

Closed-form estimates of the Gaussian and sinc semivariogram parameters

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22 March 2025

Abstract. Formulas are derived for estimates of parameters in the normal (or Gaussian) and cardinal sine (or sinc) semivariogram models, based on numerical integrals of the empirical data. First-order Taylor approximations are introduced. These estimates demand little computation, and are shown to be preferable to the iterative estimates in some cases.

Introduction. Given a set of training data (x_{ji}, y_i) , and a set of query points q_{ji} , the regression problem seeks a prediction \hat{y} for each q . The simple nearest-neighbors approach seeks the x nearest to a given q , and uses the corresponding y value. An extension of this approach is to take a weighted average of the training target values, choosing the weights according to an influence function which decreases with the distance between x and q .

The weighted-average regression scheme has a significant flaw: if the training data is sampled unevenly, areas heavily represented in the training set will have an excessive influence on the estimate. If a particular x_i is repeated enough times, the estimate will converge to y_i . This undesirable behavior can be remedied by solving the linear system $\sum A_{ij} w_j = y_i$, where A is the matrix of functions of distances between the points x , and w is a vector of weights. The estimate sought is then given by $\hat{y} = b \cdot w$, where b is the vector of functions of distance between the query point and each training point. If the influence function applied satisfies certain conditions, matrix A is positive semi-definite and this method is called *kernel regression*. A particular kind of kernel regression is *simple kriging*. (Hastie, Tibshirani & Friedman p.171) The techniques presented in this article are applicable to any kriging variant.

Kriging is an interpolation technique employed extensively in the field of geostatistics, and has applications in mining, hydrology, and epidemiology. (Col. U., 2025) It may be distinguished from kernel regression in that kriging adopts the principled approach of learning the influence function from the training data.

The original interpolation problem thus induces a second interpolation problem. For each pair of points in the training data, the distance or *lag* between them is computed, denoted h ; and the *semivariance*, denoted g , defined as $g = \frac{1}{2}(y_j - y_k)^2$. A curve-fitting problem is then undertaken to approximate each observed pair (h, g) by a function $y = f(h)$, where f is chosen

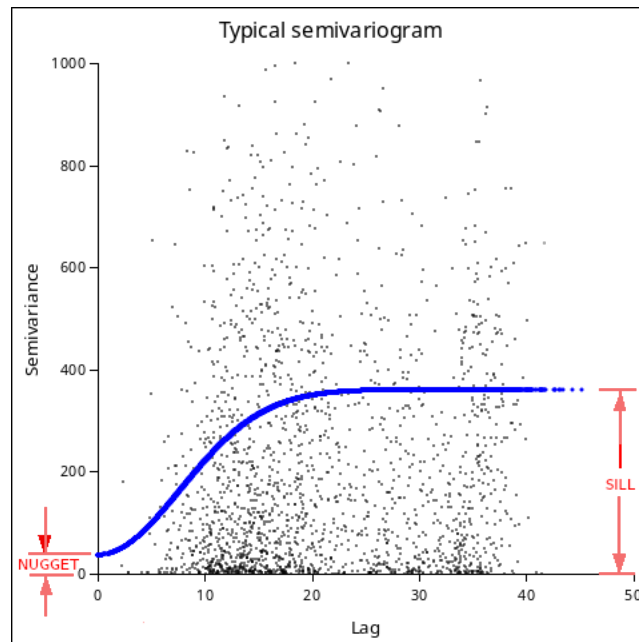
from a limited group of functions. Among these are the so-called circular and spherical semivariance models. Also in this group are the normal (or Gaussian) model, and the cardinal (or sinc) model. (Gavin and Khanal, 2021)

Next the predicted semivariances γ must be computed between each pair of points in the training set. These are converted to affinities according to the formula:

$$\alpha = 1 - \frac{\gamma}{\gamma_{max}}$$

The linear system $\sum A_{ij}w_j = y_i$ is solved for w , where the matrix A is the affinities. Then $\hat{y} = b \cdot w$ gives the estimate to the original regression problem, where the vector b is composed of the affinities between the query point and each point in the training set.

A typical semivariogram will have a plot of the form:



It is an increasing function because the farther points are away from each other, the less alike they are. One of the assumptions of kriging is that an average target value exists over the sample space, and therefore points at great separation will approach a maximum variance of their target values. The maximum semivariance is called the *sill*. It is also likely that some variance exists even at negligible distance – that is, boreholes drilled at the same location may not have identical assays. This produces a nonzero semivariance at zero lag, an effect which is called the *nugget*.

