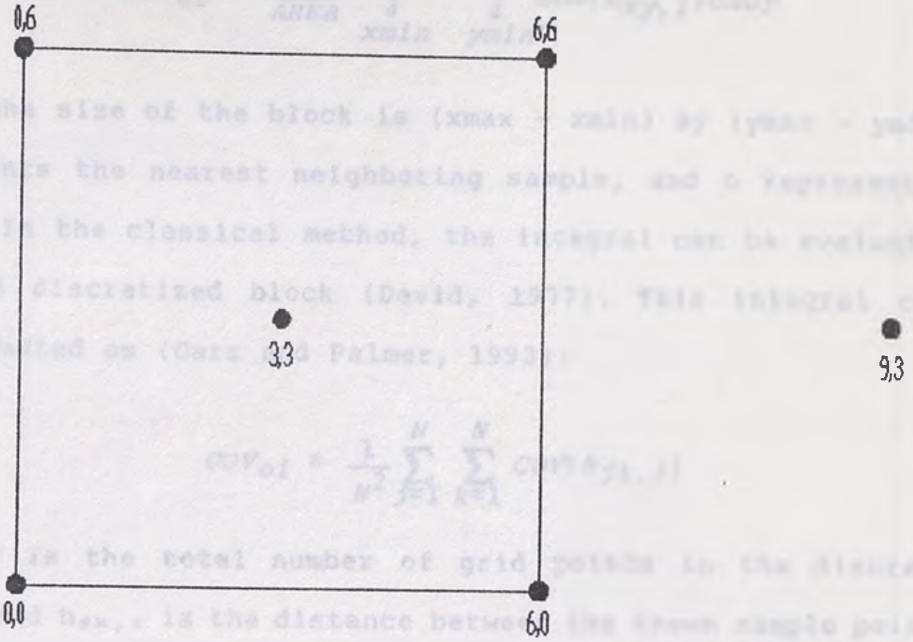


Figure IV.1. An experiment to calculate block-sample covariance between a block centered at (3,3) and a sample point located at (9,3).

the number of grid points is increased.

The covariance between the sample point and the block can be determined by evaluating the following integral:

$$COV_{oi} = \frac{1}{AREA} \int_{xmin}^{xmax} \int_{ymin}^{ymax} COV(h_{xy,i})\,dx\,dy$$

where the size of the block is (xmax - xmin) by (ymax - ymin), i represents the nearest neighboring sample, and o represents the block. In the classical method, the integral can be evaluated by using a discretized block (David, 1977). This integral can be approximated as (Carr and Palmer, 1993):

$$COV_{oi} = \frac{1}{N^2} \sum_{j=1}^{N} \sum_{k=1}^{N} COV(h_{jk,i})$$

where N is the total number of grid points in the discretized block, and $h_{jk,i}$ is the distance between the known sample point and each of the grid points. For this experiment, the values of N are 4, 50, 100, 150, and 200. This equation calculates the covariance between each grid point and the sample point and then averages the values by dividing by the number of grid points used. Figure IV.2 shows the classical method of discretizing the block into regularly spaced grid points using a 4 x 4 grid.

There are four covariance models used in the experiment to calculate the covariances using the classical method. Within the distance of the range, the four models are:

