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## Global Quantities in Space–Time

### 15.1 Introduction to Methods for Global Quantities in Space–Time

In monitoring studies with a temporal and a spatial dimension, a large variety of global target quantities can be defined. Commonly estimated target quantities are:

- the current mean, i.e., the spatial mean at the most recent sampling time;
- the change of the spatial mean from one sampling time to the other;
- the temporal trend of the spatial mean;
- the spatial mean of the temporal trend
- the spatio-temporal mean;
- the difference between the spatio-temporal means before and after an intervention.

In some cases one is interested in totals rather than means, and means can be interpreted as fractions when the target variable is a 0/1 indicator variable. Also, one may be more interested in a change of the spatial mean from one sampling time to the other than in the current level of the spatial mean. This is because the change tells more about environmental processes than the status of the environment. For instance, in a study on the greenhouse effect, one may want to estimate the change in carbon stocks in soil between now and 10 years hence. Or, to calculate the water balance of a watershed, one may want to estimate the difference in groundwater storage at the beginning and at the end of a year. The change in the spatial mean from one sampling time to the other is defined as:

$$\bar{d}_{2,1} = \frac{1}{|\mathcal{S}|} \int_{\mathbf{s} \in \mathcal{S}} z(\mathbf{s}, t_2) \, d\mathbf{s} - \frac{1}{|\mathcal{S}|} \int_{\mathbf{s} \in \mathcal{S}} z(\mathbf{s}, t_1) \, d\mathbf{s} = \frac{1}{|\mathcal{S}|} \int_{\mathbf{s} \in \mathcal{S}} \{z(\mathbf{s}, t_2) - z(\mathbf{s}, t_1)\} \, d\mathbf{s} . \quad (15.1)$$

(For model-based inference, the definition is of course the same, but the target variable  $z(\cdot)$  and the target quantity  $\bar{d}_{2,1}$  are random instead of deterministic; see (15.23).)

When sampling has been done at more than two sampling times, one may be interested in the mean change per time unit, i.e., the temporal trend. This trend may differ considerably between locations, and in that case one may want to estimate the Spatial Cumulative Distribution Function of the temporal trend, or one or more parameters of this SCDF. The spatial mean temporal trend is defined as the spatial mean of the trend parameter  $\beta(\mathbf{s})$  of a (linear) time-series model for the target variable at location  $\mathbf{s}$  at time  $t$ ,  $Z(\mathbf{s}, t)$

$$Z(\mathbf{s}, t) = \alpha(\mathbf{s}) + \beta(\mathbf{s}) \cdot (t - t_0) + \epsilon(\mathbf{s}, t) , \quad (15.2)$$

where  $t_0$  is the first time the target variable is measured.

It can be shown that this spatial mean temporal trend is equal to the temporal trend of the spatial mean, i.e., the trend parameter  $\beta$  of a time-series model for the spatial mean of  $Z$  at time  $t$ ,  $\bar{Z}(t)$  :

$$\bar{Z}(t) = \alpha + \beta \cdot (t - t_0) + \epsilon(t) . \quad (15.3)$$

A target quantity related to the spatial mean temporal trend is the temporal trend of the areal fraction where the target variable meets certain conditions, for instance the areal fraction where a quantitative target variable exceeds a given threshold. Clearly, a static type of pattern is inappropriate for estimating this quantity.

This target quantity should be distinguished from the areal fraction where the temporal trend meets a given condition. In this case the condition is in terms of the trend, whereas in the former it is in terms of the target variable. This areal fraction can be estimated by the indicator technique described before (Sect. 7.2.3). The Spatial Cumulative Distribution Function of the temporal trend is the most informative target quantity. This SCDF can simply be estimated by repeated application of the indicator technique.

The spatio-temporal mean is defined as

$$\bar{z}_{\mathcal{U}} = \frac{1}{|\mathcal{U}|} \int_{\mathbf{u} \in \mathcal{U}} z(\mathbf{u}) \, d\mathbf{u} , \quad (15.4)$$

and similarly the fraction in space and time that  $z(\mathbf{u})$  exceeds some critical threshold) is defined as

$$F_{\mathcal{U}}(z) \equiv \frac{1}{|\mathcal{U}|} \int_{\mathbf{u} \in \mathcal{U}} i(\mathbf{u}; z) \, d\mathbf{u} . \quad (15.5)$$

with

$$i(\mathbf{u}; z) = \begin{cases} 1 & \text{if } z(\mathbf{u}) \leq z \\ 0 & \text{if } z(\mathbf{u}) > z \end{cases} \quad (15.6)$$

If a change in the environmental conditions is foreseen, for instance due to the implementation of measures that have a positive or negative effect

on the quality of the environment, then one may want to assess this effect. One may choose one sampling time before and one after the intervention, and estimate the change in the spatial mean, but the difference found may strongly depend on the chosen times. Therefore this difference can be a very imprecise estimate of the difference between the spatio-temporal means before and after the intervention. Repeated measurements in time, both before and after the intervention, will increase precision. When the putatively ‘disturbed’ area has such an extent that it is unreasonable to assume that the effect is equal everywhere, it is also recommended to repeat the measurements in space. For example, assume that in an agricultural area measures are planned to reduce the leaching of nitrate to the ground and surface water. To assess the effect of these measures one may want to estimate the total amount of leached nitrate in the area where the measures are planned in the year before the intervention  $\mathcal{B}$ , and in the year after the intervention  $\mathcal{A}$ . The target quantity to be estimated is

$$\begin{aligned} d_{\mathcal{A},\mathcal{B}} &= \int_{t \in \mathcal{A}} \int_{s \in \mathcal{S}} z(\mathbf{s}, t) \, ds \, dt - \int_{t \in \mathcal{B}} \int_{s \in \mathcal{S}} z(\mathbf{s}, t) \, ds \, dt \\ &= \int_{s \in \mathcal{S}} \left\{ \int_{t \in \mathcal{A}} z(\mathbf{s}, t) \, dt - \int_{t \in \mathcal{B}} z(\mathbf{s}, t) \, dt \right\} ds . \end{aligned} \quad (15.7)$$

As for global quantities in space and global quantities in time, design-based methods are the most appropriate. Especially for regulatory monitoring, objectivity of the method and validity of the results are of great importance. For instance, if a regulation specifies a threshold value (Action Level) for the spatio-temporal mean, then a valid interval estimate of this quantity is important for statistical testing.

## 15.2 Design-Based Methods for Global Quantities in Space–Time

### 15.2.1 Introduction

The typology of sampling patterns for monitoring presented in Sect. 14.1 is equally relevant for design-based and model-based methods. In model-based methods, however, the patterns are deterministic and in design-based methods they are random, i.e., selected by probability sampling. A static-synchronous sampling design, for instance, generates random static-synchronous patterns. This section deals with sampling and estimation for spatio-temporal and current global quantities, change of global quantities and spatial mean temporal trends, by synchronous, static, static-synchronous and rotational designs.

With synchronous designs, at each sampling time one is free to choose a spatial sampling design from Sect. 7.2 that seems most appropriate given

the circumstances at that time. So one may adapt the sample size, possible stratification, clusters and/or primary units, and even the very type of design.

