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Optimal Transect Sampling Designs: Are Straight Transects Always Best?

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SUMMARY

Relatively little attention has been paid to optimal sampling design when the support of the sample is a linear transect. The D-optimality criterion allows the quantitative comparison of spatial sampling designs for samples with either point or transect support. D-optimality is applied to transects that are equally spaced point samples taken along a straight or curved path. For short transects containing three points, the optimal angle between adjacent transect segments can be determined analytically by setting the derivative of the D-optimality criterion with respect to the spatial covariance to zero. Results show that straight transects are suboptimal when the random variable being sampled has a Gaussian or spherical covariance function. By combining D-optimality with simulated annealing or Powell's algorithm, optimal spatial designs for longer transects can be determined. For a Gaussian variogram, a zigzag pattern is nearly optimal and is better than a straight transect. For a spherical variogram, a transect that bends twice to the right then twice to the left maintaining a constant interior angle is nearly optimal and is better than a straight transect. Finally, for an exponential variogram, straight transects are optimal. Implementation of these results for use in practical design of field surveys is discussed.

Keywords : Statistical design, Transects, Geostatistics, Optimization.

1. INTRODUCTION

The question of how to best locate samples across a spatial domain to meet some objective of the sampling program arises in a number of disciplines including mineral and petroleum exploration, environmental remediation, epidemiology, meteorology, forestry, ecology, hydrology, agriculture, and oceanography (for some examples see Wikle and Cressie 2011; McKenna 2009; Kumar 2009; and Saito *et al*. 2005). The largest body of work in spatial sampling design answers the question of where to locate samples from the perspective of point sampling (e.g., US EPA 2002). That is, the support of the sample is defined by a single set of coordinates and the sample volume is much less than the size of the site domain. Considerably less attention has been given to determining the optimal sampling design when the support of the sample is not a point but a linear transect.

With the availability of off-road vehicles, airplanes, helicopters, and spacecraft, along with better remote sensing sensor technology and accurate global positioning systems, it has become progressively easier to collect information while the sensors are moving. With the concurrent development of cheaper, larger data storage capabilities, collecting large amounts of data is now routine. Together these trends have led to increasing amounts of data collected as the sampling instrument moves, which produces one-dimensional samples called transects. In practice, data are collected at some temporal or spatial frequency, which makes any

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transect a sequential collection of point samples. However, spatial autocorrelation makes the measurements at these locations correlated to one another, which violates the assumptions underlying theories developed for design of independent point sampling arrangements. Therefore an extension of sampling theory specific to transects is required.

In practical applications, transects are often deployed in one of several possible ways, the most basic being a linear transect with a randomly selected orientation (Burnham *et al*. 1980). If several transects can be deployed, then parallel transects with a randomly selected orientation and individual transects each with a random orientation are two common design options. Field implementation of transect sampling is facilitated by defining each individual transect to be along a straight line. If the selected straight transect meets an obstacle in the field, e.g., a cliff along the proposed transect path, the transect would end prematurely or be diverted. Similarly, a long sampling transect of a body of water taken in a boat would be adapted so as to keep the sampling device in the water (e.g., Jassby *et al*. 1997).

The practical approach of selecting straight transects and then empirically adapting them to meet field conditions has proven useful in a number of fields, but the question remains as to whether or not these straight transect designs are optimal with respect to predicting property values at unsampled locations. For example, Palka and Pollard (1999) propose using a zigzag transect instead of the typical straight transect pattern when searching for harbor porpoises by ship. They examine the performance of using a straight transect design while the porpoise sighting rate is below a predetermined threshold, and then using a zigzag transect pattern when the sighting rate exceeds the threshold. They use an angle of approximately 60° between segments along a transect to create the zigzag pattern, and report that their design is 8% more efficient than using only a straight transect when tested in the field.

In most sampling designs, selection of straight transects has arisen from practical considerations rather than quantitative assessment of alternative transect shapes. The results of Palka and Pollard (1999) suggest that straight transects may not be optimal for all sampling situations. In this paper, we examine optimal transect sample design with respect to reducing the prediction error at unsampled locations within a spatial domain where the sampled property exhibits spatial correlation. We accomplish this examination by applying the theory of statistical design for optimal locations of point samples in a spatial domain (Fedorov and Hackl 1994) to the case of transect samples. This theory is applied to find transects containing evenly spaced samples that minimize predicted error variance for a spatial domain with a known autocorrelation structure but without prior samples. Results prove that a straight transect need not be optimal over all spatial patterns.