The number of pairs of points grows as $\frac{1}{2}N^2$; forming a histogram of average semivariance over intervals of lag reduces the computational effort. More importantly, the histogram places increased importance on the critical short lags which will have the most influence on the eventual estimate. A great deal of arbitrary discretion is possible in forming the histogram; the present effort will fix the number of histogram bins at 32 and space them evenly over the range of lags. The arithmetic mean of lag and of semivariance in each bin will be used in place of the original data, and any empty bins shall be omitted.

Plausible optimality of the cardinal kernel. The normal model is of especial interest because it is widely used in statistics as a kernel function. The cardinal function is of especial interest because it may be optimal. Viktor Epanechnikov proved that his kernel function was superior among functions which do not take on negative values. (Chill2Macht, 2018) This includes the Gaussian.

Although counterintuitive, an influence function which takes on negative values can give superior performance. It is well-known that the cardinal sine

$$\text{sinc}(h) = \begin{cases} \frac{\sin(h)}{h}, & h \neq 0 \\ 1, & h = 0 \end{cases}$$

is optimal for certain evenly-spaced interpolation problems. This function performs well empirically, takes on negative values, and produces positive-definite matrices. It is therefore a plausible conjecture that it is also the optimal kernel function for kriging regression.

Compromise made. In order to obtain a solution in closed form, exactness must be sacrificed. The estimates are given in terms of the integrals of the semivariance, which must be approximated by numerical integration. This trade is advantageous – the examples presented will show results that are generally acceptable and sometimes excellent.

Use of the result. The closed-form estimates have a very modest computational cost that is linear in the number of histogram bins. They may be used directly in the kriging process, or as starting guesses for an iterative estimate of the semivariogram parameters. In the case of the cardinal semivariogram, multiple local optima exist for fitting the parameters, but the closed-form estimate will ensure a unique solution.

For those seeking a thorough background on kriging, information can be found in the GSLIB User's Guide, Professor Nielsen's "Kriging Example," and the ArcGIS website – to suggest a few of the many worthy expositions available on the topic.

Related work. In a recent study of the topography of East Java (Sari et al., 2024), a semivariance model of the form $\gamma = c_0 + c_1 f\left(\frac{h}{c_2}\right)$ was considered, and closed form least-squares estimates were derived for the parameters c_0 and c_1 . For the critical c_2 scaling parameter, the authors resorted to a direct search method. A closed-form method to determine this parameter shall now be proposed.

Derivation. Integrals of the cardinal sine where sinc denotes the cardinal sine function and Si denotes the (cardinal) sine integral are:

$$\int \text{sinc}\left(\frac{h}{c_2}\right) dh = c_2 \text{Si}\left(\frac{h}{c_2}\right)$$

$$\int \text{Si}\left(\frac{h}{c_2}\right) dh = h \text{Si}\left(\frac{h}{c_2}\right) + c_2 \cos\left(\frac{h}{c_2}\right)$$

$$\int h \text{Si}\left(\frac{h}{c_2}\right) dh = \frac{1}{2} \left(h^2 \text{Si}\left(\frac{h}{c_2}\right) + c_2 h \cos\left(\frac{h}{c_2}\right) - c_2^2 \sin\left(\frac{h}{c_2}\right) \right)$$

$$\int h^2 \text{Si}\left(\frac{h}{c_2}\right) dh = \frac{1}{3} \left(h^3 \text{Si}\left(\frac{h}{c_2}\right) + c_2 h^2 \cos\left(\frac{h}{c_2}\right) - 2c_2^2 h \sin\left(\frac{h}{c_2}\right) - 2c_2^3 \cos\left(\frac{h}{c_2}\right) \right)$$

The cardinal sine semivariance function is defined as:

$$\gamma = c_0 + c_1 \left(1 - \text{sinc}\left(\frac{h}{c_2}\right) \right)$$

Let a_1, a_2, a_3 and a_4 denote the successive integrals of γ . Then,

$$a_1 = \int \gamma dh = (c_0 + c_1)h - c_1 c_2 \text{Si}\left(\frac{h}{c_2}\right)$$

$$a_2 = \int a_1 dh = \frac{c_0 + c_1}{2} h^2 - c_1 c_2 \left(h \text{Si}\left(\frac{h}{c_2}\right) + c_2 \cos\left(\frac{h}{c_2}\right) \right)$$

$$a_3 = \int a_2 dh = \frac{c_0 + c_1}{6} h^3 - \frac{1}{2} c_1 c_2 \left[h^2 \text{Si}\left(\frac{h}{c_2}\right) + c_2 h \cos\left(\frac{h}{c_2}\right) + c_2^2 \sin\left(\frac{h}{c_2}\right) \right]$$

$$a_4 = \int a_3 dh = \frac{c_0 + c_1}{24} h^4 - \frac{1}{6} c_1 c_2 \left[h^3 \text{Si}\left(\frac{h}{c_2}\right) + c_2 h^2 \cos\left(\frac{h}{c_2}\right) + c_2^2 h \sin\left(\frac{h}{c_2}\right) - 2c_2^3 \cos\left(\frac{h}{c_2}\right) \right]$$