Synchronous Sampling can be considered as a special case of Two-Stage Random Sampling in space–time, using spatial sections of the universe at given times as primary units, and sampling locations as secondary units (Vos, 1964). Therefore, the methods of inference for Two-Stage Random Sampling in space, given in Sect. 7.2.5, can be applied. For instance, inference about the spatio-temporal mean proceeds by first estimating the spatial mean at each sampling time (using the method associated with the spatial design at each time), and then estimating the spatio-temporal mean from these means as ‘observations’ (using the method associated with the temporal design). Inference on totals and trend parameters is similar.

With static designs the order of space and time in the two stages is reversed: sampling locations are selected as primary units and sampling times as secondary units. Now the set of sampling locations remains fixed through time, as with static-synchronous designs, which brings similar operational advantages. The difference with static-synchronous designs is that sampling is not synchronized, so that correlation due to synchronized sampling is avoided. Another difference is that the temporal design may be adapted to local circumstances. Static designs are attractive when considerable spatial variation between time series is known to exist, and when the operational advantages of fixed locations are real.

A static-synchronous design can be considered as a combination of a spatial sampling design and a temporal sampling design, so that at each sampling time all locations are sampled (see Fig. 14.4). The sampling locations can be selected by the same designs as described in Sect. 7.2 on design-based sampling in space, while the sampling times can be selected by the methods discussed in Sect. 11.2 on design-based sampling in time. The inference for static-synchronous designs depends primarily on these two constituting partial designs.

Rotational Sampling or ‘sampling with partial replacement’ represents a compromise between static and synchronous designs. The rationale is to avoid on the one hand the unbalancedness of static designs that accumulate more data only in time. On the other hand, the relative inefficiency of synchronous designs for estimating temporal trends is partially avoided because repeated measurements are made at the same locations.

The principle of Rotational Sampling is to divide the locations of an initial spatial sample into different rotational groups, and to replace each time one group by a new set of locations (see Fig. 14.5). Many different strategies of Rotational Sampling have been developed, including improved estimation procedures. In some strategies a set of locations would be re-introduced into the sample after having been rotated out for some time. See Binder and Hidirolou (1988) for a review on Rotational Sampling.

The suitabilities, from a statistical point of view, of the four design types for estimating global quantities are summarized in Table 15.1.

**Table 15.1.** Suitability of the four main types of design for estimating spatio-temporal global quantities (StGQ), current global quantities (CuGQ), change of global quantities (ChGQ), and spatial mean temporal trends (SMTT). A question mark means that estimation of the standard error may be problematic.

Type of design	StGQ	CuGQ	ChGQ	SMTT
Synchronous	+	+	+	+
Static	+	–	–	++
Static-Synchronous	+?	+	++	+?
Rotational	+?	++	+	+?

### 15.2.2 Spatio-Temporal Global Quantities

Spatio-temporal global quantities most relevant in practice are spatio-temporal means, fractions and totals, and (parameters of) spatio-temporal Cumulative Frequency Distributions. An example of a spatio-temporal total is the total emission of a pollutant in a target area during a target period. The temporal mean of the spatial fraction of the area where the emission rate exceeds a given threshold is an example of a spatio-temporal fraction.

#### Synchronous Designs

Synchronous designs can be considered as two-stage designs, and therefore the formulas of Sect. 7.2.5 can be used to calculate the number of sampling locations and sampling times. The primary units are then spatial sections of the universe at given times, and sampling locations are secondary units. The (pooled) within-unit variance in this case is the (time-averaged) spatial variance of the target variable at a given time, and the between-unit variance is the variance of the spatial means over time. Note that (7.30 – 7.32) hold for Simple Random Sampling in space and Simple Random Sampling in time, an equal number of sampling locations at all sampling times, and a linear cost function  $C = c_0 + c_1 n_t + c_2 n_t n_s$ , where  $c_0$  is the fixed costs of installing the monitoring design, for instance costs of preparing the sampling frame,  $c_1$  is the variable costs per sampling time and  $c_2$  is the variable costs per sampling location, and  $n_t$  and  $n_s$ , are the number of sampling times and locations, respectively.

Usually, more efficient types of design than Simple Random Sampling will be chosen for space and time, for instance, systematic in time and stratified in space. In that case, the above formulas can still be used, either by adopting the resulting sample sizes  $n_t$  and  $n_s$ , as conservative (safe) estimates, or by dividing them by a prior estimate of the design-effects (accounting for the higher efficiency), e.g., 1.1 or 1.2. Of course, after one or more sampling rounds

the data then collected can be used as prior information for adapting parts of the design that are still to be carried out.

Estimating the spatio-temporal mean (total, fraction) proceeds by first estimating the spatial mean at each sampling time (using the method associated with the spatial design at that time), and then estimating the spatio-temporal mean and its standard error from these means as ‘observations’ (using the method associated with the temporal design). The spatio-temporal total is obtained by multiplying the mean with the size of spatio-temporal universe ( $|\mathcal{S}| \cdot |\mathcal{T}|$ ), and similarly for the standard error.

### Static Designs

Like synchronous designs, static designs can be considered as two-stage designs, but the role of space and time are interchanged. The primary units are now temporal sections at given locations, and sampling times are secondary units. The same formulas for the number of locations and times can be used. However, now the (pooled) within-unit variance is the (space-averaged) temporal variance at a given location, and the between-unit variance is the variance of the temporal means over space. The cost function is now  $C = c_0 + c_1 n_s + c_2 n_t n_s$ , where  $c_1$  is the variable costs per sampling location and  $c_2$  is the variable costs per sampling time. The remark about using more efficient designs than Simple Random Sampling, made for synchronous designs, applies to static designs as well. Just as with synchronous designs, after some time the sample data then collected can be used as prior information in adapting parts of the design still to be carried out.

Inference about the spatio-temporal mean (total, fraction) proceeds by first estimating the temporal mean at each sampling location (using the method associated with the temporal design at that location), and then estimating the spatio-temporal mean and its standard error from these means as ‘observations’ (using the method associated with the spatial design). The spatio-temporal total is obtained by multiplying the mean with the size of spatio-temporal universe ( $|\mathcal{S}| \cdot |\mathcal{T}|$ ), and similarly for the standard error.

### Static-Synchronous Designs

Due to the two-fold alignment of the sampling events, sample optimization for static-synchronous designs is more complicated than for synchronous and static designs. With synchronous and static designs there are two variance components to take into account: the variance between and the (pooled) variance within primary units, i.e., spatial and temporal sections, respectively. With static-synchronous designs it appears that there are three variance components. Building on the early work of Quenouille (1949), Koop (1990) worked out the sampling variance in estimating (surface) areas for different combinations of two designs of point sampling in the plane, one along the X-axis and one along the Y-axis, with or without alignment of the sampling points in

either direction. Taking time for the Y-axis and space for the X-axis (or vice versa), one of Koop’s designs types, ‘random sampling with alignment in both directions’, is analogous to static-synchronous sampling with Simple Random Sampling in both space and time. Translating Koop’s variance formula for this type of design to estimation of the spatio-temporal mean gives, cf. Koop (1990, eq. 3.3.5):

$$V(\hat{z}) = \frac{S^2(z)}{n} + \left(\frac{1}{n_t} - \frac{1}{n}\right) S_t^2(\bar{z}_s) + \left(\frac{1}{n_s} - \frac{1}{n}\right) S_s^2(\bar{z}_t), \quad (15.8)$$

where  $S^2(z)$  is the spatio-temporal variance of  $z$  over space and time,  $S_t^2(\bar{z}_s)$  is the variance over time of the spatial mean, and  $S_s^2(\bar{z}_t)$  is the variance over space of the temporal mean. This formula can be used for sample optimization as follows.