2. OPTIMALITY CRITERION FOR SAMPLING DESIGN

Let R_c (c for *continuous*) be the region where the sample is to be taken. To reduce the problem to one with finite dimensionality, the continuous region R_c is replaced with a discrete subset of n points, R, which is split into two disjoint sets denoted by R_p (p for *proposed*) and R_r (r for *remainder*). The quantity being measured on R is denoted by the variable $\boldsymbol{y}$, and $\boldsymbol{y}_p$ and $\boldsymbol{y}_r$ are defined as the restriction of $\boldsymbol{y}$ to regions R_p and R_r, respectively. Fedorov and Hackl (1994) optimizes spatial sampling designs by choosing $\boldsymbol{y}_p$ such that the error of predicting $\boldsymbol{y}_r$ from $\boldsymbol{y}_p$ is minimized. If prediction is limited to linear functions of $\boldsymbol{y}_p$, then kriging gives the best linear, unbiased estimate

$$\hat{\boldsymbol{y}}_{\boldsymbol{r}} = C_{rp} C_{pp}^{-1} \boldsymbol{y}_{\boldsymbol{p}}, \tag{1}$$

where C_{pp} is the correlation matrix of $\boldsymbol{y}_p$ with itself, C_{rp} is the correlation matrix of $\boldsymbol{y}_r$ with $\boldsymbol{y}_p$, and $\hat{\boldsymbol{y}}_{\boldsymbol{r}}$ is the predicted value of $\boldsymbol{y}_r$. These correlation matrices are determined if a positive definite correlation function between spatial locations is known or can be assumed. The variance matrix of the predicted error is

$$\begin{aligned} Var(\hat{\boldsymbol{y}}_{\boldsymbol{r}} - \boldsymbol{y}_{\boldsymbol{r}}) &\equiv Var(C_{rp} C_{pp}^{-1} \boldsymbol{y}_{\boldsymbol{p}} - \boldsymbol{y}_{\boldsymbol{r}}) \\ &= C_{rr} - C_{rp} C_{pp}^{-1} C_{pr} \end{aligned} \tag{2}$$

The goal is to find a sampling design that reduces this error matrix to be as small as possible. The simplest way to do this is to minimize a scalar function of this matrix. In practice, the product of the eigenvalues is most often used (Myers and Montgomery 1995, p. 364), which corresponds to the D-optimality criteria (Mitchell 1974), and is given by

$$\min_{\mathcal{D}} |C_{rr} - C_{rp} C_{pp}^{-1} C_{pr}| \tag{3}$$

where $\mathcal{D}$ is the set of spatial locations, one for each spatial design, and $|\cdot|$ stands for the determinant. Equation (3) does not depend on the values of the measurements y_p, only on the positions of the measurements, so it can be evaluated prior to collecting the data. This aspect of the D-optimality criteria is crucial in a design setting since it is necessary to compare different proposed y_p's prior to data collection.

Fedorov and Hackl (1994) also give a computational simplification. Let **C** be the correlation matrix of $\boldsymbol{y}$ with $\boldsymbol{y}$, recalling that $\boldsymbol{y}$ is the vector of the sites $\boldsymbol{y_p}$ combined with $\boldsymbol{y_r}$, and note that $\boldsymbol{y}$ does not change for different choices of $\boldsymbol{y_p}$. **C** can be represented by the block matrix

$$\mathbf{C} = \begin{pmatrix} C_{pp} & C_{pr} \\ C_{rp} & C_{rr} \end{pmatrix}, \tag{4}$$

and from a well-known result of linear algebra

$$|\,\mathbf{C}\,| = |C_{pp}|\,|C_{rr} - C_{rp}C_{pp}^{-1}C_{pr}|. \tag{5}$$

Since **C** is fixed, the two determinants on the right hand side are inversely proportional, so the D-optimality condition is equivalent to

$$\max_{\mathcal{D}}|C_{pp}|, \tag{6}$$

which is considerably more computationally efficient than Equation (3) assuming that the proportion of sites in R_p sampled is less than 50% of n. The criterion given in Equation (6) is used below to determine the optimal interior angle between two adjacent segments of a sampling transect for a given spatial correlation functions defining the sampled property field.

