Variogram Range Estimation from Experimental Variograms with Significant Tolerance

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Calculating the experimental variogram with some tolerance parameters affects the estimated value of the maximum and minimum range of continuity. It can be shown mathematically that the maximum range of continuity is underestimated and the minimum range of continuity is overestimated. The amount of increase/decrease relates to the tolerance parameters used in variogram calculation. A procedure is presented that allows correcting experimental points. Formulas for 2D and 3D cases are presented.

Introduction

The tolerance correction is different 2D and 3D and different for whether or not a bandwidth parameter is considered in the calculation. The cases to be considered are as follows:

2D case:

1. Tolerance correction factor without bandwidth
2. Tolerance correction factor with bandwidth

3D case:

1. Tolerance correction factor without bandwidth
2. Tolerance correction factor with bandwidth
   a) Vertical bandwidth is applied but the horizontal bandwidth is not applied.
   b) Both of the vertical and horizontal bandwidths are applied.

The analytical formulas for each cases will be presented.

Tolerance correction factor in 2D without bandwidth

Assume that the ellipse in Figure 1 shows the anisotropy of the variable in a specific 2D field. The field has a maximum range of correlation of $a_{h-\max}$ (the maximum radius of the ellipse) and the minimum range of correlation of $a_{h-\min}$. If we introduce an angle tolerance of a_{tol}, then the tolerance will cause an underestimation of $a_{h-\max}$ and an overestimation of $a_{h-\min}$. Therefore the anisotropy ratio will artificially decrease just because of introducing tolerance parameters. For example if $a_{h-\max} = 4$ and $a_{h-\min} = 1$ (the anisotropy ratio would be 4:1) then introducing an angle tolerance of 22.5 degree will underestimate $a_{h-\max}$ to 3.18 and overestimate $a_{h-\min}$ to 1.02 and the apparent anisotropy ratio would be 3.1:1.

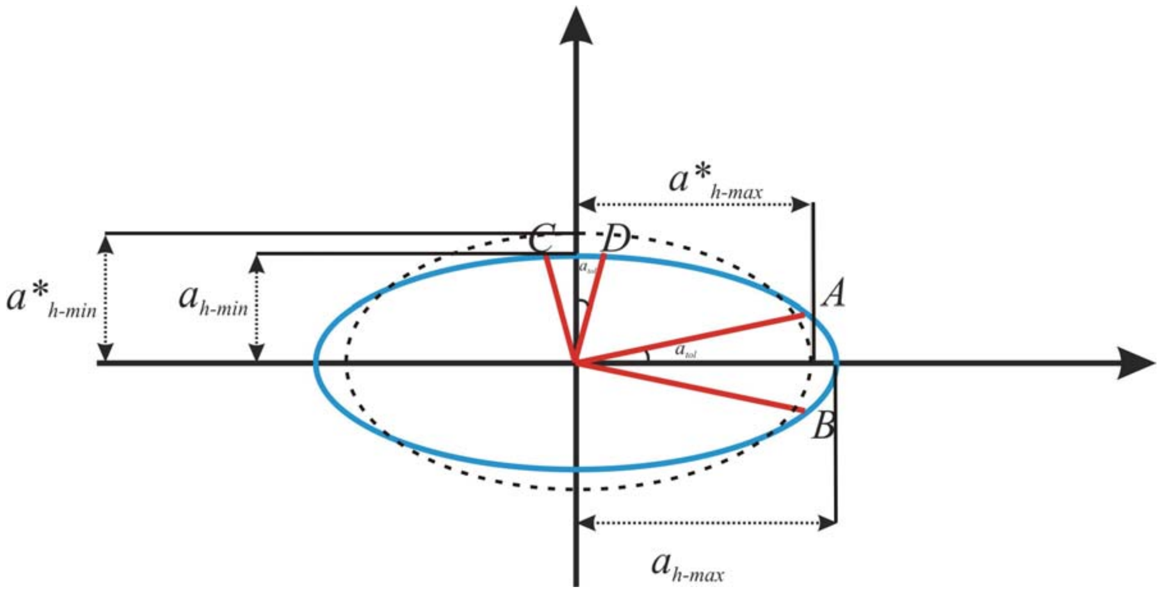

Figure 1 True Anisotropic ellipse (solid) and the estimated anisotropic ellipse (dashed) in 2D case when there is no bandwidth