From these equations, it is possible to solve for the sub-expressions:

$$\sin\left(\frac{h}{c_2}\right) = h \frac{c_0 + c_1 - \gamma}{c_1 c_2}$$

$$\text{Si}\left(\frac{h}{c_2}\right) = \frac{(c_0 + c_1)h - a_1}{c_1 c_2}$$

$$\cos\left(\frac{h}{c_2}\right) = \frac{1}{c_1 c_2^2} \left(h a_1 - a_2 - \frac{c_0 + c_1}{2} h^2 \right)$$

$$(c_0 + c_1) c_2^2 = c_2^2 \gamma - 2 \frac{a_3}{h} - \frac{c_0 + c_1}{6} h^2 + a_2$$

Substituting these expressions yields the equation for the semivariance:

$$\gamma = -(c_0 + c_1) - \frac{a_2}{c_2^2} + \frac{6 a_3 + 4 a_1}{c_2^2 h} - \frac{12 a_4 + 4 a_2}{c_2^2 h^2}$$

which is linear in the parameters c_0, c_1 , and c_2 . Parameters c_0 and c_1 occur together and may be treated as a single variable. The squared error of the estimate is:

$$f = \frac{1}{2} \sum (y_i - g_i)^2$$

where g_i are the observed semivariances, which has its optimum when

$$\frac{\partial f}{\partial c_2} = \frac{\partial f}{\partial (c_0 + c_1)} = 0$$

By aid of computer algebra (Maxima) the resulting system of two equations in two unknowns may be solved for c_2 . Care must be taken to re-enter the sums which occur in the expansion of the derivatives as distinct variables to prevent Maxima from making manipulations which are invalid on a summation. The result may be factored so as to be written :

$$\begin{aligned}
p = & 144 \sum \left(\frac{a_4}{h^2} - \frac{\bar{a}_4}{h^2} \right) \left(\frac{a_4}{h^2} \right) \\
& - 144 \sum \left(\frac{a_4}{h^2} - \frac{\bar{a}_4}{h^2} \right) \left(\frac{a_3}{h} \right) \\
& + 36 \sum \left(\frac{a_3}{h} - \frac{\bar{a}_3}{h} \right) \left(\frac{a_3}{h} \right) \\
& + 24 \sum (a_2 - \bar{a}_2) \left(\frac{a_4}{h^2} \right) \\
& - 12 \sum (a_2 - \bar{a}_2) \left(\frac{a_3}{h} \right) \\
& + \sum (a_2 - \bar{a}_2) a_2
\end{aligned}$$

$$\begin{aligned}
q = & -48 \sum \left(\frac{a_4}{h^2} - \frac{\bar{a}_4}{h^2} \right) \left(\frac{a_2}{h^2} \right) \\
& + 48 \sum \left(\frac{a_4}{h^2} - \frac{\bar{a}_4}{h^2} \right) \left(\frac{a_1}{h} \right) \\
& + 24 \sum \left(\frac{a_3}{h} - \frac{\bar{a}_3}{h} \right) \left(\frac{a_2}{h^2} \right) \\
& - 24 \sum \left(\frac{a_3}{h} - \frac{\bar{a}_3}{h} \right) \left(\frac{a_1}{h} \right) \\
& - 4 \sum (a_2 - \bar{a}_2) \left(\frac{a_2}{h^2} \right) \\
& + 4 \sum (a_2 - \bar{a}_2) \left(\frac{a_1}{h} \right) \\
& - 12 \sum (g - \bar{g}) \left(\frac{a_4}{h^2} \right) \\
& + 6 \sum (g - \bar{g}) \left(\frac{a_3}{h} \right) \\
& - \sum (g - \bar{g}) a_2
\end{aligned}$$

