

A Short Note on the Generalized Spherical Variogram Model

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The spherical model is a widely used variogram model, however the equations for the model are typically implemented for lower dimensions only (1-3) and are not commonly considered in higher dimensions. Extending this model to higher dimensions has applications in modern high dimensional geostatistical techniques. A generalized equation for the spherical variogram is presented and the properties of higher order models are described. A subroutine (`n_sph`) is presented to calculate the n -spherical variogram for $n \leq 5$. The widely used `cova3` subroutine is also modified to compute n -spherical variogram values for $n \leq 5$.

1. Spherical Variogram

Variogram models defined by the intersection of geometric bodies were first introduced by Matérn (1960). The spherical variogram has since become a widely used variogram model. The standardized spherical model is defined as one minus the volume of intersection of 2 spheres normalized by the volume of the spheres. This is shown schematically in Figure 1 and mathematically in Equation (1). The spherical variogram model in 3 dimensions is well known. The equation for a variogram with range a (sphere diameter) for lag h is given by Equation (2).

$$Sph(h) = 1 - \frac{V_{\text{intersection}}(h)}{V_{\text{sphere}}} \quad (1)$$

$$Sph_3(h) = \begin{cases} 3/2(h/a) - 1/2(h/a)^3 & \text{for } h < a \\ 1 & \text{for } h \geq a \end{cases} \quad (2)$$

This variogram is a conditional negative definite model and hence valid in a dimensional space less than or equal to the dimension of the variogram (Armstrong and Diamond, 1984; Christakos, 1984; Pyrcz and Deutsch, 2006). This three dimensional model is valid in three, two and one dimensions. To use this model in n -dimensions, an n -D (or greater) model must be used. Modern geostatistical techniques such as kriging with locally varying anisotropy (Boisvert, 2010) require high dimensional models limiting use of the spherical variogram model.

2. Generalized n -Spherical Variogram

The n -spherical variogram model can be derived using Equation (1) and n -spherical volume formulas. The equations of two n -spheres of radius r with centers separated by a distance h are given by (3) and (4).

$$x^2 + \sum_{i=1}^{n-1} y_i^2 = r^2 \quad (3)$$

$$(x-h)^2 + \sum_{i=1}^{n-1} y_i^2 = r^2 \quad (4)$$

The n -spheres intersect on the hyperplane given by the y_i 's at $x = h/2$. For the spherical variogram, this is a circle of intersection on the y - z plane. For the equal sized n -spheres, the volume of intersection is then equal to twice the volume of the spherical caps bounded by the hyperplane at $x = h/2$. The height of this cap is given by Equation (5) and shown schematically in Figure 2.

$$h' = r - h/2 \quad (5)$$

The formula for the volume of an n -sphere and associated spherical cap with height h' are known (Shetty and Ahuja, 2008) and given by Equations (6) and (7) where Γ is the gamma function given by Equation (8).

$$V_{sph} = \frac{\pi^{n/2}}{\Gamma\left(\frac{n}{2} + 1\right)} r^n \quad (6)$$

$$V_{cap} = \frac{\pi^{\frac{n-1}{2}} r^n}{\Gamma\left(\frac{n+1}{2}\right)} \int_0^{\cos^{-1}\left(\frac{r-h}{r}\right)} \sin^n(t) dt \quad (7)$$

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt \quad (8)$$

Given that the volume of intersection is equal to twice the volume of a spherical cap and using sphere diameter a instead of radius r the general formula for the n -spherical variogram can be calculated, Equation (9).

$$Sph_n(h) = 1 - \frac{2}{\sqrt{\pi}} \frac{\Gamma(n/2+1)}{\Gamma\left(\frac{n+1}{2}\right)} \int_0^{\cos^{-1}(h/a)} \sin^n(t) dt \quad (9)$$

By simplifying this general equation, the triangular, circular, spherical and n -spherical variogram equations can be calculated. The results for the 1-D to 5-D cases are shown below in Table 1.

Table 1: Simplified equations for n -spherical variogram models.