The relationship between the true range of correlations ($a_{h-\min}$, $a_{h-\max}$) and the estimated range of correlations ($a^*_{h-\min}$, $a^*_{h-\max}$) is derived. The estimated value for the range of correlation is the average of the radii in the tolerance region over the tolerance region. Therefore the estimated values can be written as:

$$a^*_{h-\max} = \frac{\int_{-a_{tol}}^{a_{tol}} r d\theta}{\int_{-a_{tol}}^{a_{tol}} d\theta} \tag{1}$$

$$a^*_{h-\min} = \frac{\int_{\frac{\pi}{2}-a_{tol}}^{\frac{\pi}{2}+a_{tol}} r d\theta}{\int_{\frac{\pi}{2}-a_{tol}}^{\frac{\pi}{2}+a_{tol}} d\theta} \tag{2}$$

By using the equation for the ellipse in polar coordinate the integrals can be solved, therefore:

$$a^*_{h-\max} = a_{h-\min} \cdot \frac{F\left(\frac{\pi}{2}, \omega\right) - F\left(\frac{\pi}{2} - a_{tol}, \omega\right)}{a_{tol}} < a_{h-\max} \tag{3}$$

$$a^*_{h-\min} = a_{h-\min} \cdot \frac{F\left(a_{tol}, \omega\right)}{a_{tol}} > a_{h-\min} .. \tag{4}$$

Where ω is the eccentricity of the ellipse and has a value between 0 and 1 and calculated as below:

$$\omega = \sqrt{1 - \frac{a_{h-\min}^2}{a_{h-\max}^2}} \quad ; \quad 0 < a_{h-\min} \le a_{h-\max} \tag{5}$$

And $F(\alpha,\omega)$ is the incomplete Legendre elliptic integral of the 1st kind and is defined as below (Abramowitz and Stegun, 1965):

$$F(\alpha,\omega) = \int_0^{\alpha} \frac{d\theta}{\sqrt{1-\omega^2 \sin^2\theta}} \tag{6}$$

The values for the incomplete Legendre elliptic integral of the 1st kind are tabulated in many mathematical handbooks (e.g. Abramowitz and Stegun, 1965). This function can be also calculated numerically by using the code provided in Numerical Recipes in Fortran 77 (Press *et al*, 1992).

By using the obtained formulas for $a_{h-\min}^*$ and $a_{h-\max}^*$, the estimated anisotropy ratio can be written as below:

$$\frac{a_{h-\max}^*}{a_{h-\min}^*} = \frac{F\left(\frac{\pi}{2},\omega\right) - F\left(\frac{\pi}{2} - a_{tol},\omega\right)}{F\left(a_{tol},\omega\right)} \tag{7}$$

We know that the true anisotropy ratio is $\frac{a_{h-\max}}{a_{h-\min}} = \frac{1}{\sqrt{1-\omega^2}}$, since $a_{h-\min}$ is overestimated and $a_{h-\max}$ is underestimated therefore $\frac{a_{h-\max}^*}{a_{h-\min}^*}$ will be decreased, therefore:

$$\frac{a_{h-\max}}{a_{h-\min}} > \frac{a_{h-\max}^*}{a_{h-\min}^*} \tag{8}$$

It can be proved that, $F\left(\frac{\pi}{2},\omega\right) - F\left(\frac{\pi}{2} - a_{tol},\omega\right) = F\left(\arctan\left(\frac{\tan a_{tol}}{\sqrt{1-\omega^2}}\right),\omega\right)$ (Abramowitz and Stegun, 1965) therefore the equations (3) and (4) can be written as below:

$$a_{h-\max}^* = a_{h-\min} \cdot \frac{F\left(\arctan\left(\frac{\tan a_{tol}}{\sqrt{1-\omega^2}}\right),\omega\right)}{a_{tol}} \tag{9}$$

$$\frac{a_{h-\max}^*}{a_{h-\min}^*} = \frac{F\left(\arctan\left(\frac{\tan a_{tol}}{\sqrt{1-\omega^2}}\right),\omega\right)}{F\left(a_{tol},\omega\right)} \tag{10}$$