$$c_2 = \sqrt{\frac{p}{q}}$$

where the bar terms denote the arithmetic mean, for example $\frac{\bar{a}_4}{h^2} = \frac{1}{M} \sum \frac{a_4}{h^2}$, where M is the number of histogram bins. Since h_i and g_i are observed data; a_1 , a_2 , a_3 and a_4 may be determined by numerical integration and c_2 may be evaluated. The trapezoidal rule will suffice. Specifically,

$$(a_1)_1 = 0$$

$$(a_1)_i = (a_1)_{i-1} + \frac{1}{2} (g_i + g_{i-1}) (h_i - h_{i-1})$$

and

$$(a_2)_1 = 0$$

$$(a_2)_i = (a_2)_{i-1} + \frac{1}{2} ((a_1)_i + (a_1)_{i-1}) (h_i - h_{i-1})$$

and so forth.

Having obtained an estimate for the critical scale parameter c_2 , estimates for c_0 and c_1 may be gotten with considerably less difficulty, as the original equation for the semivariance may be used and no integration is required. Let s_i denote the cardinal sine expression

$$s_i = \text{sinc}\left(\frac{h_i}{c_2}\right)$$

The squared-error loss is:

$$f = \frac{1}{2} \sum (\gamma_i - g_i)^2 = \frac{1}{2} \sum (c_0 + c_1(1 - s_i) - g_i)^2$$

where g_i is the observed semivariance. Then at the optimum,

$$\frac{\partial f}{\partial c_0} = \sum [c_0 + c_1(1 - s_i) - g_i] = 0$$

$$\frac{\partial f}{\partial c_1} = \sum [c_0 + c_1(1 - s_i) - g_i](1 - s_i) = 0$$

This system of two equations in two unknowns may be solved to yield

$$c_1 = - \frac{\sum (g_i - \bar{g}) s_i}{\sum (s_i - \bar{s}) s_i}$$

$$c_0 = \bar{g} - c_1(1 - \bar{s})$$

which completes the estimate of the cardinal semivariogram parameters. It may be desired to have no nugget effect, for example, if the value of c_0 as determined above is negative. In that case the semivariogram model is:

$$\gamma = c_1 \left(1 - \text{sinc}\left(\frac{h}{c_2}\right)\right)$$

and c_1 will be found to be:

$$c_1 = \frac{\sum (1 - s_i) g_i}{\sum (1 - s_i)^2}$$

Normal semivariogram parameters. The derivation of the normal semivariogram parameters follows a similar strategy as the cardinal. The defining equation is

$$\gamma = c_0 + c_1 \left(1 - \exp\left(-\left(\frac{h}{c_2}\right)^2\right)\right)$$

Let a_1 , a_2 , and a_3 denote the successive integrals of γ . Then,

$$\begin{aligned}
a_1 &= \int y dh = (c_0 + c_1)h - \frac{\sqrt{\pi}c_1c_2}{2} \operatorname{erf}\left(\frac{h}{c_2}\right) \\
a_2 &= \int a_1 dh = \frac{c_0+c_1}{2}h^2 - \frac{c_1c_2}{2} \left[\sqrt{\pi} h \operatorname{erf}\left(\frac{h}{c_2}\right) + c_2 \exp\left(-\left(\frac{h}{c_2}\right)^2\right) \right] \\
a_3 &= \int a_2 dh = \frac{c_0+c_1}{6}h^3 - \frac{c_1c_2}{8} \left[\sqrt{\pi} (2h^2+c_2^2) \operatorname{erf}\left(\frac{h}{c_2}\right) + 2c_2h \exp\left(-\left(\frac{h}{c_2}\right)^2\right) \right]
\end{aligned}$$

From these equations, it is possible to solve for the sub-expressions:

$$\exp\left(-\left(\frac{h}{c_2}\right)^2\right) = \frac{c_0+c_1-y}{c_1}$$

$$\operatorname{erf}\left(\frac{h}{c_2}\right) = \frac{(c_0+c_1-a_1)}{c_1c_2 \frac{\sqrt{\pi}}{2}}$$

$$(c_0+c_1)c^2 = 2ha_1 - 2a_2 - (c_0+c_1)h^2 + c_2^2y$$

Substituting to eliminate the nonlinear terms yields:

$$y = \frac{a_1}{h} - \frac{\left(\frac{4a_3}{h} - 4a_2 + 2a_1h - \frac{2}{3}(c_0+c_1)h^2\right)}{c_2^2}$$