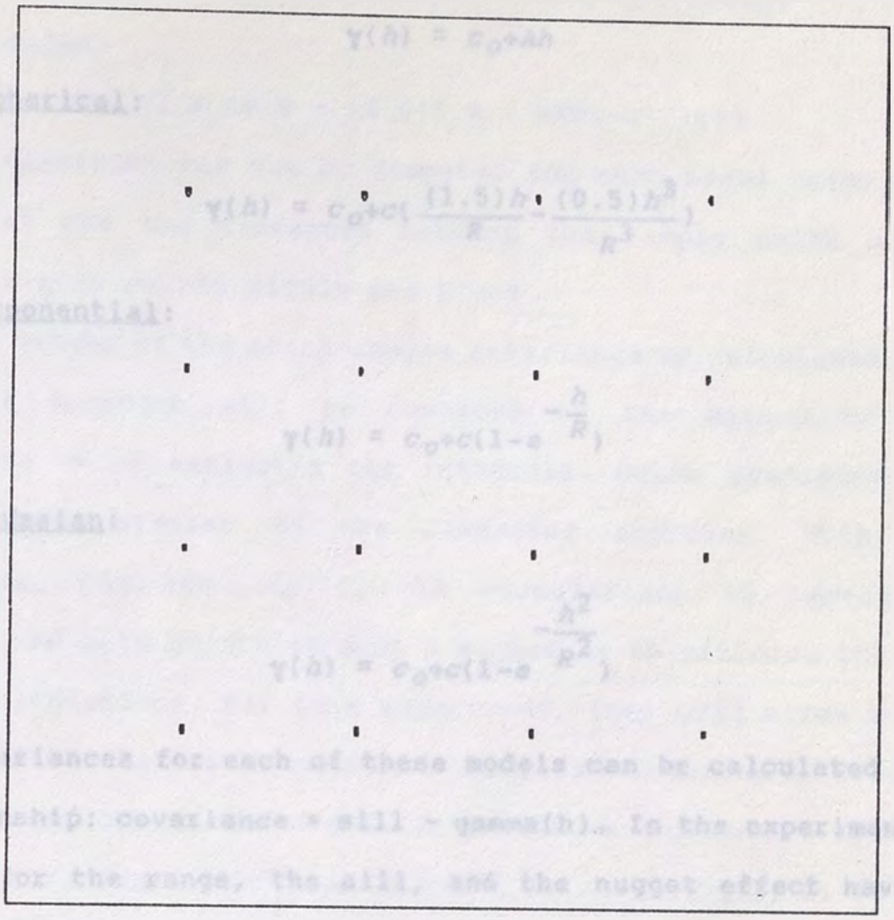


Figure IV.2. The classical method of block kriging by discretizing a block into a regularly spaced grid. The case of a 4 x 4 grid is shown.

linear:

$$\gamma(h) = c_o + Ah$$

spherical:

$$\gamma(h) = c_o + c\left(\frac{(1.5)h}{R} - \frac{(0.5)h^3}{R^3}\right)$$

exponential:

$$\gamma(h) = c_o + c\left(1 - e^{-\frac{h}{R}}\right)$$

Gaussian:

$$\gamma(h) = c_o + c\left(1 - e^{-\frac{h^2}{R^2}}\right)$$

The covariances for each of these models can be calculated by the relationship: covariance = sill - gamma(h). In the experiment, the values for the range, the sill, and the nugget effect have been arbitrarily chosen. These values using arbitrary units are:

R = range = 10

c_o = nugget effect = 0

c = sill = 10

The covariance values for each model becomes:

linear:

COV(h) = 10.0 - h

spherical:

COV(h) = 10.0 - 10.0(0.15h - 0.0005h^3)

<u>exponential</u>:

$$COV(h) = 10.0 - 10.0(1.0 - EXP(-h/3.3333))$$

<u>Gaussian</u>:

$$COV(h) = 10.0 - 10.0(1.0 - EXP(-h^2/36))$$

These covariances can now be computed for each model using values of h that are the distances between the sample point and the different grid points within the block.

The values of the block-sample covariance as calculated by the classical approach will be compared to the method of Gauss quadrature which evaluates the integrals. Gauss quadrature also uses a grid similar to the classical approach. With Gauss quadrature, the accuracy of the calculations is improved by locating the grid points in such a manner as to minimize the error of the calculations. For this experiment, four grid sizes will be used to calculate the block-sample covariance. The grid sizes are 3 x 3, 4 x 4, 5 x 5, and 6 x 6. In the Gauss quadrature approach, the grid locations correspond to Gauss points using 3, 4, 5, and 6 Gauss points. The grid point locations are not regularly spaced but are symmetrically spaced about the center of the block. Figure IV.3 shows the discretized block using 3, 4, 5, and 6 Gauss points.

Using the Gauss quadrature method, the covariance between the block and the sample point can be calculated with the following approximation:

$$COV_{oi} = \frac{1}{AREA} \sum_{j=1}^{N} \sum_{k=1}^{N} W_j W_k COV(h_{i,jk})$$