For example if $a_{h-\max} = 4$, $a_{h-\min} = 1$, $a_{tol} = 22.5^\circ = \frac{\pi}{8}$ then the eccentricity is, $\omega = \frac{\sqrt{15}}{4}$ and by using the derived formulas for the estimated ranges of correlations, we have:

$$a^*_{h-\max} = 1 \times \frac{F\left(\frac{\pi}{2}, \frac{\sqrt{15}}{4}\right) - F\left(\frac{3\pi}{8}, \frac{\sqrt{15}}{4}\right)}{\left(\frac{\pi}{8}\right)} = 3.184601$$

$$a^*_{h-\min} = 1 \times \frac{F\left(\frac{\pi}{8}, \frac{\sqrt{15}}{4}\right)}{\left(\frac{\pi}{8}\right)} = 1.024952$$

It can be seen that $a^*_{h-\min} > a_{h-\min}$ and $a^*_{h-\max} < a_{h-\max}$ therefore the anisotropy ratio is also decreased:

$$\frac{a^*_{h-\max}}{a^*_{h-\min}} = \frac{3.184601}{1.024952} \cong 3.107073 < \frac{a_{h-\max}}{a_{h-\min}} = 4 \quad \Rightarrow \quad \frac{a^*_{h-\max}}{a^*_{h-\min}} < \frac{a_{h-\max}}{a_{h-\min}}$$

The more important problem in the case of the variogram calculations is what the true values for the minor and major direction of continuity are if we know the estimated values for them. In almost all of the cases we know the estimated values. To do that we should solve the derived relations for calculating the $a_{h-\min}$ and $a_{h-\max}$ by knowing, $a^*_{h-\min}$, $a^*_{h-\max}$ and a_{tol}.

We know that:

$$\frac{a^*_{h-\max}}{a^*_{h-\min}} = \frac{F\left(\arctan\left(\frac{\tan a_{tol}}{\sqrt{1-\omega^2}}\right), \omega\right)}{F\left(a_{tol}, \omega\right)}$$

After rearranging:

$$f\left(\omega\right) = \left(\frac{a^*_{h-\max}}{a^*_{h-\min}}\right) \cdot F\left(a_{tol}, \omega\right) - F\left(\arctan\left(\frac{\tan a_{tol}}{\sqrt{1-\omega^2}}\right), \omega\right) = 0 \tag{11}$$

The values for, $a^*_{h-\min}$, $a^*_{h-\max}$ and a_{tol} are known therefore the above equation can be solved to calculate ω which has the value between 0 and 1. Bisection method can be used for finding the root of $f\left(\omega\right)$. After finding the actual eccentricity, the true $a_{h-\min}$ and $a_{h-\max}$ can be calculated as below:

$$a_{h-\min} = \frac{a^*_{h-\min} \cdot a_{tol}}{F\left(a_{tol}, \omega\right)} \tag{12}$$

$$a_{h-\max} = \frac{a_{h-\min}}{\sqrt{1-\omega^2}} \tag{13}$$

Tolerance correction factor in 2D with bandwidth

In this case since a bandwidth is introduced therefore two different apparent angle tolerances should be used instead of the true angle tolerance in both of the minimum and maximum directions of continuity. These two apparent angle tolerances are calculated as below. The apparent angle tolerance for maximum direction, $a^{app}_{tol,\max}$, is shown in Figure 2.

$$a_{tol,\max}^{app} = \arctan\left(\frac{b}{a_{h-\max}\sqrt{1-\frac{b^2}{a_{h-\min}^2}}} \right) \tag{14}$$

$$a_{tol,\min}^{app} = \arctan\left(\frac{b}{a_{h-\min}\sqrt{1-\frac{b^2}{a_{h-\max}^2}}} \right) \tag{15}$$

where *b* is the bandwidth.