The least-squares estimate for the scaling parameter is

$$\begin{aligned}
p = & 8 \left(\sum \frac{a_2a_3}{h} \sum h^4 - \sum a_2h^2 \sum a_3h \right) \\
& + 4 \left(\left(\sum a_3h \right)^2 - \sum \frac{a_3^2}{h^2} \sum h^4 \right) \\
& + 4 \left(\sum a_1h^3 \sum a_3h - \sum a_1a_3 \sum h^4 \right) \\
& + 4 \left(\left(\sum a_2h^2 \right)^2 - \sum a_2^2 \sum h^4 \right) \\
& + 4 \left(\sum a_1a_2h \sum h^4 - \sum a_1h^3 \sum a_2h^2 \right) \\
& + \left(\left(\sum a_1h^3 \right)^2 - \sum a_1^2h^2 \sum h^4 \right)
\end{aligned}$$

$$\begin{aligned}
q = & 2 \left(\sum a_1h \sum a_3h - \sum \frac{a_1a_3}{h^2} \sum h^4 \right) \\
& + 2 \left(\sum \frac{a_1a_2}{h} \sum h^4 - \sum a_1h \sum a_2h^2 \right) \\
& + \left(\sum a_1h \sum a_1h^3 - \sum a_1^2 \sum h^4 \right) \\
& + 2 \left(\sum \frac{a_3g}{h} \sum h^4 - \sum a_3h \sum gh^2 \right) \\
& + 2 \left(\sum a_2h^2 \sum gh^2 - \sum a_2g \sum h^4 \right) \\
& + \left(\sum a_1gh \sum h^4 - \sum a_1h^3 \sum gh^2 \right)
\end{aligned}$$

$$c_2 = \sqrt{2\frac{p}{q}}$$

Let e_i denote the exponential expression $e_i = \exp(-(\frac{h_i}{c_2})^2)$

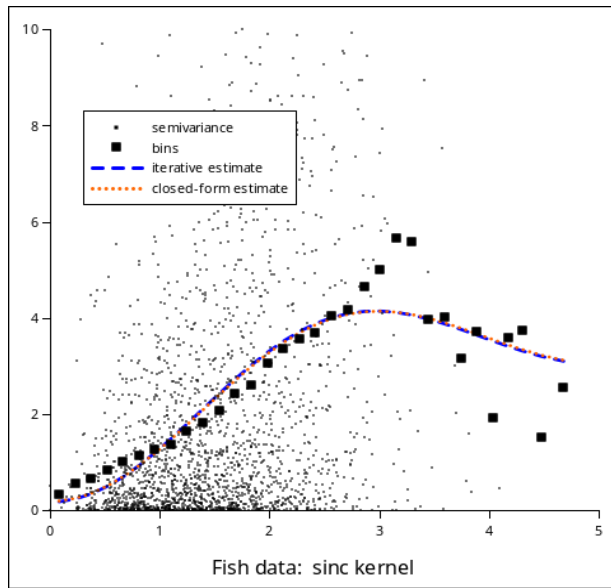
Then

$$c_1 = -\frac{\sum (g_i - \bar{g})e_i}{\sum (e_i - \bar{e})e_i}$$

$$c_0 = \bar{g} - c_1(1 - \bar{e})$$

which completes the estimate of the normal semivariogram parameters. If c_0 is to be held to zero, the estimate for c_1 is instead:

$$c_1 = \frac{\sum (1 - e_i)g_i}{\sum (1 - e_i)^2}$$

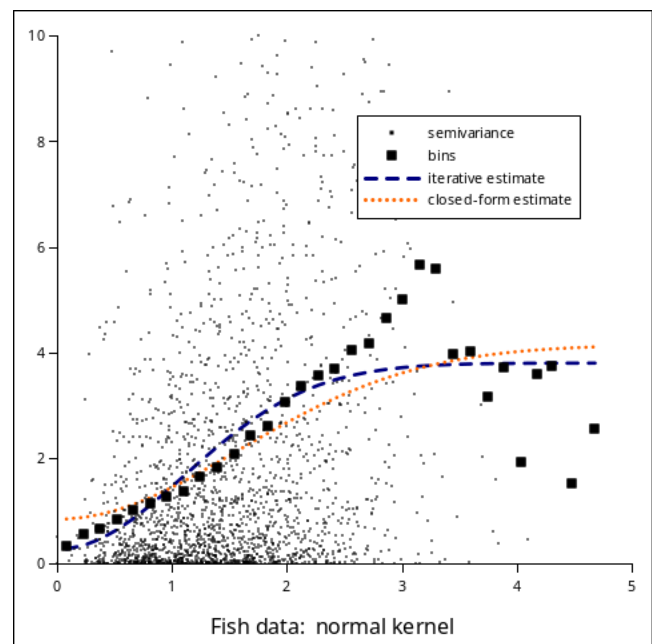


Favorable examples. To demonstrate the accuracy of the approximation, consider the fish toxicity data (Cassotti et al.) Each variable was assigned an importance weight of its linear regression coefficient, and the distance between each pair of observations was taken to be weighed Euclidean. A sample of one seventh of possible semivariance pairs was collected into a histogram of 32 bins, and the cardinal and normal semivariogram parameters were estimated according to the above method. The result was then compared to that obtained by the iterative solution available in the spreadsheet Gnumeric. The semivariances plotted here are of a much smaller sample for illustrative purposes. The agreement in this case is excellent.

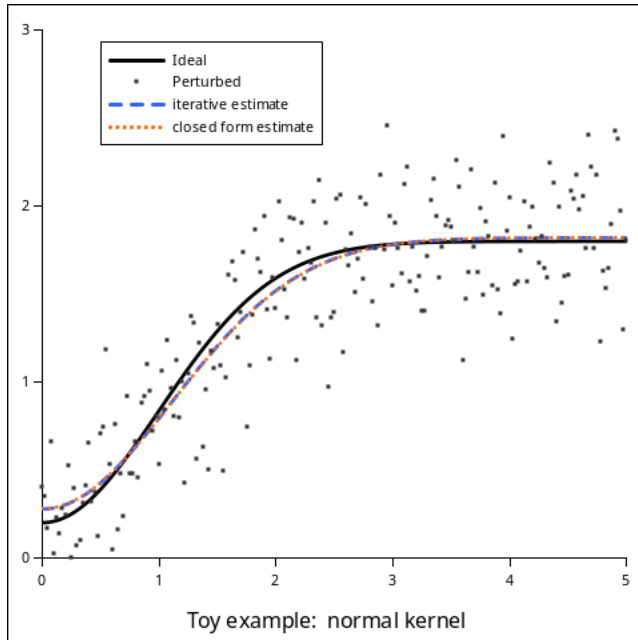
	Iterative estimate	Closed-form estimate
C_0	0.175	0.191
C_1	3.267	3.252
C_2	0.658	0.665
Squared error	13.198	13.222
Comparative error	-	0.175%

The normal parameter estimate on this problem is less impressive, but still useful.

	Iterative estimate	Closed-form estimate
C_0	0.273	0.833
C_1	3.533	3.310
C_2	1.553	2.201
Squared error	21.935	27.534
Comparative error	-	25.524%

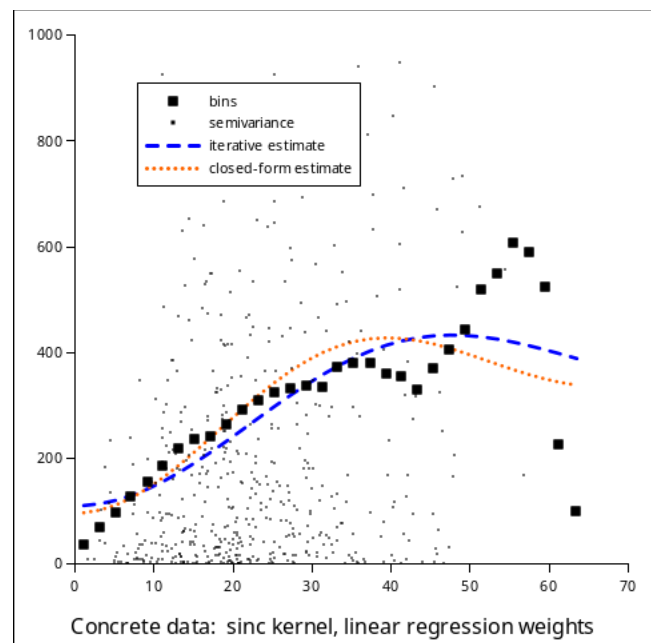


For a better validation of the correctness of the estimate in the normal case, construct the artificial test case in which the semivariance is given from the formula with known parameters with some added Gaussian noise. With parameters $c_0=0.2$, $c_1=1.6$, $c_2=1.4$, and noise level $\sigma = 0.3$, a draw from the random number generator is shown below.