1. Make prior estimates of the three variance components.
2. Make estimates of the cost components in a linear cost function such as those mentioned under synchronous and static designs.
3. Choose relevant ranges for  $n_s$  and  $n_t$  and calculate for each combination of  $n_s$  and  $n_t$  the expected sampling variance and costs.
4. In case of quality maximization under a given budget constraint, select  $n_s$  and  $n_t$  for which the expected sampling variance is smallest and the expected costs are still within the budget.
5. In case of costs minimization under a given quality requirement, select  $n_s$  and  $n_t$  for which the expected costs is smallest and the expected sampling variance still meets the requirement.

Estimation can be done in two steps, the order of which may be reversed. First, for each sampling location the quantity over time is estimated from the data at that location, using the method associated with the temporal design. Then the spatio-temporal quantity and its standard error are estimated using these temporal values as ‘observations’, using the method associated with the spatial design. This standard error accounts automatically for errors due to sampling in space and sampling in time, but not for possible spatial correlations between the estimated temporal quantities due to synchronized sampling at the locations. This will generally lead to underestimation of the standard error. Due to the two-fold alignment of the sampling events, there is no unbiased estimator of the sampling variance available (Koop, 1990). One option is to substitute posterior estimates of the variance components in (15.8). Another possibility is to form, by random partitioning, a number of smaller static-synchronous subsamples. The variance between the means of these subsamples could be then used as an estimate of the variance for the original sample.

### 15.2.3 Current Global Quantities

#### Synchronous Designs

The choice of the sampling design and the inference are as for global quantities in space (see Sect. 7.2). The inference depends only on the current type of spatial design. There is no overlap between the spatial samples at different sampling times, and as a result, there is no simple way of exploiting the information in the previous samples to estimate the current quantity. This is a drawback of synchronous designs compared to rotational designs, which do create such overlap, see Sect. 15.2.1.

#### Static-Synchronous Designs

Inference on a current global quantity, such as the spatial mean, fraction, total or (a parameter of) the Spatial Cumulative Distribution Function at any given sampling time, can be done by applying the appropriate method from Sect. 7.2 on the data collected at that time. To estimate the current quantity, only measurements taken at the current sampling time need to be used. There is no additional information in the measurements from the previous sampling times, because the locations coincide.

#### Rotational Designs

In Rotational Sampling there is partial overlap between samples of successive sampling times, and consequently the sample of the previous sampling time can be used in estimating a current spatial mean, fraction or total. We present the procedure for the mean; fractions are estimated by applying the same procedure to indicator variables, and totals are estimated by multiplying the estimated mean and its standard error with the size of the spatial universe (surface area in case of 2D).

To start with, two sampling times are considered. The sample of the first sampling time is subsampled, and on the locations of this subsample the target variable is also measured at the second sampling time. This subsample with measurements at both sampling times is referred to as the matched sample; the unmatched sample consists of the locations with measurements at the first sampling time only. At the second sampling time, the target variable is also measured on a set of new locations. The spatial mean at the second sampling time  $\bar{z}_2$ , is estimated by the composite estimator (Cochran, 1977, p. 346)

$$\hat{z}_{2c} = \hat{w}_1 \hat{z}_{2gr}^{(m)} + \hat{w}_2 \hat{z}_{2\pi}^{(u)}, \quad (15.9)$$

where  $\hat{w}_1$  and  $\hat{w}_2$  are weights summing to 1,  $\hat{z}_{2\pi}^{(u)}$  is the  $\pi$ -estimator for the mean of  $z_2$  estimated from the unmatched sample, and  $\hat{z}_{2gr}^{(m)}$  is the Two-Phase



Random Sampling regression estimator for the mean of  $z_2$  estimated from the matched (remeasured) sample (see Sect. 7.2.12)

$$\hat{z}_{2\text{gr}}^{(m)} = \hat{z}_{2\pi}^{(m)} + b \left( \hat{z}_{1\pi} - \hat{z}_{1\pi}^{(m)} \right), \tag{15.10}$$

where  $\hat{z}_{2\pi}^{(m)}$  is the second sampling time mean estimated from the matched sample,  $b$  is the estimated slope coefficient,  $\hat{z}_{1\pi}$  is the first sampling time mean estimated from the entire first-phase sample (matched plus unmatched), and  $\hat{z}_{1\pi}^{(m)}$  is the first sampling time mean estimated from the matched sample. The estimated optimal weights  $\hat{w}_1$  and  $\hat{w}_2$  equal

$$\hat{w}_1 = 1 - \hat{w}_2 = \frac{\hat{V} \left( \hat{z}_{2\pi}^{(u)} \right)}{\hat{V} \left( \hat{z}_{2\text{gr}}^{(m)} \right) + \hat{V} \left( \hat{z}_{2\pi}^{(u)} \right)}, \tag{15.11}$$

where  $\hat{V} \left( \hat{z}_{2\text{gr}}^{(m)} \right)$  is the estimated variance of the regression estimator, and  $\hat{V} \left( \hat{z}_{2\pi}^{(u)} \right)$  is the estimated variance of the  $\pi$ -estimator for the mean of  $z_2$  for the unmatched sample. For Simple Random Sampling of  $n$  locations at both sampling times and  $m$  matched (remeasured) locations this variance is given by

$$\hat{V} \left( \hat{z}_{2\text{gr}}^{(m)} \right) = \frac{\widehat{S}^2(e)}{m} + \frac{\widehat{S}^2(z_2) - \widehat{S}^2(e)}{n}, \tag{15.12}$$

where  $\widehat{S}^2(e)$  is the estimated variance of the residuals  $e = z_2 - z_1 b$ , and

$$\hat{V} \left( \hat{z}_{2\pi}^{(u)} \right) = \frac{\widehat{S}^2(z_2)}{n - m}. \tag{15.13}$$

The variance of the composite estimator can be estimated by (Schreuder et al., 1987):

$$\hat{V} \left( \hat{z}_{2c} \right) = \frac{1 + 4 \hat{w}_1 \hat{w}_2 \left( \frac{1}{m-1} + \frac{1}{n-m-1} \right)}{\hat{w}_1 + \hat{w}_2}. \tag{15.14}$$

The variance depends on the proportion of matched sampling locations. The optimal matching proportion can be calculated with (Cochran, 1977)

$$\frac{m}{n} = \frac{\sqrt{1 - \rho^2}}{1 + \sqrt{1 - \rho^2}}, \tag{15.15}$$

where  $\rho$  is the correlation coefficient between  $z_1$  and  $z_2$ . For  $\rho = 0.9, 0.8$  and  $0.5$  the optimum matching proportion equals 0.30, 0.38 and 0.48 respectively. When  $\rho$  goes to 0,  $m/n$  approaches 0.5. Given these correlation coefficients the gain in precision, calculated as the ratio of the variance with no matching (Synchronous Sampling) and the variance with the optimum matching

proportion, equals 1.39, 1.25 and 1.07, respectively. When the costs of remeasuring a location are lower than the costs of measuring a new location, the optimum matching proportion increases. When choosing a matching proportion one must take care that the number of matched locations is large enough to obtain reliable estimates of the regression coefficient and the variance of the regression estimator, say  $m > 10$ .