It is obvious that *b* should have a maximum value, if we want to see its effect on variogram calculation in the presence of anisotropic ellipse. For calculating $a_{tol,\max}^{app}$, the maximum value of *b* is equal to $b_{\min}^*$. It is function of the a_{tol}, $a_{h-\min}$ and $a_{h-\max}$. $b_{\min}^*$ is calculated as:

$$b_{\min}^* = \frac{\tan a_{tol}}{\sqrt{\frac{1}{a_{h-\max}^2} + \frac{\tan^2 a_{tol}}{a_{h-\min}^2}}} \tag{16}$$

The bandwidth, *b*, in this case is satisfied in below inequality:

$$b \le b_{\min}^* \le a_{h-\min}$$

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$$b_{\min}^* = \frac{\tan a_{tol}}{\sqrt{\frac{\tan^2 a_{tol}}{a_{h-\max}^2} + \frac{1}{a_{h-\min}^2}}} \tag{17}$$

The bandwidth, *b*, in this case is satisfied in below inequality:

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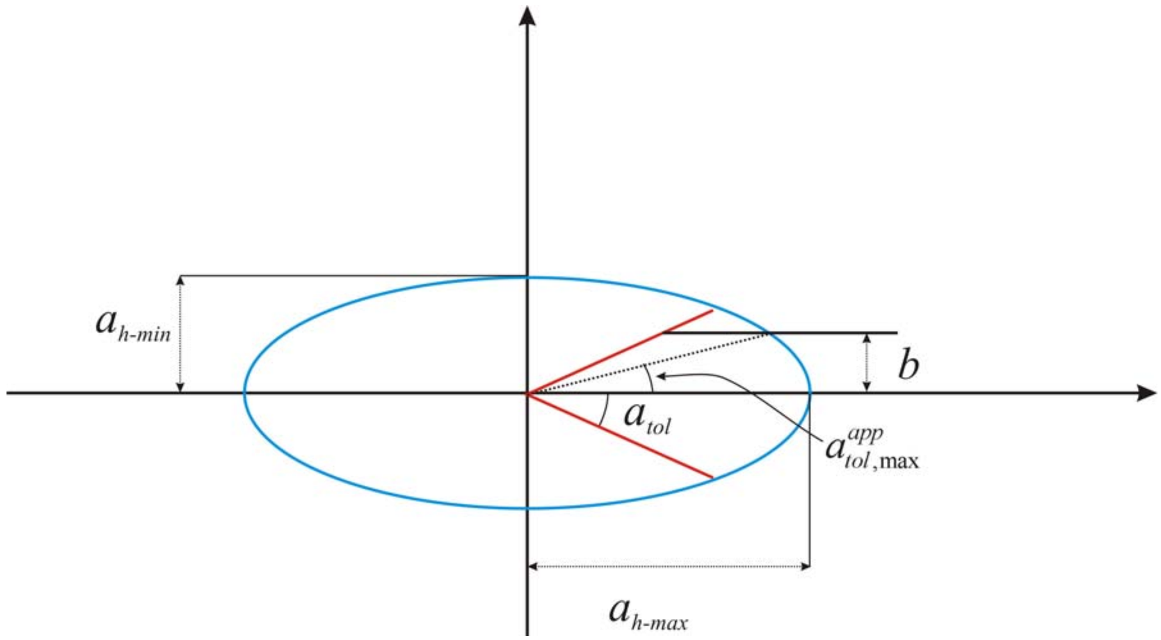

Figure 2 Anisotropic ellipse in 2D case with bandwidth for maximum direction of continuity

The formulas for estimated range of correlation in two major directions in the case of bandwidth reduce to:

$$a_{h-\max}^{*} = a_{h-\min} \cdot \frac{F\left(\frac{\pi}{2}, \omega\right) - F\left(\frac{\pi}{2} - a_{tol,\max}^{app}, \omega\right)}{a_{tol,\max}^{app}} \tag{18}$$

$$a_{h-\min}^{*} = a_{h-\min} \cdot \frac{F\left(a_{tol,\min}^{app}, \omega\right)}{a_{tol,\min}^{app}} > a_{h-\min} \tag{19}$$

To obtain $a_{h-\min}$ and $a_{h-\max}$ a system of non-linear equations should be solved. In addition to above two formulas for $a_{h-\min}$ and $a_{h-\max}$, there are three auxiliary equations for calculating $a_{tol,\min}^{app}$, $a_{tol,\max}^{app}$ and ω which were given before. The known parameters are the values for the bandwidth, angle tolerance and the estimated ranges.