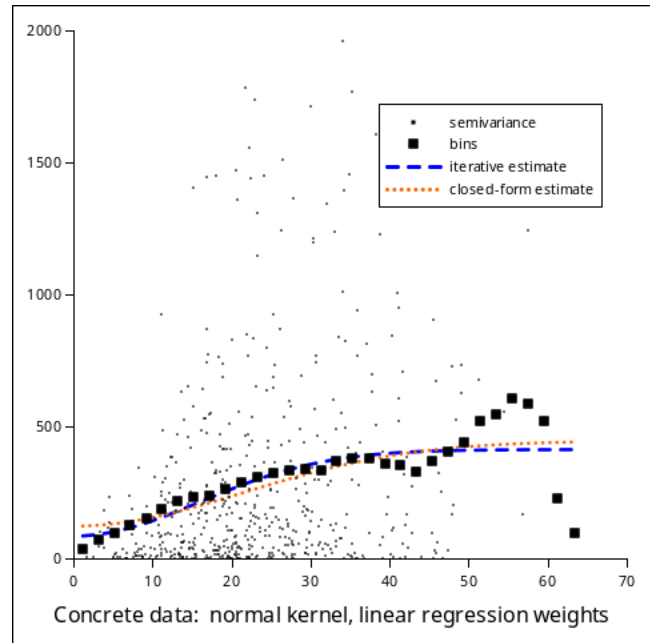


	Iterative estimate	Closed-form estimate
C_0	0.278	0.280
C_1	1.543	1.542
C_2	1.562	1.568
Squared error	17.705	17.706
Comparative error	-	0.003%

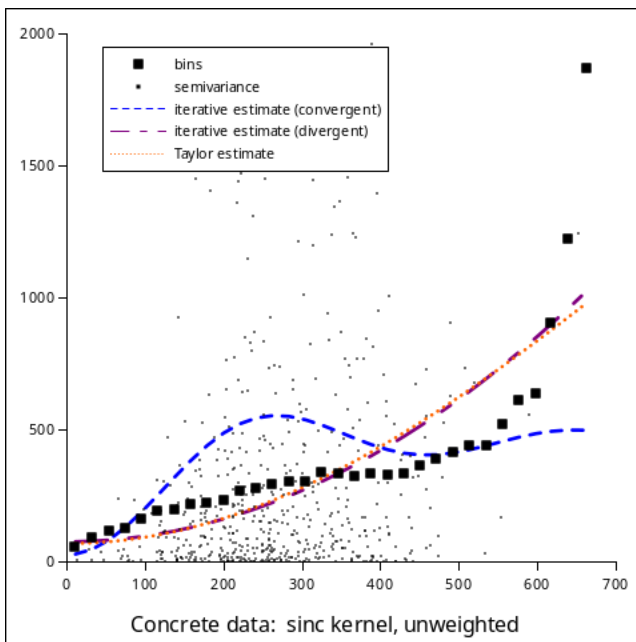
As a further example, consider the concrete compressive strength data (Yeh, 1998), using the Euclidean distance with the linear regression weights. The histogram bins are averages over all semivariance pairs, and the plotted dots are a sample of each thousandth pair. For the cardinal model, reasonable agreement is attained between the closed-form solution and the iterative solution. The difference in squared error is within 20%.



The closed-form estimate for the normal model also performs reasonably well on this problem, achieving a relative error of less than 10%.



Unsatisfactory example. When distances in the concrete data are computed without importance weights on the variables, the semivariogram shows an increasing trend that does not approach a sill. In this case the closed-form estimates for c_2 fail completely, with the quantity inside the square root being negative. The iterative solution will depend on the starting values and may fail to converge, with c_1 and c_2 increasing indefinitely.



Taylor series approximation. If the data do not show a sill, it is not reasonable to expect to fit a curve with a sill to the data. Recalling the Epanechnikov kernel, try to fit the data to a parabola instead.

Make use of the first-order Taylor series approximation

$$\text{sinc}(x) \approx 1 - \frac{x^2}{6}$$

Then

$$y = c_0 + c_1 \left(1 - \text{sinc}\left(\frac{h}{c_2}\right)\right) \approx c_0 + \frac{c_1}{6c_2^2} h^2$$