With three or more sampling times, the current mean  $\bar{z}_0$  is estimated by substituting the composite estimator for the mean at the previous sampling time,  $\hat{z}'_{-1}$  (15.9), for the  $\pi$ -estimator for the previous mean,  $\hat{z}_{-1\pi}$ , in the regression estimator (15.10):

$$\hat{z}_{0\text{gr}}^{(m)} = \hat{z}_{0\pi}^{(m)} + b \left( \hat{z}_{-1\text{c}} - \hat{z}_{-1\pi}^{(m)} \right) , \tag{15.16}$$

and then weighting this regression estimator and the  $\pi$ -estimator for the current mean inversely proportional to the variance (15.11). Cochran (1977) shows that the optimal matching proportion increases rapidly with the sampling time. For the fifth sampling time the optimal matching proportion is close to 0.5 for a correlation coefficient  $\leq 0.95$ .

Once the matching proportion is chosen, one can calculate the sample size needed for a given precision (15.14). Prior estimates of the residual variance and the variance of the target variable at the current time are needed to calculate the weights.

### 15.2.4 Change of Global Quantities

#### Synchronous Designs

Change of the spatial mean (total, fraction) can be estimated as with static-synchronous designs (Eq. 15.19). Because the samples taken at different times are mutually independent, the estimated means  $\hat{z}(t_1)$  and  $\hat{z}(t_2)$  are uncorrelated. The sampling variance of  $\hat{d}_{2,1}$  equals

$$V \left( \hat{d}_{2,1} \right) = V \left( \hat{z}(t_2) \right) + V \left( \hat{z}(t_1) \right) , \tag{15.17}$$

which can be simply estimated by:

$$\hat{V} \left( \hat{d}_{2,1} \right) = \hat{V} \left( \hat{z}(t_2) \right) + \hat{V} \left( \hat{z}(t_1) \right) . \tag{15.18}$$

Note that, contrary to (15.20), there is no covariance-term, which makes synchronous designs in general less efficient than static-synchronous designs. In the case of classical testing, this procedure leads to the common two-sample *t*-test. Change of spatial fractions and totals can be estimated in the same way as change of spatial means.

If both sampling rounds are still to be designed, one has to decide on the sampling design type and the sample size at both sampling times. In general

there will be no reason for choosing different design types for the two sampling times. Also, in general prior estimates of the spatial variance components for the target variable will be equal for the two sampling times. In that case the optimal ratio of sizes of the first and second sample will be 0.5. The sample size per sampling time required to estimate the change with prescribed precision can then be calculated by the formulas of Sect. 7.2, substituting half the maximum allowed variance of the estimated change for the variance of the estimated mean of the target variable.

After the first sampling time, one has new information that can be used to redesign the sample of the second time. The estimated sampling variance of the mean at the first sampling time can be subtracted from the variance of the estimated change to obtain the variance of the mean at the second sampling time. Also, estimates of the spatial variance components at the first sampling time can be used as prior estimates to calculate the sample size needed to meet this updated constraint on the sampling variance of the estimated mean at the second sampling time.

### Static-Synchronous Designs

The change of the spatial mean or fraction from one sampling time to the other,  $\bar{d}_{2,1}$  (15.1), can be estimated straightforwardly by

$$\hat{\bar{d}}_{2,1} = \hat{z}(t_2) - \hat{z}(t_1) . \quad (15.19)$$

In static-synchronous samples, the locations of the first and the second sampling time coincide. This implies that in estimating the sampling variance of the change, a possible temporal correlation between the estimated means  $\hat{z}(t_1)$  and  $\hat{z}(t_2)$  must be taken into account. The true sampling variance equals

$$V \left( \hat{\bar{d}}_{2,1} \right) = V \left( \hat{z}(t_2) \right) + V \left( \hat{z}(t_1) \right) - 2C \left( \hat{z}(t_2), \hat{z}(t_1) \right) . \quad (15.20)$$

So, the stronger (more positive) the temporal correlation between the two estimated spatial means, the smaller the sampling variance of the change. In general this correlation will be largest when the sampling locations at the first and second sampling time coincide, as is the case with static designs and nondestructive sampling. With destructive sampling, the shifts should be kept as small as possible. Also, if a spatial trend is suspected, then the direction of the separation vector must be randomized to avoid bias (Papritz and Flühler, 1994). A simple way to estimate the variance (15.20) is first calculating the difference  $d_i = z_i(t_2) - z_i(t_1)$  at each sampling location  $i$ , and then applying the appropriate method of inference from Sect. 7.2 to those differences. (If change of a fraction is to be estimated,  $z$  is an indicator variable, and  $d$  can take the values -1, 0 or 1.) In the case of classical testing, this procedure leads to the common  $t$ -test for paired observations.

The change of a spatial total from one sampling time to the other can be estimated by multiplying the estimated change of the spatial mean with the

size of the target universe (area in case of 2D), and similarly for the standard error.

The required sample size can be calculated with the formulas from Sect. 7.2, substituting spatial variances of the differences for the spatial variances of the target variable. From the third sampling time onwards, these variance components can be estimated from the data of the previous sampling times.

## Rotational Designs

The change of the spatial mean from the previous to the latest sampling time can be estimated by:

$$\hat{d} = \hat{z}_{0c} - \hat{z}_{-1c}, \quad (15.21)$$

where  $\hat{z}_{0c}$  and  $\hat{z}_{-1c}$  are the composite estimators at the latest and the previous sampling time, respectively (see (15.9)). An alternative, more precise but more complicated estimator of the change is to combine two estimators of change, one built on the matched sample and one built on the unmatched sample, into a composite estimator with optimized weights (Schreuder et al., 1993, p. 180). Change fractions can be estimated by applying this method to indicator variables, and change of totals are obtained by multiplying estimated change of means with the size of the spatial universe.

### 15.2.5 Spatial Mean Temporal Trend

#### Synchronous Designs

With synchronous designs the spatial mean temporal trend (temporal trend of spatial mean) is estimated by first estimating the spatial means at time  $t$ ,  $\bar{z}(t)$ , and then estimating the model parameter  $\beta$  in (15.3) and the variance of  $\hat{\beta}$  by Weighted Least Squares fitting, with weights inversely proportional to the variances of spatial means. The variance accounts for uncertainty about  $\beta$  due to the residual term  $\epsilon(t)$ , and for uncertainty about the spatial means due to sampling errors.

#### Static Designs

Compared with synchronous designs, the inference proceeds in reversed order. First the temporal trend parameters are estimated for each sampling location separately, then these estimates are averaged to a spatial mean, using the method associated with the spatial design. To estimate the temporal trend of an areal fraction static designs are inappropriate.

### Static-Synchronous Designs

To estimate the spatial mean temporal trend, first the model parameter  $\beta(\mathbf{s})$  is estimated at all sampling locations, and then these estimates are used to estimate the spatial mean of the model parameter,  $\bar{\beta}$ . The variance of the estimated spatial mean temporal trend can be estimated straightforwardly by the estimators of Sect. 7.2. This variance accounts automatically for uncertainty about  $\bar{\beta}$  due to sampling error, and for uncertainty about the model parameters due to the residual term  $\epsilon(\mathbf{s}, t_i)$ , but not for spatial correlations (due to synchronized sampling) between these two error-components.