Tolerance correction factor in 3D without bandwidth

In 3D tolerance case in addition to obtaining the relation between the true and the estimated ranges in horizontal (maximum and minimum directions of continuity) direction, the relationship should be obtained for vertical direction as well. The idea for calculating the estimated ranges are the same as in 2D case but the relations are more complicated. The required integrals are written in spherical coordinates, therefore for horizontal direction we have:

$$a^*_{h-\max} = \frac{\int_{-a^h_{tol}}^{a^h_{tol}} \int_{\phi_1(\theta)}^{\pi-\phi_1(\theta)} \rho d\phi d\theta}{\int_{-a^h_{tol}}^{a^h_{tol}} \int_{\phi_1(\theta)}^{\pi-\phi_1(\theta)} d\phi d\theta} \tag{20}$$

$$a^*_{h-\min} = \frac{\int_{\frac{\pi}{2}-a_{tol}}^{\frac{\pi}{2}+a^h_{tol}} \int_{\phi_2(\theta)}^{\pi-\phi_2(\theta)} \rho d\phi d\theta}{\int_{\frac{\pi}{2}-a^h_{tol}}^{\frac{\pi}{2}+a^h_{tol}} \int_{\phi_2(\theta)}^{\pi-\phi_2(\theta)} d\phi d\theta} \tag{21}$$

And for vertical direction:

$$a^*_{ver} = \frac{\int_0^{2\pi} \int_0^{a_{tol}} \rho d\phi d\theta}{\int_0^{2\pi} \int_0^{a_{tol}} d\phi d\theta} \tag{22}$$

Where ρ is the distance from the centre of the ellipsoid to its circumference in spherical coordinate and $\phi_1(\theta)$ and $\phi_2(\theta)$ are:

$$\phi_1(\theta) = \operatorname{arccot}\left(\tan^2 a^v_{tol} \cdot \sqrt{1-\left(1+\cot^2 a^h_{tol}\right)\cdot \sin^2\theta}\right) \tag{23}$$

$$\phi_2(\theta) = \operatorname{arccot}\left(\tan^2 a^v_{tol} \cdot \sqrt{1-\left(1+\cot^2 a^h_{tol}\right)\cdot \cos^2\theta}\right) \tag{24}$$

After integrating and applying the boundaries of the integrals for horizontal direction we will have:

$$a^*_{h-\max} = \frac{a_{ver}}{\pi \cdot a^h_{tol} - 2\int_0^{a^h_{tol}} \phi_1(\theta)\cdot d\theta} \cdot \int_0^{a^h_{tol}} \left[F\left(\pi-\phi_1(\theta),\omega_1(\theta)\right) - F\left(\phi_1(\theta),\omega_1(\theta)\right)\right]\cdot d\theta \tag{25}$$

$$a^*_{h-\min} = \frac{a_{ver}}{\pi \cdot a^h_{tol} - 2\int_0^{a^h_{tol}} \phi_1(\theta)\cdot d\theta} \cdot \int_0^{a^h_{tol}} \left[F\left(\pi-\phi_1(\theta),\omega_2(\theta)\right) - F\left(\phi_1(\theta),\omega_2(\theta)\right)\right]\cdot d\theta \tag{26}$$

And for vertical direction we have:

$$a^*_{ver} = \frac{a_{ver}}{2\pi \cdot a_{tol}} \cdot \int_0^{2\pi} F\left(a_{tol},\omega_1(\theta)\right)\cdot d\theta \tag{27}$$