Dimension		Equation
1	Triangular	$Sph_1(h) = h/a$
2	Circular	$Sph_2(h) = 1 + (2/\pi)(h/a)\sqrt{1-(h/a)^2} - (2/\pi)\cos^{-1}(h/a)$
3	Spherical	$Sph_3(h) = 3/2(h/a) - 1/2(h/a)^3$
4	4-Spherical	$Sph_4(h) = 1 - (1/6\pi)\left(12\cos^{-1}(h/a) - 8\sin\left(2\cos^{-1}(h/a)\right) + \sin\left(4\cos^{-1}(h/a)\right)\right)$
5	5-Spherical	$Sph_5(h) = 15/8(h/a) - 5/4(h/a)^3 + 3/8(h/a)^5$
		For $h \geq a$: $Sph_n(h) = 1$

It is noteworthy that the odd n -D variograms have relatively simple equations governing them while the even n -D variograms have complicated equations involving the arccosine term in the integral from the general equation. This is because of the $\sin^n(t)$ term in the integral which is complicated to integrate for even n and simple for odd n . Sample plots of variograms that would be obtained using these equations are shown in Figure 3. Note that initial slope at $h=0$ increases with increasing dimensions for the cases shown. Because of this it is not a simple matter to use the same range for a higher order variogram model. All of the variogram models shown in Figure 3 are range normalized (ie: $a=1$). To calculate the intercept with the sill using the initial slope, Equation (10) is applied. The intercept values using the initial slope at are listed in Table 2.

$$\text{Intercept} = \left[\frac{dSph}{d(h/a)} \Big|_{(h/a)=0} \right]^{-1} \quad (10)$$

Table 2: List of sill intercept values using the initial slope at $h=0$ as a function of dimension.

	Dimension	Sill Intercept	$\left. \frac{dSph}{d(h/a)} \right _{(h/a)=0}$
1	Triangular	1	1
2	Circular	$\pi/4 \sim 0.785$	$4/\pi \sim 1.273$
3	Spherical	$2/3 \sim 0.667$	$3/2 \sim 1.500$
4	4-Spherical	$3\pi/16 \sim 0.589$	$16/3\pi \sim 1.698$
5	5-Spherical	$8/15 \sim 0.533$	$15/8 \sim 1.875$
	Exponential	∞	3.000

Table 2 shows that the amount which the slope increases with increasing dimension decreases with higher dimensions; so while the difference between triangular and circular variogram models is very large, the difference between the 4-spherical and 5-spherical models is considerably smaller.

3. Computational Aspects

A Fortran subroutine (Figure 4) was written to calculate the n -Spherical variogram values using the equations detailed here. For a lag h greater than range a , a value 1.0 is returned automatically. This could be changed depending on the use of the subroutine. The commonly used `cova3` subroutine was also modified to compute the n -spherical variogram values for up to 5 dimensions (see the electronic files accompanying this paper). This subroutine can replace the currently used version of `cova3` with no loss of functionality or change in input parameters.

The effects of using a higher dimensional spherical variogram model with the same range as a lower rank spherical variogram were tested using the familiar `2DWellData.dat`. For simplicity, all variograms were generated using the same range (see the accompanying electronic files for complete parameters). Sample variograms are plotted in Figure 5. The variograms do not differ significantly, although the high dimensional spherical variograms are “bowed-out” as was previously illustrated. These variograms were used to krig normal-score transformed porosity values from the `2DWellData`. Plots of the kriged data are compiled in Figure 6. All of the n -spherical variograms produced very similar kriging outputs.

As the number of dimensions increases, the equation for the spherical variogram becomes increasingly complex requiring greater computation times (see Table 1). To calculate the equation for a n -spherical variogram at an arbitrary n , Equation (9) has to be solved. Numerical integration techniques are only effective at low n as $\sin^n(t)$ in the integral domain converges to a sharp peak for which ordinary numerical integration techniques are not effective, so solutions to the hypergeometric function should be used. Equation (9) can be expanded to Equation (11) where ${}_2F_1$ is the hypergeometric function; however, this still requires solving the gamma function and hypergeometric function for large values of n . For this reason it is recommended that for large values of n , variograms should be modeled using the exponential variogram, which is valid for any n .

$$Sph_n(h) = \frac{2(h/a)}{\sqrt{\pi}} \frac{\Gamma(n/2+1)}{\Gamma((n+1)/2)} {}_2F_1\left(\frac{1}{2}, \frac{1-n}{2}; \frac{3}{2}; (h/a)^2\right) \quad (11)$$

4. Conclusions

The general equation for a n -Spherical variogram was derived. The Fortran subroutine, `cova3` was coded to include spherical variograms less than or equal to five dimensions.