3. OPTIMAL TRANSECTS FOR THREE LOCATIONS

The interior angle is the minimum of the two possible ways to measure the angle between two adjacent segments of a transect (Fig. 1). The maximum possible interior angle is 180 degrees and corresponds to a straight transect, and with the D-optimality criterion, the optimal value of the interior angle can be calculated. For simplicity we restrict transects so that the spacing between samples is fixed at one unit of distance.

For the simplest possible case, three samples as shown in Fig. 1, the optimal transect shape can be calculated analytically. Assume that the spatial autocorrelation is isotropic and given by $c(s)$, where s is the distance between two locations. Since the distance between two successive samples is fixed at one unit, the distance between the two endpoints of the three point transect is $s = \sqrt{2 - 2\cos(\theta)}$, where s ranges between zero and two. Note that $s = 2$ corresponds to a straight transect. Solving for the interior angle gives: $\theta = \arccos(1 - s^2/2)$. So the D-optimality criterion for a correlation function with a normalized variance is given by

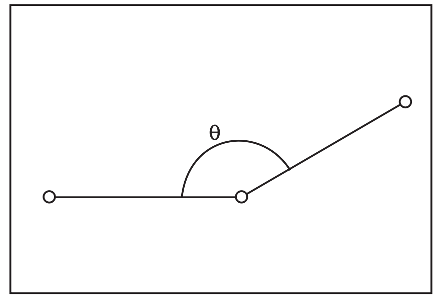

Fig. 1. Shortest transect of interest with three samples spaced one unit apart and interior angle of θ.

$$\begin{vmatrix} 1 & c(1) & c(s) \\ c(1) & 1 & c(1) \\ c(s) & c(1) & 1 \end{vmatrix} = -c(s)^2 + 2c(1)^2c(s) + 1 - 2c(1)^2$$

$$\equiv f(c(s)), \tag{7}$$

where f is a quadratic polynomial in $c(s)$ with a negative quadratic term. For s between zero and two if it can be assumed that: 1) $c(s)$ strictly decreases with increasing s; 2) is positive; and 3) is differentiable, then the maximum of f occurs either at an interior point where the first derivative of f with respect to $c(s)$ is zero, or if no such point exists, it must occur at $c(0)$ or $c(2)$.

The fact that $c(s)$ decreases as s increases means $c(0) = 1 > c(1) > c(1)^2 > 0$, which implies that $c(1)^2 - 1 < 0$, so the following derivative is negative

$$\left.\frac{df}{dc(s)}\right|_{s=0} = 2c(1)^2 - 2c(s)|_{s=0} = 2(c(1)^2 - 1) < 0. \tag{8}$$

Since df/dc and dc/ds are both negative,

$$\left.\frac{df}{ds}\right|_{s=0} = \left.\frac{df}{dc}\frac{dc}{ds}\right|_{s=0} > 0, \tag{9}$$

which implies that $f(c(0))$ is a local minimum. Since $f(c(s))$ is a quadratic in $c(s)$ with leading term negative, there can be only two ways that the transect can be optimal: $f(c(2))$ is the maximum, which corresponds to a straight transect, or the maximum occurs at $f(c(s))$, where $0 < s < 2$, which corresponds to a bent transect.

To determine which of these two cases occurs, we set the derivate of $f(c(s))$ with respect to $c(s)$ in Equation (7) to zero and obtain

$$\frac{df(c(s))}{dc(s)} = -2c(s) + 2c(1)^2 = 0 \Rightarrow c(s) = c(1)^2 \quad (10)$$

Because c is continuous and strictly decreases to 0 as s goes from 0 to infinity and because $c(0) > c(1)^2 > 0$, Equation (10) must have a unique solution. If this solution satisfies $s \in (0, 2)$, then the straight transect is suboptimal. Otherwise $f(c(s))$ is strictly increasing for $s \in (0, 2)$, and the straight transect is optimal.