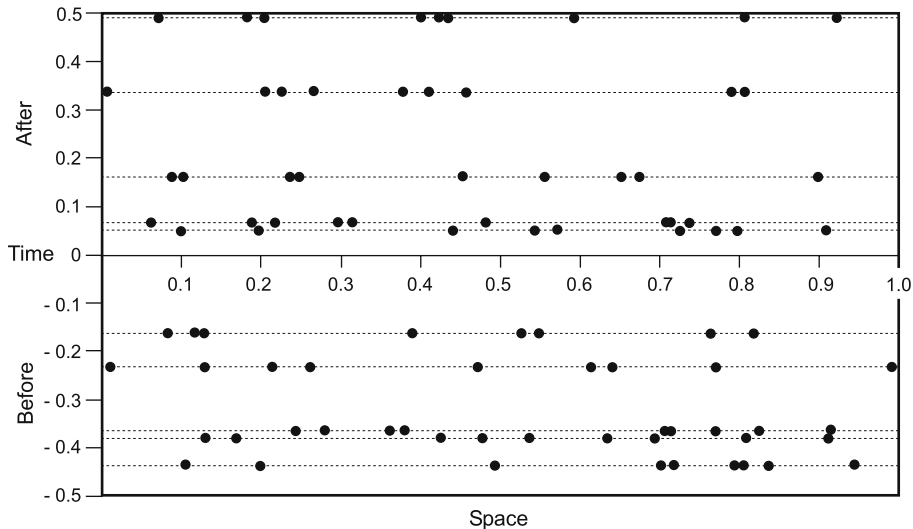
If systematic sampling in time, i.e., sampling at constant time-intervals is applied, then the sampling frequency to be optimized, see Fig. 15.4. For the required number of sampling locations the formulas from Sect. 7.2 can be used. A prior estimate of the spatial variance of the temporal trend at locations (within the target area, strata, primary units or clusters) is needed. The (averaged) estimation variance of the temporal trend at locations must be added to this spatial variance, see (13.20).

### Rotational Designs

Similarly to static designs, the spatial mean temporal trend can be estimated by first estimating the temporal trend  $\beta(\mathbf{s})$  at the sampling locations, and then estimating the spatial mean of the model parameter,  $\bar{\beta}$ . However, compared to static designs, considerable time elapses before all sampling locations have been observed repeatedly. For instance, in the 4-period rotational sample of Fig. 14.7 one must wait for the seventh sampling time until all locations have been sampled three times. The alternative is to estimate the spatial means (areal fractions, totals) first, and then the trend of the spatial mean (areal fraction, total). With this procedure an estimate of the spatial mean temporal trend (trend of areal fraction or total) can already be obtained after the third sampling time. Successive estimates of the current mean (areal fraction, total) estimated by the composite estimator evidently are correlated because measurements of the previous time are used to estimate the current global quantity. Therefore, it is recommendable not to use the measurements of the previous sampling time to estimate the current status of the global quantity, i.e., use the  $\pi$ -estimator. Due to overlap of successive samples the estimated global quantities at successive times still can be correlated, but this correlation will be much less serious a problem.

#### 15.2.6 Estimating Effects with BACI designs

Figure 15.1 shows a monitoring design composed of two independent synchronous designs, one before and one after an intervention. The difference in spatio-temporal means before and after the intervention  $\bar{d}_{\mathcal{A},\mathcal{B}}$  can be estimated by estimating the two space–time means with the design-based estimators mentioned in the previous sections. The sampling variance of the



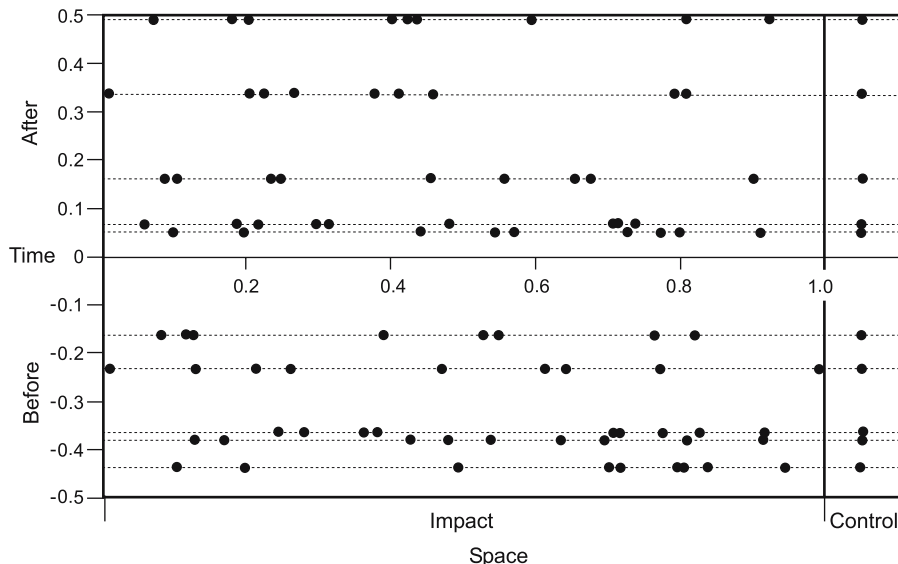
**Fig. 15.1.** Notional example of a synchronous sample before and after an intervention

estimated difference can be estimated simply by the sum of the variances of the two estimated space–time means. As stated above, Synchronous Sampling can be considered as a special case of Two-Stage Random Sampling in space–time, using spatial sections of the universe at given times as primary units, and sampling locations as secondary units. Assuming that the variance within and between primary units before and after the intervention are equal, the formulas of Sect. 7.2.5 can be used to determine the optimal number of sampling times and sampling locations before and after the intervention.

Suppose that the target variable shows a linear trend in time due to processes working in an area that is much larger than the area where the measures are planned. Then one will find a difference between the space–time means before and after the intervention which has nothing to do with the intervention. To overcome this problem, one can measure the target variable at one or more reference (control) sites, i.e., locations more or less similar to the impact sites but outside the area with the planned measures. The target quantity is now defined as

$$\bar{\delta}_{\mathcal{A},\mathcal{B}} = \frac{1}{|\mathcal{S} \times \mathcal{A}|} \int_{t \in \mathcal{A}} \int_{\mathbf{s} \in \mathcal{S}} \delta(\mathbf{s},t) \, d\mathbf{s} \, dt - \frac{1}{|\mathcal{S} \times \mathcal{B}|} \int_{t \in \mathcal{B}} \int_{\mathbf{s} \in \mathcal{S}} \delta(\mathbf{s},t) \, d\mathbf{s} \, dt, \quad (15.22)$$

where  $\delta(\mathbf{s},t) = z(\mathbf{s},t) - \bar{z}_C(t)$ , with  $\bar{z}_C(t)$  being equal to the mean of  $z$  at the control sites at time  $t$ . The control sites can be restricted to one or more purposely selected locations outside the impact area. In that case the mean



**Fig. 15.2.** Notional example of a synchronous sample before and after an intervention, with simultaneous sampling of a control site (a BACI design)

$\bar{z}_C(t)$  is known without error. It is convenient to measure the impact and control sites simultaneously, because then estimating or testing the quantity (15.22) is analogous to that of (15.7). Figure 15.2 shows an example of a synchronous sampling pattern in the impact area, and one purposely selected control site. One may also select the control sites randomly from a bounded control area. In that case one can account for uncertainty in the spatial means  $\bar{z}_C(t)$ . Random sampling in the control area can be synchronized with the sampling in the impact-area. Besides possible operational advantages, this also leads to higher precision when the estimated spatial means at time  $t$  in the control area and in the impact area are positively correlated.