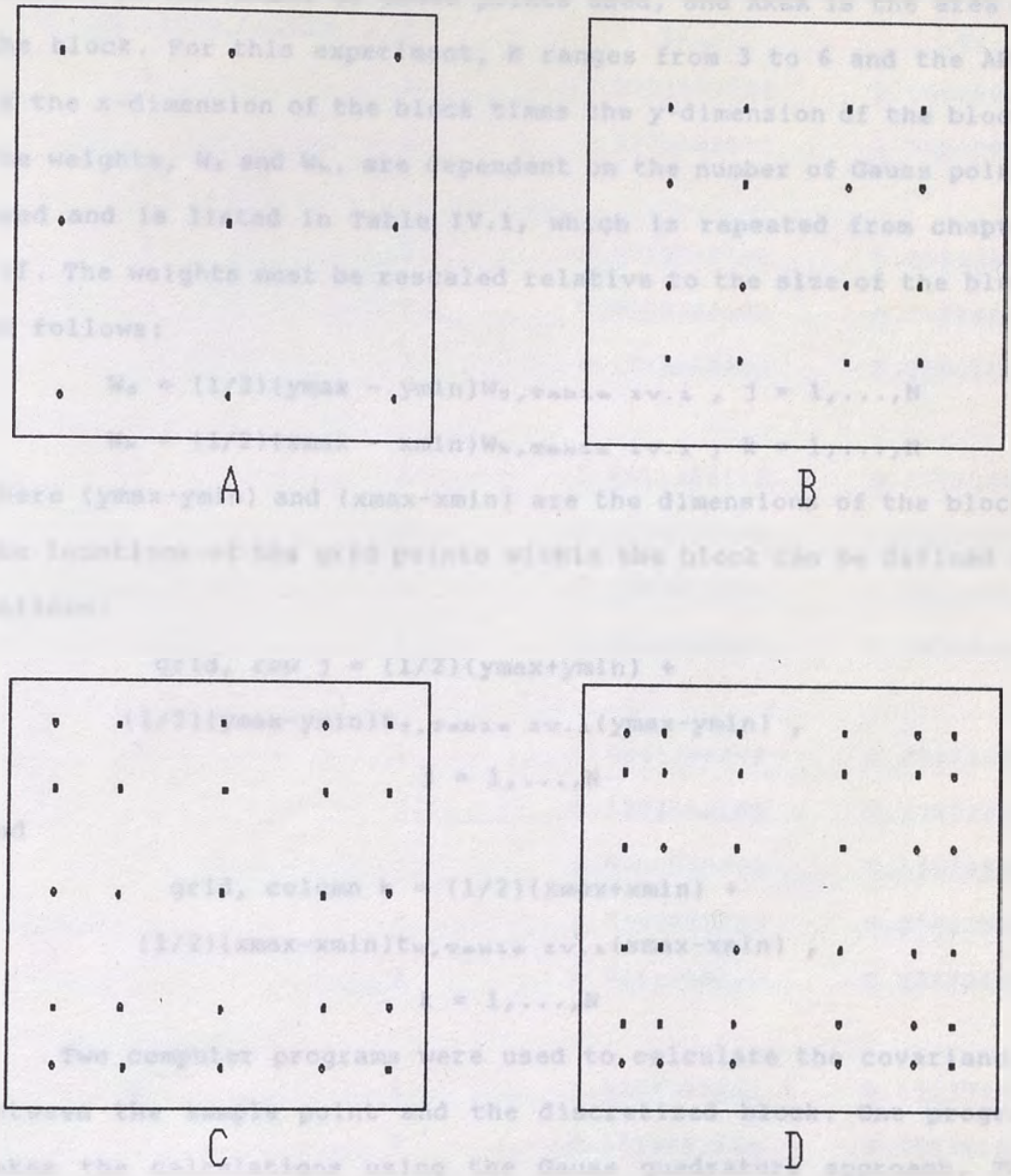


Figure IV.3. The Gauss quadrature method of using a symmetrically spaced grid: A) a 3 x 3 grid, B) a 4 x 4 grid, C) a 5 x 5 grid, and D) a 6 x 6 grid.

where N is the number of Gauss points used, and AREA is the area of the block. For this experiment, N ranges from 3 to 6 and the AREA is the x-dimension of the block times the y-dimension of the block. The weights, W_j and W_k, are dependent on the number of Gauss points used and is listed in Table IV.1, which is repeated from chapter III. The weights must be rescaled relative to the size of the block as follows:

$$W_j = (1/2)(ymax - ymin)W_{j,\text{Table IV.1}} \ , \ j = 1,\ldots,N$$

$$W_k = (1/2)(xmax - xmin)W_{k,\text{Table IV.1}} \ , \ k = 1,\ldots,N$$

where (ymax-ymin) and (xmax-xmin) are the dimensions of the block. The locations of the grid points within the block can be defined as follows:

$$\text{grid, row } j = (1/2)(ymax+ymin) + (1/2)(ymax-ymin)t_{j,\text{Table IV.1}}(ymax-ymin) \ , \ j = 1,\ldots,N$$

and

$$\text{grid, column } k = (1/2)(xmax+xmin) + (1/2)(xmax-xmin)t_{k,\text{Table IV.1}}(xmax-xmin) \ , \ k = 1,\ldots,N$$

Two computer programs were used to calculate the covariances between the sample point and the discretized block. One program makes the calculations using the Gauss quadrature approach. The other uses block kriging to calculate the covariances. Subroutines for the Gauss quadrature approach for calculating block-sample covariances are reprinted from Carr and Palmer, 1993 in the appendix A and B at the end of this thesis. The subroutines are for

Table IV.1. Gauss point locations and weights.

No. of Gauss Points	i	t_i	W_i
2	1	-0.5773502692	1.0000000000
	2	0.5773502692	1.0000000000
3	1	-0.7745966692	0.5555555556
	2	0.0000000000	0.8888888889
	3	0.7745966692	0.5555555556
4	1	-0.8611363116	0.3478548452
	2	-0.3399810436	0.6521451548
	3	0.3399810436	0.6521451548
	4	0.8611363116	0.3478548452
5	1	-0.9061798460	0.2369268850
	2	-0.5384693102	0.4786286704
	3	0.0000000000	0.5688888889
	4	0.5384693102	0.4786286704
	5	0.9061798460	0.2369268850
6	1	-0.9324695142	0.1713244924
	2	-0.6612093864	0.3607615730
	3	-0.2386191860	0.4679139346
	4	0.2386191860	0.4679139346
	5	0.6612093864	0.3607615730
	6	0.9324695142	0.1713244924

the case of two and three dimensional Gauss quadrature integration of block-sample covariance.

The results of the covariance calculations for the four covariance models are listed in Table IV.2 for both the classical block kriging approach and the Gauss quadrature approach. In the comparison of the accuracy between the two approaches, the Gauss quadrature approach using four Gauss points achieves equivalent or greater accuracy than the classical approach using a 50x50 or a 100x100 grid block. The use of four Gauss points in a 4x4 grid is optimal in all experiments with the four models. Three Gauss points in a 3x3 grid fails to achieve the accuracy needed to make the calculations. For the case of five Gauss points in a 5x5 grid, and six Gauss points in a 6x6 grid, the accuracy is only improved by a small amount. The use of five or six Gauss points is not necessary to use due to the increase in computational effort and cost to achieve a small increase in accuracy.