In general, if the range of the autocorrelation function, a, is less than one, then $c(1) = 0$ and the optimality criterion reduces to $1 - c(s)^2$. This criterion is maximized if $c(s) = 0$, which happens for all s larger than a. Hence, straight transects are equally good as any transect with s larger than a. Since $c(a) = 0$ holds for the range, a, if $1 < a < 2$, then Equation (10) has a unique solution, and a meandering transect that is more optimal than a straight transect exists. If $a > 2$, then more knowledge of $c(s)$ is required to determine the optimality criterion. We examine the D-optimality criterion as a function of the distance between the endpoints of a short sampling transect where the spatial correlation of the field is described by each of three commonly used autocorrelation models: Gaussian, spherical and exponential.

(i) Gaussian autocorrelation model

The Gaussian model given by

$$c(s) = \exp\left(\frac{-3s^2}{a^2}\right), \; s \geq 0, \quad (11)$$

where the practical range is a. Once a is specified, it is possible to solve for $c(s) = c(1)^2$ for s, which can be done numerically. A plot of the D-optimality criterion, $f(c(s))$, as a function of the distance between the ends of the transect, is given in the upper left of Fig. 2. Here the variogram range is 3. Table 1 lists the optimal s, which equals $\sqrt{2}$, a value that corresponds to an

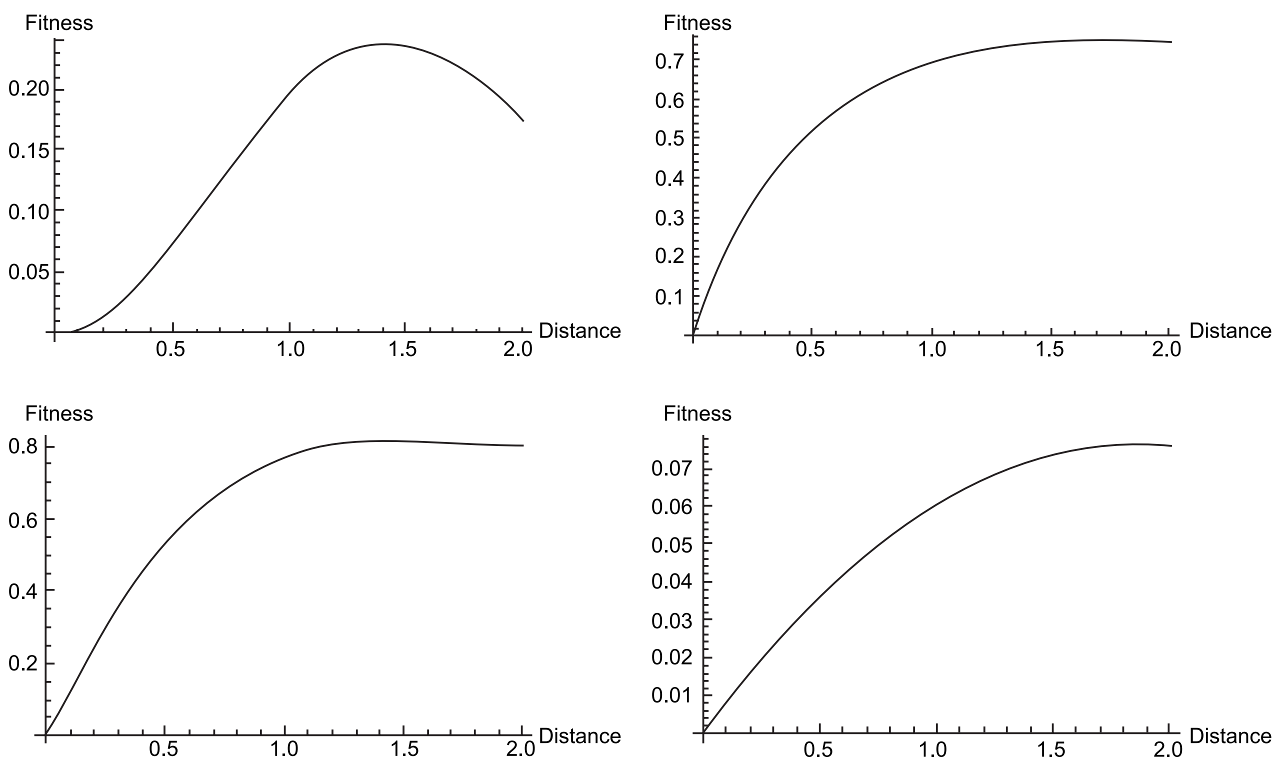

Fig. 2. Plots of D-optimality fitness defined by Equation (7) vs. the distance between the endpoints of the transect, which is given by $\sqrt{2-2\cos(\theta)}$. The top left plot shows Gaussian autocorrelation with range equals 3, and the top right plot shows exponential autocorrelation with range equals 3. The bottom two plots show spherical correlation: the left has range equals 2, while the right range equals 10.