Note that if the estimator of (15.22) differs significantly from zero, then still one cannot conclude that this is caused by the intervention. The treatment levels (impact versus control) are not randomly allocated to the sites as in experimental design, and as a consequence one must be careful to interpret the estimated target quantity as the effect of the treatment (intervention).

Underwood (1994) considers the case of a single impact location that is not randomly selected, but predetermined by the source of the disturbance. To introduce randomness, Underwood proposes selecting the control sites randomly. However, Stewart-Oaten and Bence (2001) pointed out that in this case the estimation of the effect of the intervention at the impact site must be based necessarily on a geostatistical model. The measurements after the intervention at the control sites are used to predict the target variable at the

impact site. These predictions are used as possible values if no intervention would have occurred at the impact site. Note that this strategy can be used if before-measurements at the impact site are unavailable. If one does have measurements before the intervention at the impact site, the alternative is to describe the temporal variation at the impact site with a time-series model and use the synchronized measurements at the control sites as covariates.

## 15.3 Model-Based Methods for Global Quantities in Space–Time

### 15.3.1 Introduction

This section describes sampling in space and time for prediction of global quantities (e.g., spatio-temporal means or spatio-temporal cumulative distribution functions), where a model is used for statistical inference. If prior to sampling a reasonable model can be postulated, then this model can also be used to guide the sampling, i.e., to optimize the pattern of sampling events. Although design-based methods generally are well suited for global quantities, there may be reasons to prefer model-based methods. An example is where one has prior monitoring data from purposive samples in space–time that need to be extended with additional data. Another example is where the global target quantity is related to a detection problem (Sect. 2.2.6).

The first two sections deal with optimization of the sampling locations at two given sampling times. The target quantities considered are the change of the mean between two successive sampling times (Sect. 15.3.2), and the current mean, i.e., the mean at the latest sampling time (Sect. 15.3.3). Both target quantities are predicted by co-kriging. The optimal patterns for the two target quantities will generally be different.

The following two sections deal with the situation where more than two sampling times are to be considered. In that case co-kriging becomes cumbersome, because a co-regionalization model for more than two co-variables is hard to obtain. The alternative is then to postulate a relatively simple geo-statistical model for the variation in space–time. In Sect. 15.3.4 such a model is used to optimize the spacing and interval length of a space–time grid for predicting the spatio-temporal mean. Sect. 15.3.5 elaborates on optimization of the sample pattern for the current mean with this model.

Finally, Sect. 15.3.6 deals with sampling for predicting the spatial mean temporal trend. A simple model is postulated for the residuals of the temporal trend, which is used to optimize the spacing and interval length of a space–time grid.

In some situations one may have knowledge about the dynamics of the target variable, described by a process model. If this model can be used to predict the spatio-temporal evolution of the target variable, then the predicted spatio-temporal images can be used to direct sampling effort in space and



time. For instance, a groundwater flow and transport model could be used to describe the development of a contaminant plume by a series of concentration maps that are subsequently used to determine where and when concentrations can best be measured. Examples of the use of a process model for sampling in space–time can be found in Meyer and Brill (1988), Cieniawski et al. (1995) and Bierkens (2002). When a realistic process model is available, its use in sampling is recommendable because this is likely to increase the efficiency. The reason that we do not treat this type of model-based sampling is that it is highly application-specific and therefore beyond the scope of this book.

### 15.3.2 Co-Kriging the Change of Spatial Mean

This section deals with sampling for predicting the change of the spatial mean between two sampling times. What should be optimized are the sampling locations at these two times. The target quantity is predicted by block co-kriging. In co-kriging the change of the mean, there is not a primary variable and a secondary variable, but the cross-correlation between the random variable at sampling time 1,  $Z(\mathbf{s}, t_1)$ , and at sampling time 2,  $Z(\mathbf{s}, t_2)$  is used to improve the predicted change of the spatial means.

Hereafter, we denote  $Z_1(\mathbf{s}) = Z(\mathbf{s}, t_1)$  and  $Z_2(\mathbf{s}) = Z(\mathbf{s}, t_2)$ , and assume that  $Z_1(\mathbf{s})$  and  $Z_2(\mathbf{s})$  are two second-order stationary functions with unknown means  $\mu_1$  and  $\mu_2$  and with the following covariance functions:  $C_{11}(\mathbf{h}) = \text{Cov}[Z_1(\mathbf{s}), Z_1(\mathbf{s} + \mathbf{h})]$ ,  $C_{22}(\mathbf{h}) = \text{Cov}[Z_2(\mathbf{s}), Z_2(\mathbf{s} + \mathbf{h})]$  and cross-covariance function  $C_{12}(\mathbf{h}) = \text{Cov}[Z_1(\mathbf{s}), Z_2(\mathbf{s} + \mathbf{h})]$ .

Here we use covariances rather than semivariances, because the estimation of the cross-variogram requires that data at two sampling times are observed at the same location<sup>1</sup> (see Goovaerts, 1997).

The change of the spatial mean

$$\bar{D}_{2,1} = \frac{1}{|\mathcal{S}|} \int_{\mathbf{s} \in \mathcal{S}} Z_2(\mathbf{s}) \, d\mathbf{s} - \frac{1}{|\mathcal{S}|} \int_{\mathbf{s} \in \mathcal{S}} Z_1(\mathbf{s}) \, d\mathbf{s}, \quad (15.23)$$

is predicted by (Papritz and Flühler, 1994)

$$\tilde{\bar{D}}_{2,1} = \sum_{i=1}^{n_2} \lambda_{2i} Z_2(\mathbf{s}_{2i}) - \sum_{i=1}^{n_1} \lambda_{1i} Z_1(\mathbf{s}_{1i}), \quad (15.24)$$

where  $n_1$  and  $n_2$  are the number of sampling locations at  $t_1$  and  $t_2$ , respectively. The co-kriging weights  $\lambda_{1i}$  and  $\lambda_{2i}$  are obtained by solving the following sets of linear equations:

<sup>1</sup> An alternative formulation in terms of so-called pseudo cross-variograms is possible, which is also suitable for intrinsic Stochastic Functions. This however yields much more complicated expressions (see Papritz and Flühler, 1994).