For the case of the exponential model, the exponential term is approximated by into a Taylor series. The Taylor series is then truncated which introduces an error equal to the value of the truncated terms. The experiment for the exponential model achieved a satisfactory accuracy using four Gauss points which is close to the accuracy of the classical approach using a grid of 50x50.

The classical approach using a grid size of 4x4, as used in David (1977), results in a large error for this problem. The accuracy loses precision at the hundredths or thousands place after

Table IV.2. Comparison of Gauss quadrature and classical approaches to block-sample covariance calculation, Figure IV.1 experiment.

Linear Covariance Model:

Gauss Quadrature	Classical
3.739813 (N=3)	3.755674 (4x4)
3.739456 (N=4)	3.739573 (50x50)
3.739479 (N=5)	3.739499 (100x100)
3.739476 (N=6)	3.739485 (150x150)
	3.739482 (200x200)

Spherical Covariance Model:

Gauss Quadrature	Classical
2.100078 (N=3)	2.097473 (4x4)
2.099511 (N=4)	2.099530 (50x50)
2.099547 (N=5)	2.099537 (100x100)
2.099543 (N=6)	2.099536 (150x150)
	2.099535 (200x200)

Gaussian Covariance Model:

Gauss Quadrature	Classical
3.643188 (N=3)	3.648052 (4x4)
3.643265 (N=4)	3.643297 (50x50)
3.643266 (N=5)	3.643270 (100x100)
3.643266 (N=6)	3.643270 (150x150)
	3.643265 (200x200)

Exponential Covariance Model:

Gauss Quadrature	Classical
1.730243 (N=3)	1.724465 (4x4)
1.729411 (N=4)	1.729432 (50x50)
1.729468 (N=5)	1.729457 (100x100)
1.729462 (N=6)	1.729463 (150x150)
	1.729462 (200x200)

the decimal. For this experiment, the classical approach for all four models using a 4x4 grid has the least accuracy.

The data listed in Table IV.2 has been plotted in Figure IV.4. The four graphs shown are for the four different covariance models used. Graph A is the linear model, graph B is the spherical model, graph C is the Gaussian model, and graph D is the exponential model. Each graph shows both the Gauss quadrature and the classical approaches. Both approaches achieve greater accuracy as the number of Gauss points or grid points increase as shown in the graphs.

The experiment also included three other geometries besides the intermediate sample location test to see if the accuracy of the Gauss quadrature approach is superior to the classical approach. The three geometries included the oblique test, the close test, and the near range test. These geometries are shown in Figure IV.5. The coordinate locations for the sample test are (7,6) for the oblique test, (6.1,3) for the close test, and (9,3) for the near range test. Tables IV.3, IV.4, and IV.5 show the results of the experiments for each of the three tests.

The oblique test experiment shows accurate results for four Gauss points which is comparable to the classical results using a 50 x 50 size grid. For the linear covariance model, three Gauss points shows the same accuracy as the classical approach using a 50 x 50 grid size.

The close test experiment shows less accuracy for the Gauss quadrature approach in comparison to other geometries tested. It

Figure IV.4. A) Linear model B) spherical model.