References

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 Shetty, S. and Ahuja, N., 2008, A Uniformity Criterion and Algorithm for Data Clustering, *19th International Conference on Pattern Recognition*, Tampa, FL, article number 4761239, 4 pp.

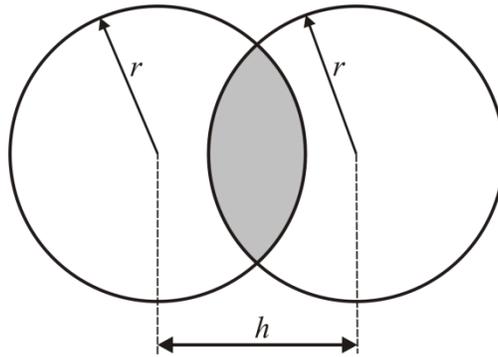


Figure 1: Schematic cross section of the intersection of two spheres for constructing spherical variogram model.

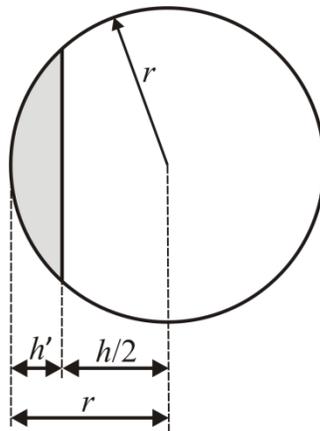


Figure 2: Schematic of height of spherical cap.

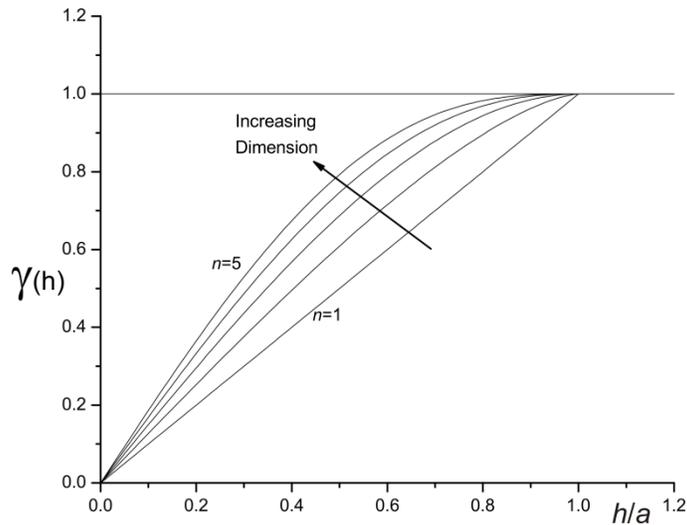


Figure 3: Range normalized variogram models showing the effect of increasing dimension.

```

subroutine nsph(n,a,h,sph)
c-----
c
c      Calculate the n-Spherical Variogram
c      *****
c Calculate the n-spherical variogram up to and including 5 dimensions
c The formulas are hard-coded so does not require use of the gamma
c function. On error returns sph = -1.0
c ***Note that for h > a function returns sph = 1.0 exactly***
c
c      Parameters for nsph
c      *****
c      n          -number of dimensions
c      a          -variogram range (sphere diameter)
c      h          -lag value (sphere center separation distance)
c      sph        -calculated spherical variogram value
c-----
parameter(PI=3.14159265)
integer n
real a,h,sph,ha
ha = h/a
if (h .ge. a) then
  sph = 1.0
  return
end if

select case (n)
case (1)
  sph = ha
case (2)
  sph = 1.+2./PI*ha*SQRT(1.-ha*ha)-2./PI*ACOS(ha)
case (3)
  sph = 1.5*ha-0.5*ha*ha*ha
case (4)
  sph = 1.-1./6./PI*(12.*ACOS(ha)-8*SIN(2.*ACOS(ha))
+      +SIN(4.*ACOS(ha)))
case (5)
  sph = 1.875*ha-1.25*ha*ha*ha+0.375*ha*ha*ha*ha*ha
case default
  sph = -1.0
end select

return
end

```

Figure 4: Fortran subroutine for calculated *n*-Spherical variogram values up to and including *n*=5.