$$\begin{aligned}
 & \sum_{j=1}^{n_1} \lambda_{1j} C_{11}(\mathbf{s}_{1j} - \mathbf{s}_{1i}) - \sum_{j=1}^{n_2} \lambda_{2j} C_{21}(\mathbf{s}_{2j} - \mathbf{s}_{1i}) - \nu_1 \\
 & = C_{11}(\mathcal{S}, \mathbf{s}_{1i}) - C_{21}(\mathcal{S}, \mathbf{s}_{1i}) \quad i = 1, \dots, n_1 \\
 & \sum_{j=1}^{n_2} \lambda_{2j} C_{22}(\mathbf{s}_{2i} - \mathbf{s}_{2j}) - \sum_{j=1}^{n_1} \lambda_{1j} C_{21}(\mathbf{s}_{2i} - \mathbf{s}_{1j}) - \nu_2 \\
 & = C_{22}(\mathbf{s}_{2i}, \mathcal{S}) - C_{21}(\mathbf{s}_{2i}, \mathcal{S}) \quad i = 1, \dots, n_2 \\
 & \sum_{i=1}^{n_1} \lambda_{1i} = 1 \quad \sum_{i=1}^{n_2} \lambda_{2i} = 1,
 \end{aligned} \tag{15.25}$$

where  $\nu_1$  and  $\nu_2$  are Lagrange multipliers, and where two unbiasedness constraints are included to assure that the predictor (15.24) is unbiased.  $C_{11}(\mathcal{S}, \mathbf{s}_{1i})$ ,  $C_{21}(\mathcal{S}, \mathbf{s}_{1i})$ ,  $C_{21}(\mathbf{s}_{2i}, \mathcal{S})$  and  $C_{22}(\mathbf{s}_{2i}, \mathcal{S})$  are point-to-block averaged covariances. With  $C_{11}(\mathcal{S}, \mathcal{S})$ ,  $C_{21}(\mathcal{S}, \mathcal{S})$  and  $C_{22}(\mathcal{S}, \mathcal{S})$ , the within-block ( $\mathcal{S}$ -averaged) (cross-)covariances, the variance of the prediction error (block co-kriging variance) can be calculated as

$$\begin{aligned}
 V(\widetilde{D}_{2,1} - \overline{D}_{2,1}) & = C_{11}(\mathcal{S}, \mathcal{S}) + C_{22}(\mathcal{S}, \mathcal{S}) - 2C_{21}(\mathcal{S}, \mathcal{S}) + \nu_1 + \nu_2 \\
 & - \sum_{i=1}^{n_1} \lambda_{1i} [C_{11}(\mathcal{S}, \mathbf{s}_{1i}) - C_{21}(\mathcal{S}, \mathbf{s}_{1i})] - \sum_{i=1}^{n_2} \lambda_{2i} [C_{22}(\mathbf{s}_{2i}, \mathcal{S}) - C_{21}(\mathbf{s}_{2i}, \mathcal{S})].
 \end{aligned} \tag{15.26}$$

As can be seen from (15.26), the prediction-error variance depends only on the sampling locations at the sampling times  $t_2$  and  $t_1$  and can thus be used for optimization of the sampling locations. Papritz and Webster (1995) have shown that if the observations at the two times are positively correlated, then the prediction-error variance is minimal when the sampling locations at the two times coincide. When sampling is destructive (e.g., soil sampling), it is impossible to exactly sample the same location. In that case it is advisable to sample at sampling time  $t_2$  as closely as possible to the sampling locations at sampling time  $t_1$ .

Some additional remarks about co-kriging of differences are in order. First, if the sampling locations at the two sampling times do not coincide, then co-kriging always yields more accurate predictions than first ordinary kriging separately at both sampling times and then subtracting the two predicted means. If the observations at the two sampling times coincide and the cross-covariance structure is intrinsic, i.e.,  $C_{11}(\mathbf{h}) = \alpha C_{22}(\mathbf{h}) = \beta C_{12}(\mathbf{h})$ , where  $\alpha$  and  $\beta$  are positive real valued constants for all lags  $\mathbf{h}$ , then co-kriging yields the same results as kriging for each sampling time first and then obtaining differences. The system is called ‘autokrigeable’. If the system is autokrigeable, the kriging weights will also be the same for each sampling time. In this case,  $\overline{D}_{2,1}$  can simply be estimated by direct ordinary block-kriging of differences:

$$\widetilde{D}_{2,1} = \sum_{i=1}^{n_s} \lambda_i [Z_2(\mathbf{s}_i) - Z_1(\mathbf{s}_i)] = \sum_{i=1}^{n_s} \lambda_i D_{2,1}(\mathbf{s}_i), \tag{15.27}$$

with  $\lambda_i$  obtained from solving the ordinary block-kriging equations (see Appendix B)

$$\begin{aligned} \sum_{j=1}^{n_s} \lambda_j \gamma_D(\mathbf{h}_{ij}) + \nu &= \gamma_D(\mathbf{s}_i, \mathcal{S}) & i = 1, \dots, n_s \\ \sum_{i=1}^{n_s} \lambda_i &= 1, \end{aligned} \quad (15.28)$$

with  $\gamma_D(\mathbf{h}_{ij})$  the variogram of  $D_{2,1}$ , which should be estimated directly from the differences. The block-kriging variance of the predicted mean difference is given by:

$$V\left(\tilde{D}_{2,1} - \bar{D}_{2,1}\right) = \sum_{i=1}^{n_s} \lambda_i \gamma_D(\mathbf{s}_i, \mathcal{S}) + \nu - \gamma_D(\mathcal{S}, \mathcal{S}). \quad (15.29)$$

In conclusion, model-based sampling for predicting the change of the mean can be treated as a special case of model-based sampling in space because it is optimal to sample the same locations at the two times. The pattern with minimum block co-kriging variance (15.26) can be searched for by simulated annealing, see Sect. 7.3.3 for further details. Optimization becomes even more simple when an intrinsic covariance model is postulated. In that case block co-kriging is equivalent to block-kriging the differences, and the pattern can be optimized by minimization of the block-kriging variance of the predicted mean difference (15.29). A simple alternative for situations where one is not able to postulate a model for the variation in space–time, is to design a spatial coverage sample (Sect. 8.3.3) or a regular grid (Sect. 7.3.2).

### 15.3.3 Co-Kriging Current Means

In co-kriging the current mean, the measurement of the target variable at the previous sampling time is used as a secondary variable, i.e., a co-variable. The current mean is predicted by the ordinary block co-kriging predictor:

$$\tilde{Z}_2 = \sum_{i=1}^{n_2} \lambda_{2i} Z_2(\mathbf{s}_{2i}) + \sum_{i=1}^{n_1} \lambda_{1i} Z_1(\mathbf{s}_{1i}), \quad (15.30)$$

The co-kriging weights  $\lambda_{1i}$  and  $\lambda_{2i}$  are obtained by solving the following sets of linear equations:

$$\begin{aligned} \sum_{j=1}^{n_2} \lambda_{2j} C_{22}(\mathbf{s}_{2i} - \mathbf{s}_{2j}) + \sum_{j=1}^{n_1} \lambda_{1j} C_{21}(\mathbf{s}_{2i} - \mathbf{s}_{1j}) + \nu_1 \\ &= C_{22}(\mathbf{s}_{2i}, \mathcal{S}) & i = 1, \dots, n_2 \\ \sum_{j=1}^{n_2} \lambda_{2j} C_{12}(\mathbf{s}_{1i} - \mathbf{s}_{2j}) + \sum_{j=1}^{n_1} \lambda_{1j} C_{11}(\mathbf{s}_{1i} - \mathbf{s}_{1j}) + \nu_2 \\ &= C_{12}(\mathbf{s}_{1i}, \mathcal{S}) & i = 1, \dots, n_1 \\ \sum_{j=1}^{n_2} \lambda_{2j} &= 1 & \sum_{j=1}^{n_1} \lambda_{1j} &= 0, \end{aligned} \quad (15.31)$$

Finally, the block co-kriging variance of the predicted current mean equals

$$\begin{aligned}
V\left(\widetilde{Z}_2\right) &= C_{22}(\mathcal{S}, \mathcal{S}) - \nu_1 \\
&\quad - \sum_{i=1}^{n_2} \lambda_{2i} C_{22}(\mathbf{s}_{2i}, \mathcal{S}) - \sum_{i=1}^{n_1} \lambda_{1i} C_{12}(\mathbf{s}_{1i}, \mathcal{S}).
\end{aligned}
\tag{15.32}$$

The optimal sampling pattern for the current mean may differ from the change of the mean. Whereas for the change of mean it is optimal to sample the same locations at the two times, for the current mean this will be optimal only when the spatial autocorrelation strongly dominates the temporal autocorrelation.