Table 1. Values of s that maximize f, with corresponding angle θ, for Gaussian autocorrelation. The last column compares a straight transect to the optimal transect using the D-optimality criterion.

Range	d	θ (degrees)	$f(s)$	$f(2)/f(s)$
2	1.41	90	0.60	0.95
3	1.41	90	0.24	0.74
5	1.41	90	0.045	0.38
10	1.41	90	0.0034	0.11

interior angle of 90°. For the larger ranges, a straight transect is significantly inferior to the optimal L-shaped transect. As the value of the range increases, the superiority of the bent transect relative to the straight transect increases.

(ii) Spherical autocorrelation model

Next, the spherical model given by

$$c(s) = \begin{cases} 1-\dfrac{3}{2}\left(\dfrac{s}{a}\right)+\dfrac{1}{2}\left(\dfrac{s}{a}\right)^3, & 0 \le s \le a \\ 0, & s > a \end{cases} \tag{12}$$

is examined. The bottom two plots of Fig. 2 show the D-optimality function, $f(c(s))$, vs. s for variogram ranges of 2 and 10. Table 2 shows that the value of s corresponding to the maximum of f along with the interior angle of the transect. Notice that once f reaches its maximum at s_{max}, $f(s)$ is nearly constant for $s > s_{max}$, so while a straight transect is not optimal, it is close to optimal since $f(2)/f(s)$ is close to 1.0 for all s in Table 2.

Table 2. Values of s that maximize f, with corresponding angle θ, for spherical autocorrelation. The last column compares a straight transect to the optimal transect using the D-optimality criterion.

Range	d	θ (degrees)	$f(s)$	$f(2)/f(s)$
2	1.47	94	0.81	0.988
3	1.62	108	0.53	0.973
5	1.75	122	0.25	0.984
10	1.87	138	0.077	0.995

(iii) Exponential autocorrelation model

The third example shows that straight transects can be optimal with the exponential autocorrelation given by

Table 3. Values of s that maximize f, with corresponding angle θ, for exponential autocorrelation. Unlike the results for Gaussian and spherical autocorrelations, straight transects are optimal.

Range	d	θ (degrees)	$f(s)$	$f(2)/f(s)$
2	2	180	0.90	1.00
3	2	180	0.75	1.00
5	2	180	0.49	1.00
10	2	180	0.20	1.00

$$c(s) = \exp\left(\frac{-3s}{a}\right), \; s \ge 0 \tag{13}$$

The results in the upper right of Fig. 2 and Table 3 show that straight transects are the optimal transect shape for sampling a property described by an exponential covariance function. Similar to the results for the Gaussian model, the exponential model produces the same shape of the transect independent of the range of the autocorrelation function.

Fig. 2 demonstrates that straight transects may or may not be optimal depending on the correlation function. Fig. 3 shows the plots of Gaussian, spherical and exponential autocorrelations, and by comparing the slopes of these curves at the point (0, 1) to how close straight transects come to being optimal, a pattern emerges. First, the less negative the slope at (0, 1), the less the data satisfying such an autocorrelation vary at short distances. Hence, data satisfying the Gaussian

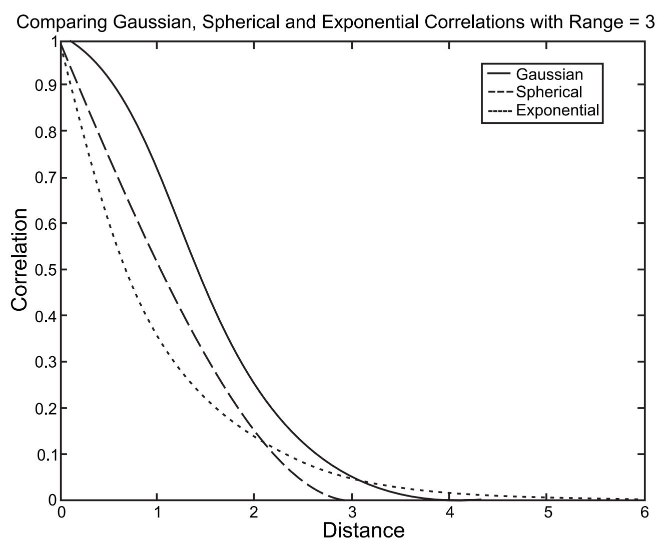

Fig. 3. Comparison of Gaussian, spherical and exponential correlation functions. All have an effective range equal to three units.