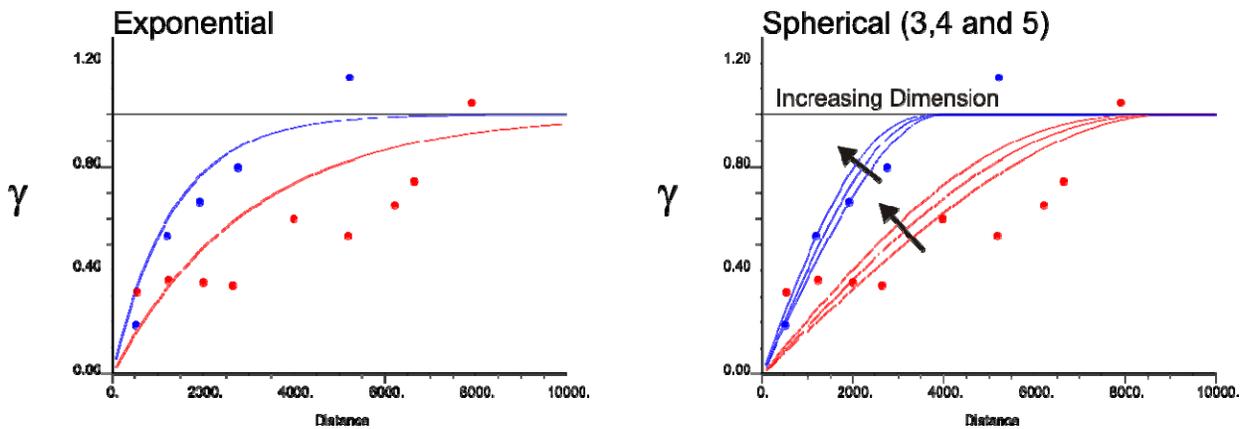


Figure 5: Variograms models for 2DWellData.dat, all with identical ranges.

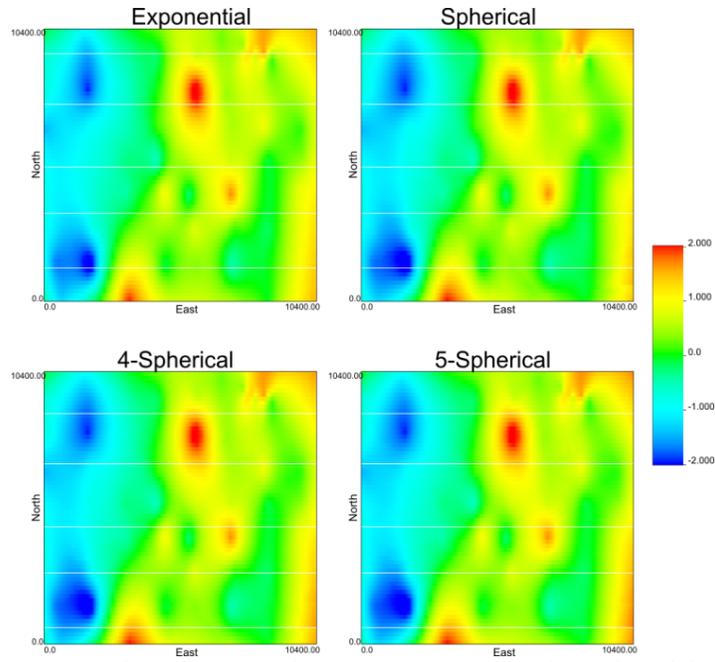


Figure 6: Kriged 2D WellData using the variograms shown in Figure 5. All spherical models give similar results.