Where $\omega_1(\theta)$ and $\omega_2(\theta)$ are calculated as:

$$\omega_1(\theta)=1-\left(\frac{a_{ver}^2}{a_{h-\max}^2}\right)-\left(\frac{a_{ver}^2}{a_{h-\min}^2\cdot a_{h-\max}^2}\right)\cdot\left(a_{h-\max}^2-a_{h-\min}^2\right)\cdot\sin^2\theta \tag{28}$$

$$\omega_2(\theta)=1-\left(\frac{a_{ver}^2}{a_{h-\max}^2}\right)-\left(\frac{a_{ver}^2}{a_{h-\min}^2\cdot a_{h-\max}^2}\right)\cdot\left(a_{h-\max}^2-a_{h-\min}^2\right)\cdot\cos^2\theta \tag{29}$$

In the case that the angle tolerances and the estimated values for the ranges are known then by solving the three non-linear equations (equations for $a_{h-\min}^*$, $a_{h-\max}^*$ and a_{ver}^*) simultaneously, the three unknowns($a_{h-\min}$, $a_{h-\max}$ and a_{ver}) can be determined.

Tolerance correction factor in 3D with bandwidth

In the case of bandwidth in 3D, for horizontal direction, two cases might happen:

1. There is vertical bandwidth (b_{ver}) but no horizontal bandwidth (b_{hor}) is applied.

   In this case the vertical bandwidth introduces two apparent angle tolerances, $a_{tol,\min}^{v,app}$ and $a_{tol,\max}^{v,app}$ instead of a_{tol}^{v}. These two apparent angles are different because of the minimum and maximum directions of continuity and calculated as:

$$a_{tol,\min}^{v,app}=\arctan\left(\frac{b_{ver}}{a_{h-\min}\sqrt{1-\frac{b_{ver}^2}{a_{ver}^2}}}\right) \tag{30}$$

$$a_{tol,\max}^{v,app}=\arctan\left(\frac{b_{ver}}{a_{h-\max}\sqrt{1-\frac{b_{ver}^2}{a_{ver}^2}}}\right) \tag{31}$$

   The equations for $a_{h-\min}^*$ and $a_{h-\max}^*$ are

$$a_{h-\max}^*=\frac{a_{ver}}{\pi\cdot a_{tol}^h-2\int_0^{a_{tol}^h}\phi_1(\theta)\cdot d\theta}\cdot\int_0^{a_{tol}^h}\left[F\left(\pi-\phi_1(\theta),\omega_1(\theta)\right)-F\left(\phi_1(\theta),\omega_1(\theta)\right)\right]\cdot d\theta \tag{32}$$

$$a_{h-\min}^*=\frac{a_{ver}}{\pi\cdot a_{tol}^h-2\int_0^{a_{tol}^h}\phi_2(\theta)\cdot d\theta}\cdot\int_0^{a_{tol}^h}\left[F\left(\pi-\phi_2(\theta),\omega_2(\theta)\right)-F\left(\phi_2(\theta),\omega_2(\theta)\right)\right]\cdot d\theta \tag{33}$$

   where $\phi_1(\theta)$ and $\phi_2(\theta)$ are calculated as

$$\phi_1(\theta)=\operatorname{arccot}\left(\tan^2 a_{tol,\max}^{v,app}\cdot\sqrt{1-\left(1+\cot^2 a_{tol}^h\right)\cdot\sin^2\theta}\right) \tag{34}$$

$$\phi_2(\theta) = \operatorname{arccot}\left(\tan^2 a_{tol,\min}^{v,app} \cdot \sqrt{1-\left(1+\cot^2 a_{tol}^{h}\right)\cdot \cos^2\theta}\right) \tag{35}$$

2. Both of the horizontal and vertical bandwidths are present.

In this case four apparent angle tolerances are introduced two in minimum directions, $a_{tol,\min}^{v,app}$ and $a_{tol,\min}^{h,app}$, and two in maximum directions, $a_{tol,\max}^{v,app}$ and $a_{tol,\max}^{h,app}$. The equations for $a_{tol,\min}^{v,app}$ and $a_{tol,\max}^{v,app}$ are the same as before but for $a_{tol,\min}^{h,app}$ and $a_{tol,\max}^{h,app}$ we have:

$$a_{tol,\min}^{h,app} = \arctan\left(\frac{b_{hor}}{a_{h-\min}\sqrt{1-\dfrac{b_{hor}^2}{a_{h-\max}^2}}}\right) \tag{36}$$

$$a_{tol,\max}^{h,app} = \arctan\left(\frac{b_{hor}}{a_{h-\max}\sqrt{1-\dfrac{b_{hor}^2}{a_{h-\min}^2}}}\right) \tag{37}$$