autocorrelation vary the least, and by Table 1, straight transects perform the worst. Data satisfying a spherical autocorrelation vary intermediately, and by Table 2, straight transects are close to optimal. Data satisfying exponential autocorrelation vary the most, and by Table 3, straight transects are optimal. That is, the more variable the data at small scales, the better straight transects perform.

This result is surprising because when autocorrelation is present, the clustering of sample locations would seem to be redundant, and so one would guess that the best transect is a straight line. Nonetheless, the superiority of meandering transects over straight transects can occur with short or long transects for both Gaussian and spherical autocorrelations.

4. NEAR-OPTIMAL LONG TRANSECTS

For longer transects with more samples that cannot be computed analytically, we use Equation (6) as a fitness function for optimization algorithms, which is used for the rest of this article. Long transects can be defined by specifying all the interior angles, so finding the D-optimal transect requires optimization over all these angles. Since there are likely to be many local optima, one can use either a global optimization algorithm or a local optimization algorithm using a number of initial starting values. Both approaches are tested here. For global optimization, simulated annealing is used, which is an algorithm that searches the space of transects by repeatedly applying random perturbations to the interior angles of a transect and initially allowing a chance for inferior perturbations to be kept. As the number of iterations increases, the probability of keeping an inferior perturbation goes to zero. Since random perturbations are used, results vary from one solution to the next, which produces a distribution of solutions about the true optimal solution. Since finding an explicit function returning the derivative of the D-optimality criterion is impractical for long transects, and since evaluating the D-optimal criterion is computationally inexpensive, local optimization is performed by Powell's algorithm, which uses multiple function evaluations to determine a set of linearly independent directions within the parameter space to search for a minimum (see details in Gumley 2002).

Although one cannot prove a given transect design optimal by these two algorithms, similar designs via different methods provide confidence that a given design is superior. Moreover, it is possible to prove that straight transects are sub-optimal for the spherical and Gaussian autocorrelations because these optimization routines found designs with better fitness than the straight transect (see Figs. 4 through 7.)

(i) Gaussian autocorrelation model

We examine the Gaussian autocorrelation closely because in the short transect calculations done above, straight transects performed the worst. For a transect consisting of ten samples and a range equaling three, a straight transect has fitness of 2.31e-5. The best design found by simulated annealing has fitness 6.95e-4, as shown on the left in Fig. 4, about 30 times better than the straight transect. The best design found by Powell's algorithm also has a fitness 6.95e-4, as shown on the right in Fig. 4, nearly identical to the simulated annealing result. For both optimizations, transects are considered to be on an infinite plane, so there are no boundary effects.

Fig. 4 show transects with nearly equal interior angles. Since such a pattern would be tedious to execute precisely in the field, one might rather use the best transect that has constant interior angles in a zigzag pattern. Since this is now a single parameter optimization, it is easy to solve, and the best angle is 109° with a fitness of 6.77e-4, only 2.6% worse than the design found by the two optimization algorithms mentioned above.

This zigzag pattern holds true for longer transects of 20 samples. Fig. 5 shows designs found by simulated annealing and Powell's algorithm. Note that simulated annealing has the zigzag pattern locally and has fitness equaling 1.31 e-7, but has trouble maintaining the zigzag pattern along the entire transect. Powell's algorithm produces a design that has nearly equal interior angles, but by adjusting the angles towards the endpoints, achieves the higher fitness of 1.60 e-7. A separate one-dimensional optimization shows that a design with constant interior angles of 110° has fitness 1.55e-7, only 3.1% lower than the design found by Powell's algorithm. A straight transect has fitness 4.37e-11, which is three orders of magnitude lower than any of the other designs specified above.