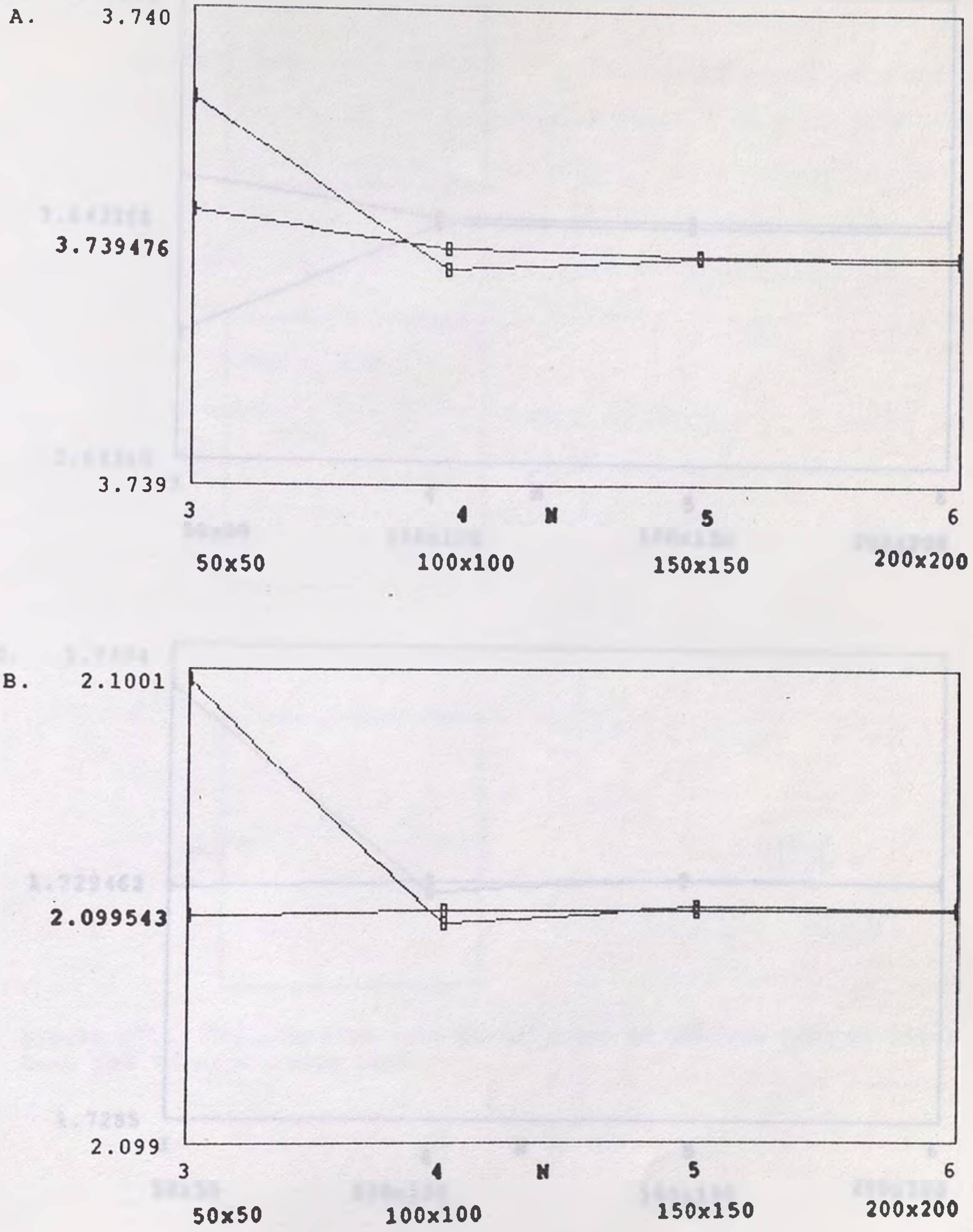
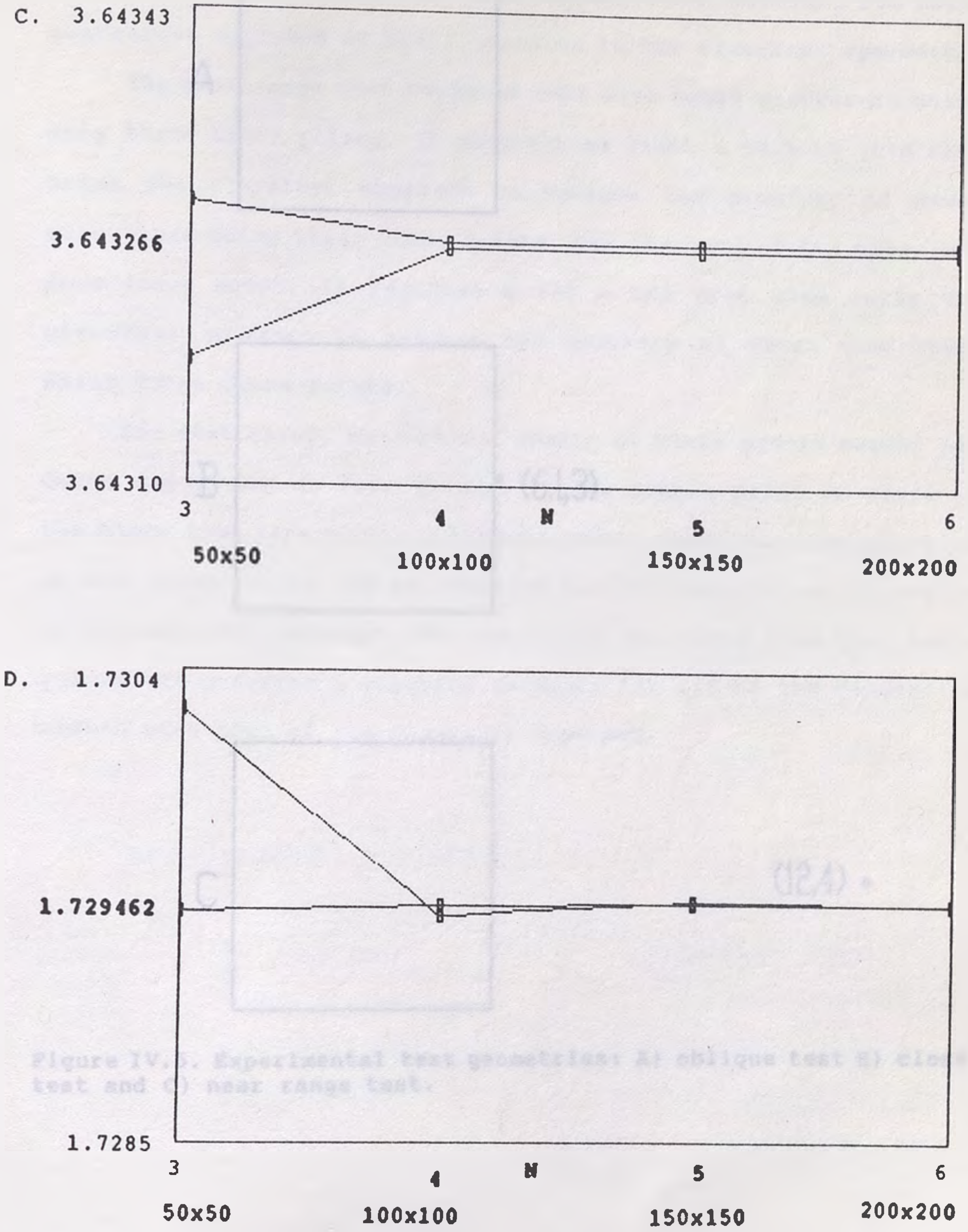


Figure IV.4. (Continued). C) Guassian model D) exponential model.