And finally the formulas for $a_{h-\min}^{*}$ and $a_{h-\max}^{*}$ are

$$a_{h-\max}^{*} = \frac{a_{ver}}{\pi \cdot a_{tol,\max}^{h,app} - 2\int_0^{a_{tol,\max}^{h,app}} \phi_1(\theta)\cdot d\theta} \cdot \int_0^{a_{tol,\max}^{h,app}} \left[F\left(\pi-\phi_1(\theta),\omega_1(\theta)\right) - F\left(\phi_1(\theta),\omega_1(\theta)\right)\right]\cdot d\theta \tag{38}$$

$$a_{h-\min}^{*} = \frac{a_{ver}}{\pi \cdot a_{tol,\min}^{h,app} - 2\int_0^{a_{tol,\min}^{h,app}} \phi_2(\theta)\cdot d\theta} \cdot \int_0^{a_{tol,\min}^{h,app}} \left[F\left(\pi-\phi_2(\theta),\omega_2(\theta)\right) - F\left(\phi_2(\theta),\omega_2(\theta)\right)\right]\cdot d\theta \tag{39}$$

where $\phi_1(\theta)$ and $\phi_2(\theta)$ are calculated as

$$\phi_1(\theta) = \operatorname{arccot}\left(\tan^2 a_{tol,\max}^{v,app} \cdot \sqrt{1-\left(1+\cot^2 a_{tol,\max}^{h,app}\right)\cdot \sin^2\theta}\right) \tag{40}$$

$$\phi_2(\theta) = \operatorname{arccot}\left(\tan^2 a_{tol,\min}^{v,app} \cdot \sqrt{1-\left(1+\cot^2 a_{tol,\min}^{h,app}\right)\cdot \cos^2\theta}\right) \tag{41}$$

Rescaling the experimental variogram points

In 2D case, the tolerance correction factor in the two minor and major directions of continuity can be calculated as:

$$f_{\min} = \frac{a_{h-\min}}{a_{h-\min}^{*}} \tag{42}$$

$$f_{\max} = \frac{a_{h-\max}}{a^*_{h-\max}} \tag{43}$$

These factors in minor and major directions should be applied on all of the calculated experimental points therefore the lag distance axis on variogram plot for major and minor directions should be rescaled:

$$\mathbf{h}_{new} = f_{\min} \cdot \mathbf{h} \tag{44}$$

$$\mathbf{h}_{new} = f_{\max} \cdot \mathbf{h} \tag{45}$$

It should be noted that the variogram values are not changed, the plot is just shifted horizontally to the left or to the right depending on the minor or major directions of continuity.

For 3D the optimal experimental lag distances should be updated and a variogram should be fitted again. The new lag distance should be obtained for three different directions: minor, major and vertical directions. The tolerance correction factors for minor and major directions are the same as equations (42) and (43), respectively. For the vertical direction, the correction factor is:

$$f_{ver} = \frac{a_{ver}}{a^*_{ver}} \tag{46}$$

And the corresponding rescaled lag distance in vertical direction is:

$$\mathbf{h}_{new} = f_{ver} \cdot \mathbf{h} \tag{47}$$

After rescaling the lag distance axis in all of three directions and updating the experimental points, a variogram should be fitted by using `varfit` (Neufeld and Deutsch, 2004).

Conclusion

Introducing tolerance parameters in variogram calculation underestimates the range of correlation in the major direction and overestimates the range of correlation in minor direction. The amount of underestimation and overestimation are determined analytically. The correction factor in major, minor (in both 2D and 3D data set) and vertical direction (in 3D) should be determined and then the lag distances should be rescaled by using these correction factors.

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