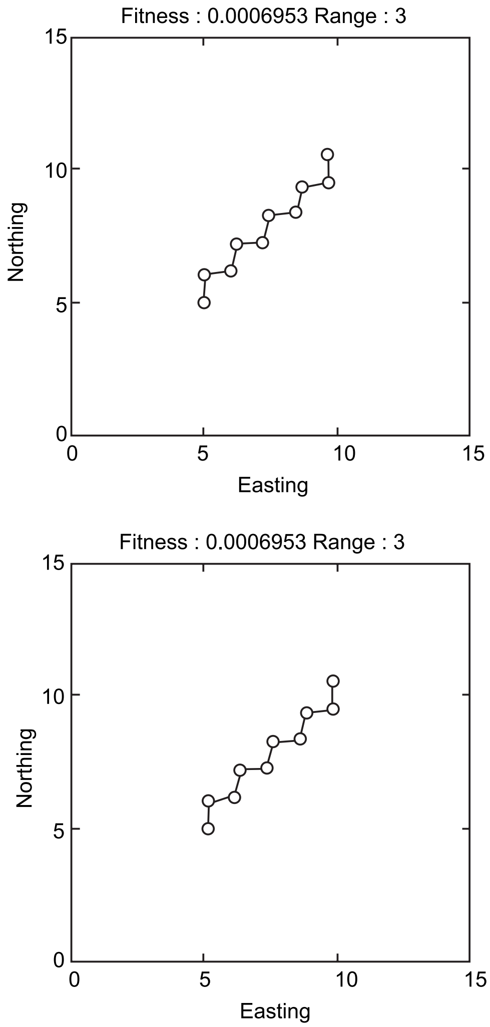

Fig. 4. Two transects derived with a Gaussian autocorrelation function having a range of three. The transect in the left graph is found by simulated annealing, and the transect in the right graph is found by Powell's algorithm. Both transects consist of 10 samples.

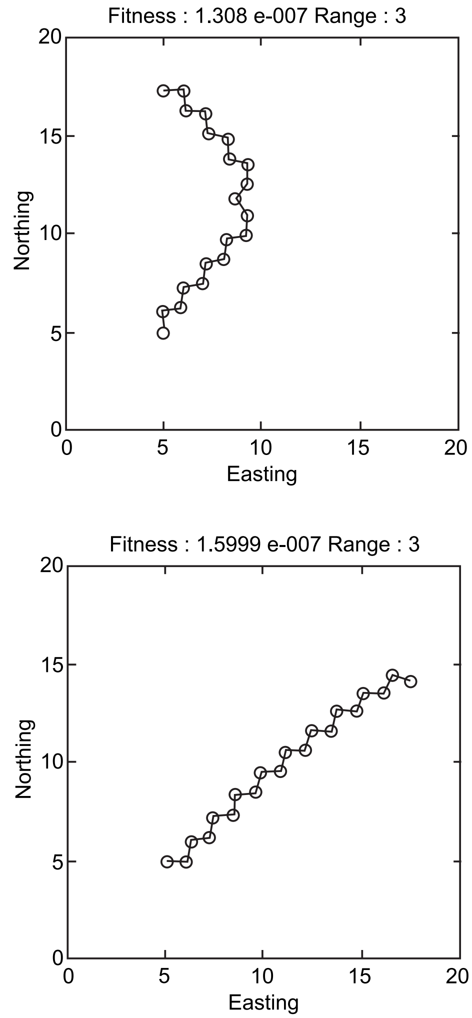

Fig. 5. Two transects derived with Gaussian autocorrelation with range of three. The transect in the left graph is found by simulated annealing, and the transect in the right graph is found by Powell's algorithm. Both transects consist of 20 samples.

(ii) Spherical autocorrelation model

Now we consider the spherical autocorrelation function, again with a range of three. For ten samples, simulated annealing and Powell's algorithm find essentially the same solution (Fig. 6). Again there is an obvious pattern, and again the interior angle is nearly constant, though instead of a zigzag, the transect bends left twice then right twice. Since collecting data along this transect design in the field would be tedious, it may be of practical interest to find the optimal transect with the restriction that interior angles are constant, and the transect bends left twice then right twice. The best transect obtained under this restriction has an interior angle of 125° and a fitness of 5.53e-2, only 0.18% less than the best case. A straight transect has a fitness of 4.73e-2, which is 15% less than optimal.