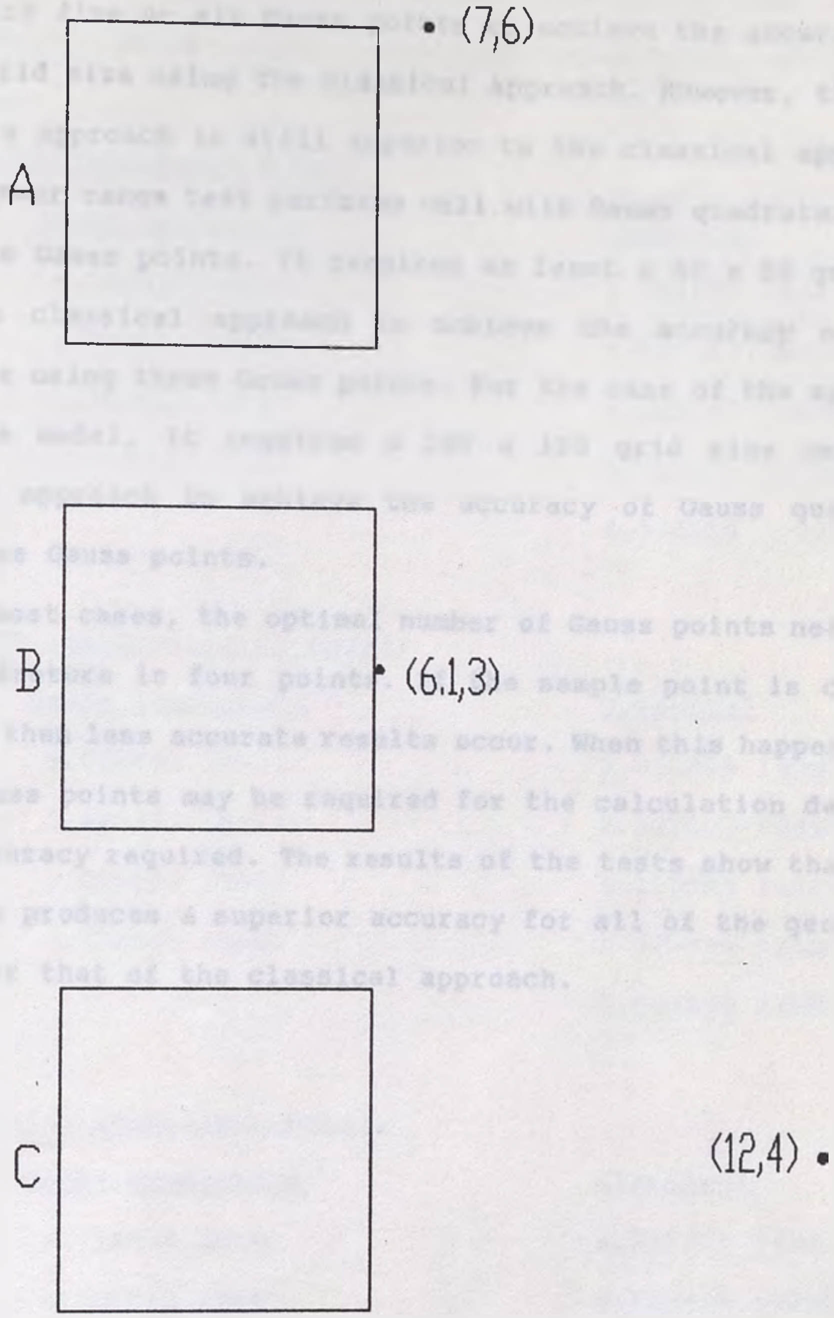


Figure IV.5. Experimental test geometries: A) oblique test B) close test and C) near range test.

may require five or six Gauss points to achieve the accuracy of a 50 x 50 grid size using the classical approach. However, the Gauss quadrature approach is still superior to the classical approach.

The near range test performs well with Gauss quadrature using only three Gauss points. It requires at least a 50 x 50 grid size using the classical approach to achieve the accuracy of Gauss quadrature using three Gauss points. For the case of the spherical covariance model, it requires a 100 x 100 grid size using the classical approach to achieve the accuracy of Gauss quadrature using three Gauss points.

For most cases, the optimal number of Gauss points needed for Gauss quadrature is four points. If the sample point is close to the block then less accurate results occur. When this happens, five or six Gauss points may be required for the calculation depending on the accuracy required. The results of the tests show that Gauss quadrature produces a superior accuracy for all of the geometries tested over that of the classical approach.