Defining $c_3 = \frac{c_1}{6c_2^2}$, the parabolic model to be fit is

$$y = c_0 + c_3 h^2$$

To minimize the squared error, solve the equations

$$\frac{\partial f}{\partial c_0} = \sum (c_0 + c_3 h_i^2 - g_i) = 0$$

$$\frac{\partial f}{\partial c_3} = \sum (c_0 + c_3 h_i^2 - g_i) h_i^2 = 0$$

resulting in:

$$c_3 = \frac{\sum g_i h_i^2 - \bar{g} \sum h_i^2}{\sum h_i^4 - \frac{(\sum h_i^2)^2}{N}}$$

$$c_0 = \bar{g} - c_3 \frac{\sum h_i^2}{N}$$

unless a zero nugget $c_0=0$ is imposed, in which case

$$c_3 = \frac{\sum g_i h_i^2}{\sum h_i^4}$$

The parabolic model thus obtained may be used as itself, or it may be used to find the corresponding cardinal sine model. Taking a reasonable guess for the sill, such as the maximum observed semivariance

$$c_0 + c_1 = g_{max}$$

from the definition of c_3 ,

$$c_2 = \sqrt{\frac{c_1}{6c_3}}$$

and c_0 and c_1 may be recomputed by the method given before.

Taylor approximation of the normal model. The first-order Taylor series approximation of the exponential function is

$$e^x = \sum_{i=0}^{\infty} \frac{x^i}{i!} \approx 1 + x$$

Thus, the parabolic approximation of the normal semivariance model is:

$$y = c_0 + c_1 \left(1 - \exp\left(-\left(\frac{h}{c_2}\right)^2\right)\right) \approx c_0 + \frac{c_1}{c_2^2} h^2$$

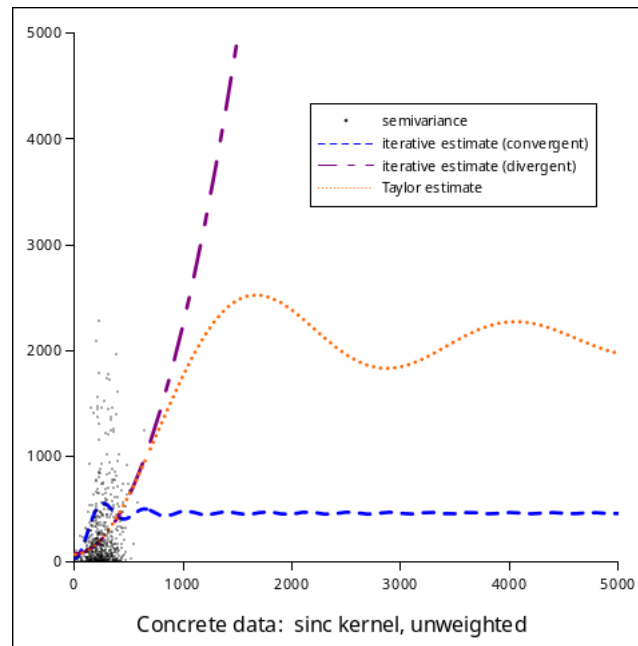
Defining $c_3 = \frac{c_1}{c_2^2}$, parameters c_0 and c_3 may be determined as before. If the corresponding normal semivariogram is desired, take the maximum observed semivariance as a reasonable guess for the sill, and

$$c_1 = g_{max} - c_0$$

$$c_2 = \sqrt{\frac{c_1}{c_3}}$$

and c_0 and c_1 may be recomputed by the method given before.

Parabolic example. The concrete problem is illustrated with lags extrapolated out to 5000. Depending on the initial guess, the iterative solution may converge, or it may diverge with values for c_1 and c_2 increasing indefinitely. The estimate given by converting the Taylor approximation to the cardinal model extrapolates better than the divergent iterative estimate.



It is also much more accurate than the convergent estimate. In this case, the closed-form method would seem preferable to the iterative method, even as a final result.

	Convergent estimate	Divergent estimate	Taylor estimate
c_0	26.970	76.329	69.257
c_1	433.613	16041331.615	2018.960
c_2	59.439	35147.543	371.586
Squared error	3.211×10^6	1.202×10^6	1.313×10^6
Comparative error	167.240%	-	9.308%

Implementation. Efficient programs in FORTRAN and C for estimating the cardinal semivariogram parameters are placed in the public domain in the package `variogram`, available at <http://13olive.net/code/variogram.zip>

Programming the estimates of the normal semivariogram parameters is left as a project for the interested reader.

Conclusions. The closed-form parameter estimates may be used themselves or may serve as initial guesses in an iterative technique. These estimates are not exact, but can be made as accurate as the numerical integration of the empirical semivariance data.

The estimate for the cardinal sine semivariogram parameters is especially valuable since this curve does not have a unique local minimum of least-squared error. The Taylor series approximations introduced provide a feasible solution in cases in which iterative estimates do not converge. The technique used in the derivation may offer an avenue of attack to other challenging problems.

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