Finally, with a spherical autocorrelation function and a transect length of 20 samples, simulated annealing again has trouble finding the global pattern. Fig. 7 shows the transect found by Powell's algorithm that clearly has the same design as Fig. 6. The best design for the 20 sample transect restricted so that the interior angles are constant and satisfy the two left then two right pattern, has an interior angle of 126° and fitness 2.16e-3, which is only 0.5% less than optimal. The straight transect has fitness of 1.54e-3, which is 29% less than optimal.

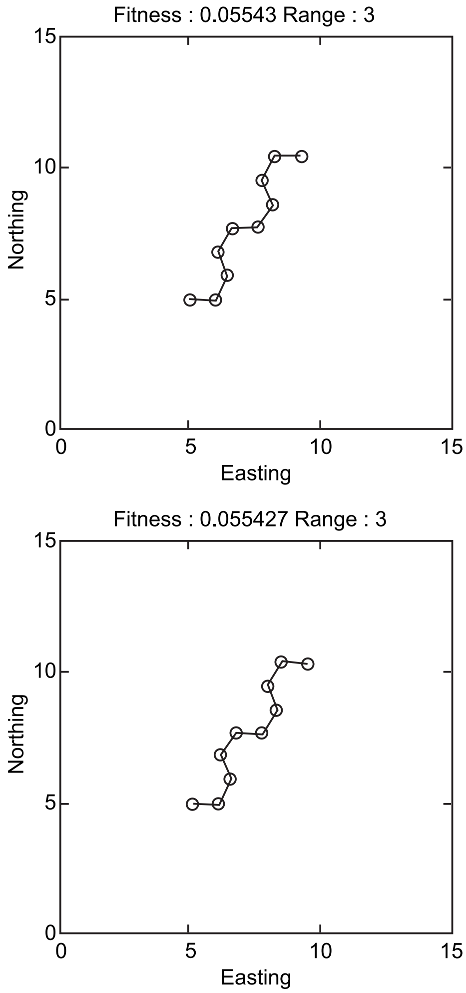

Fig. 6. Two transects derived with spherical autocorrelation with range of three. The transect in the left graph is found by simulated annealing, and the transect in the right graph is found by Powell's algorithm. Both transects consist of 10 samples.

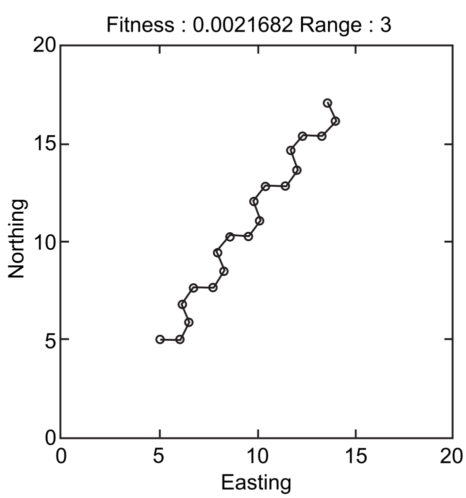

Fig. 7. A sampling transect with 20 points designed using Powell's algorithm. This transect is calculated for samples defined with a spherical autocorrelation with range of three.

5. CONCLUSION

Using both D-optimality and spatial sampling design for point samples, it is possible to define a fitness function for transects, one that minimizes the prediction error at unsampled locations within a spatial domain.

With this objective function to compare two transects, simulated annealing and Powell's algorithm can find nearly optimal transects.

The optimal transect design depends on the autocorrelation function of the region being sampled. For exponential autocorrelation, straight transects are optimal for three samples, and appear to be optimal for ten and twenty samples. However, for spherical autocorrelation, although straight transects are close to optimal, they are inferior to a transect design that turns left twice, then turns right twice by as much as 29%. For Gaussian autocorrelations, straight transects are far from optimal. The best design is a zigzag with an alternating interior angle close to 109° and can provide as much as a 99.97% improvement in the optimality criterion over straight transects. These results for spherical and Gaussian autocorrelations are surprising since straight transects are the least clustered, and intuition suggests that lack of clustering should produce optimal transects.

For spherical and Gaussian autocorrelations, the optimal transect design has roughly constant interior angles. Although transects with precisely constant interior angles are not optimal, they are close, and they have the advantage of being easier to implement in the field, especially if samples are collected on a moving vehicle that can turn easily. A zigzag pattern has already been field tested with favorable results in the literature, so further field applications of non-straight sampling transects should be contemplated.

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