Table IV.3. Comparison of Gauss quadrature and classical approaches to block-sample covariance calculation, oblique test experiment.

Linear Covariance Model:

Gauss Quadrature	Classical
4.702337 (N=3)	4.722692 (4x4)
4.702168 (N=4)	4.702343 (50x50)
4.702204 (N=5)	4.702247 (100x100)
4.702212 (N=6)	4.702231 (150x150)
	4.702219 (200x200)

Spherical Covariance Model:

Gauss Quadrature	Classical
3.023693 (N=3)	3.031969 (4x4)
3.023477 (N=4)	3.023603 (50x50)
3.023533 (N=5)	3.023549 (100x100)
3.023545 (N=6)	3.023549 (150x150)
	3.023545 (200x200)

Gaussian Covariance Model:

Gauss Quadrature	Classical
4.730015 (N=3)	4.747771 (4x4)
4.730313 (N=4)	4.730424 (50x50)
4.730306 (N=5)	4.730335 (100x100)
4.730306 (N=6)	4.730319 (150x150)
	4.730316 (200x200)

Exponential Covariance Model:

Gauss Quadrature	Classical
2.337662 (N=3)	2.335201 (4x4)
2.336874 (N=4)	2.336991 (50x50)
2.336975 (N=5)	2.336996 (100x100)
2.336998 (N=6)	2.337009 (150x150)
	2.336998 (200x200)

Table IV.4. Comparison of Gauss quadrature and classical approaches to block-sample covariance calculation, close test experiment.

Linear Covariance Model:

Gauss Quadrature	Classical
6.376933 (N=3)	6.394145 (4x4)
6.355317 (N=4)	6.361050 (50x50)
6.364159 (N=5)	6.360880 (100x100)
6.359231 (N=6)	6.360845 (150x150)
	6.360832 (200x200)

Spherical Covariance Model:

Gauss Quadrature	Classical
4.935266 (N=3)	4.945596 (4x4)
4.902568 (N=4)	4.911107 (50x50)
4.915894 (N=5)	4.910905 (100x100)
4.908484 (N=6)	4.910913 (150x150)
	4.910909 (200x200)

Gaussian Covariance Model:

Gauss Quadrature	Classical
6.792079 (N=3)	6.838635 (4x4)
6.791795 (N=4)	6.792103 (50x50)
6.791799 (N=5)	6.791877 (100x100)
6.791797 (N=6)	6.791843 (150x150)
	6.791796 (200x200)

Exponential Covariance Model:

Gauss Quadrature	Classical
3.775079 (N=3)	3.744226 (4x4)
3.712529 (N=4)	3.728738 (50x50)
3.738496 (N=5)	3.728641 (100x100)
3.723887 (N=6)	3.728634 (150x150)
	3.728588 (200x200)

Table IV.5. Comparison of Gauss quadrature and classical approaches to block-sample covariance calculation, near range test experiment.

Linear Covariance Model:

Gauss Quadrature	Classical
0.775966 (N=3)	0.786477 (4x4)
0.775943 (N=4)	0.776011 (50x50)
0.775943 (N=5)	0.775959 (100x100)
0.775943 (N=6)	0.775951 (150x150)
	0.775947 (200x200)

Spherical Covariance Model:

Gauss Quadrature	Classical
0.491383 (N=3)	0.468259 (4x4)
0.491340 (N=4)	0.491193 (50x50)
0.491341 (N=5)	0.491304 (100x100)
0.491341 (N=6)	0.491324 (150x150)
	0.491332 (200x200)

Gaussian Covariance Model:

Gauss Quadrature	Classical
1.219044 (N=3)	1.208357 (4x4)
1.218904 (N=4)	1.218840 (50x50)
1.218907 (N=5)	1.218892 (100x100)
1.218907 (N=6)	1.218900 (150x150)
	1.218901 (200x200)

Exponential Covariance Model:

Gauss Quadrature	Classical
0.714381 (N=3)	0.710812 (4x4)
0.714352 (N=4)	0.714331 (50x50)
0.714352 (N=5)	0.714348 (100x100)
0.714352 (N=6)	0.714349 (150x150)
	0.714352 (200x200)

Chapter V

Conclusions

Block-sample covariance can be calculated using the classical method by discretizing the block into regularly spaced grid points, calculating the covariance between the sample point and each point in the block, and then averaging the values. An alternate method of calculating the covariance between the sample point and the block is Gauss quadrature. The Gauss quadrature method discretizes the block into grid points which are symmetrically spaced about the center of the block and uses weighted coefficients to minimize the error of the calculation.

The covariance between a sample point and a block is defined by an integral equation over area or volume. Gauss quadrature is a method which can approximate the solution to this integral. This thesis has shown by experimentation that the Gauss quadrature method is superior to the classical method in calculating covariances between a sample point and a block.

In the experiment, the Gauss quadrature method uses a 3 x 3 grid, a 4 x 4 grid, a 5 x 5 grid, and a 6 x 6 grid. This is compared to the classical method using a 4 x 4 grid, a 50 x 50 grid, a 100 x 100 grid, a 150 x 150 grid, and a 200 x 200 grid. The experiment shows that the Gauss quadrature method using a 4 x 4 grid yields a superior accuracy to the classical method using a 4 x 4 grid for approximately the same computational cost. The classical method needs at least a 50 x 50 grid, and sometimes a 100 x 100 grid to achieve the accuracy of the Gauss quadrature method using a 4 x 4 grid.

The experiment uses four different geometries for the sample point and the block. The geometries that have been tested are the oblique test, the close test, the near range test, and the intermediate location test. Each geometry that has been tested shows similar results. For most geometries, the optimum number of Gauss points is four points. For all geometries, the Gauss quadrature method is superior to the classical method.

Another factor that is varied in the test was the covariance model. Four different covariance models are tested. The models that are tested are the linear covariance model, the spherical covariance model, the Gaussian covariance model, and the exponential covariance model. Each of these models shows superior accuracy using the Gauss quadrature method to the classical method.

In conclusion, this thesis has shown by experimentation that the Gauss quadrature method is a superior method to the classical method for calculating the covariances between a sample point and a block. The degree of accuracy between the two methods is small. For an application which requires a high degree of accuracy, the Gauss quadrature method is the necessary method to use.

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APPENDIX A

This appendix is presented to show a computer algorithm for the implementation of Gauss quadrature for the calculation of two-dimensional block-sample covariances. This computer algorithm is a modification of a subroutine, COVAR (David, 1977, p. 264). A 4 x 4 Gauss point rule is implemented.

The computer algorithm:

```
      function covar (x, y, xcen, ycen, dx, dy)
c
c     this function is a modified version of a function, COVAR,
c     presented in David(1977, p. 264).
c
c     x,y  are the coordinates of the sample
c     xcen, ycen  are the coordinates of the center of the block
c     dx =  xmax - xmin  =  x dimension of the block
c     dy =  ymax - ymin  =  y dimension of the block
c
c     required routine:  function gammb (David, 1977, p. 265).
c
      dimension tj(4), wj(4), tk(4), wk(4), t(4), w(4)
c
c     n = number of gauss points = 4
c
      n = 4
      t(1)  =  -.8611363116
      t(4)  =  - t(1)
      t(2)  =  -.3399810436
      t(3)  =  - t(2)
      w(1)  =   .3478548452
      w(4)  =    w(1)
      w(2)  =   .6521451548
      w(3)  =    w(2)
c
c     rescale t and w relative to the size of the block
c
      do i = 1,n
       tj(i) = ycen + t(i) * dy/2.
       tk(i) = xcen + t(i) * dx/2.
       wj(i) = w(i) * dy/2.
       wk(i) = w(i) * dx/2.
      end do
c
c     compute covariance
c
```

```
      somg = 0.0
      do i = 1,n
        do j = 1,n
          somg = somg + gammb(x, tk(i), y, tj(j)) * wk(i) * wj(j)
        end do
      end do
c
c     compute covariance by dividing somg by the area of the block
c
      covar = somg/(dx * dy)
      return
      end
```

APPENDIX B

This appendix is presented to show a computer algorithm for the implementation of Gauss quadrature for the calculation of three-dimensional block-sample covariances. This computer algorithm is a modification of a subroutine, COVAR (David, 1977, p. 264). A 4 x 4 Gauss point rule is implemented.

The computer algorithm:

```
      function covar (x, y, z, xcen, ycen, zcen, dx, dy, dz)
c
c     this function is a modified version of a function, COVAR,
c     presented in David(1977, p. 264).
c
c     x,y,z  are the coordinates of the sample
c     xcen,ycen,zcen are the coordinates of the center of the block
c     dx =  xmax - xmin  =  x dimension of the block
c     dy =  ymax - ymin  =  y dimension of the block
c     dz =  zmax - zmin  =  z dimension of the block
c
c     required routine:  function gammb (David, 1977, p. 265) (must
c                         be modified to compute 3D distances).
c
      dimension tj(4), wj(4), tk(4), wk(4), tm(4), wm(4), t(4), w(4)
c
c     n = number of gauss points = 4
c
      n = 4
      t(1)  =  -.8611363116
      t(4)  =  - t(1)
      t(2)  =  -.3399810436
      t(3)  =  - t(2)
      w(1)  =   .3478548452
      w(4)  =    w(1)
      w(2)  =   .6521451548
      w(3)  =    w(2)
c
c     rescale t and w relative to the size of the block
c
      do i = 1,n
       tj(i) = ycen + t(i) * dy/2.
       tk(i) = xcen + t(i) * dx/2.
       tm(i) = zcen + t(i) * dz/2.
       wj(i) = w(i) * dy/2.
       wk(i) = w(i) * dx/2.
       wm(i) = w(i) * dz/2.
```

```
      end do
c
c     compute covariance
c
      somg = 0.0
      do i = 1,n
       do j = 1,n
        do k = 1,n
        somg = somg+gammb(x,tk(i),y,tj(j),z,tm(k))*wk(i)*sj(j)*wm(k)
        end do
       end do
      end do
c
c     divide somg by the volume of the block
c
      covar = somg/(dx * dy * dz)
      return
      end
```