In the reverse case, it is optimal to sample at time  $t_2$  at locations farthest from those at time  $t_1$ . This is because at these intermediate locations one has the least information on the current values, whereas at or near to a location sampled at  $t_1$  a more precise estimate of the current value could be obtained with the observation at time  $t_1$ . In this case a simple solution is two interpenetrating grids, one for each sampling time. An alternative for irregularly shaped areas is to optimize the locations at time  $t_2$  with k-means using the locations of time  $t_1$  as prior locations, leading to a spatial infill sample (Sect. 8.3.3).

If neither the temporal nor the spatial autocorrelation is dominant, then the pattern of the locations might be optimized with simulated annealing, using the locations at the previous sampling time as prior data. The quality measure to be minimized is the block co-kriging variance of the predicted current mean.

### 15.3.4 Space–Time Kriging the Spatio-Temporal Mean

This section deals with the design of a space–time sample for the whole monitoring period, to predict the spatio-temporal mean. The sampling pattern will be optimized for the space–time block-kriging predictor.

Space–time kriging is a simple extension to spatial kriging, treating time as an extra dimension (e.g., Heuvelink et al., 1997). The spatio-temporal variation is modelled with a Stochastic Function  $Z(\mathbf{s}, t)$ ,  $\mathbf{s} \in \mathcal{S}$  and  $t \in \mathcal{T}$ , which is assumed to be second-order stationary in both space and time. We model the space–time semivariance between  $Z(\mathbf{s}_i, t_i)$  and  $Z(\mathbf{s}_j, t_j)$  with the following variogram model, assuming isotropy in space and space–time geometric anisotropy (see Heuvelink et al., 1997):

$$\gamma(\mathbf{u}_i, \mathbf{u}_j) = \gamma(\mathbf{s}_i - \mathbf{s}_j, t_i - t_j) = \gamma(\mathbf{h}_{ij}, \tau_{ij}) = \gamma\left(\sqrt{\frac{|\mathbf{h}_{ij}|^2}{a_s^2} + \frac{\tau_{ij}^2}{a_t^2}}\right), \tag{15.33}$$

with  $|\mathbf{h}_{ij}| = |\mathbf{s}_i - \mathbf{s}_j|$  and  $\tau_{ij} = |t_i - t_j|$  the Euclidian distances in space and time, respectively, and  $a_s$  and  $a_t$  the variogram range parameters in space and time, respectively. The target quantity is the spatio-temporal mean  $\overline{Z}_U$  of  $Z(\mathbf{s}, t)$  over  $\mathcal{U}$  (15.4).

If the mean value  $\mu = E[Z(\mathbf{u})]$  is not known,  $\overline{Z}_U$  can be predicted with ordinary block-kriging:

$$\tilde{Z}_{\mathcal{U}} = \sum_{i=1}^n \lambda_i Z(\mathbf{u}_i), \quad (15.34)$$

where the weights  $\lambda_i$  are obtained by solving the following set of equations

$$\sum_{j=1}^n \lambda_j \gamma(\mathbf{u}_i, \mathbf{u}_j) + \nu = \gamma(\mathbf{u}_i, \mathcal{U}) \quad i = 1, \dots, n$$

$$\sum_{i=1}^n \lambda_i = 1 \quad (15.35)$$

and the variance of the prediction error is given by

$$V[\tilde{Z}_{\mathcal{U}} - \bar{Z}_{\mathcal{U}}] = \sigma_{\text{obk}}^2 = \sum_{i=1}^n \lambda_i \gamma(\mathbf{u}_i, \mathcal{U}) + \nu - \gamma(\mathcal{U}, \mathcal{U}), \quad (15.36)$$

with

$$\gamma(\mathbf{u}_i, \mathcal{U}) = \frac{1}{|\mathcal{U}|} \int_{\mathbf{u} \in \mathcal{U}} \gamma(\mathbf{u}_i, \mathbf{u}) \, d\mathbf{u} \quad (15.37)$$

$$\gamma(\mathcal{U}, \mathcal{U}) = \frac{1}{|\mathcal{U}|^2} \int_{\mathbf{u}_2 \in \mathcal{U}} \int_{\mathbf{u}_1 \in \mathcal{U}} \gamma(\mathbf{u}_1, \mathbf{u}_2) \, d\mathbf{u}_1 \, d\mathbf{u}_2. \quad (15.38)$$

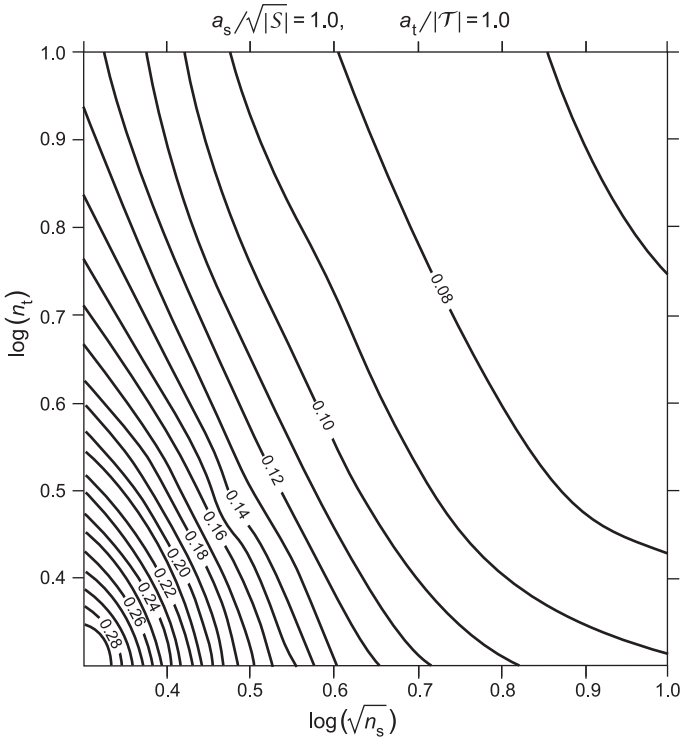
In practice, the integrals (15.37) and (15.38) are approximated by discretizing  $\mathcal{U}$  with a grid and averaging semivariances between locations on the grid (see Appendix B). The prediction-error variance (15.36) can be used as a quality measure to be minimized through sampling. It can be seen that this depends only on the projected  $n$  sampling locations. Thus, it can be used for sample optimization when new sampling locations are projected.

A simple and practical type of sampling pattern for space–time kriging the spatio-temporal mean is a space–time grid. The trade-off between the sampling effort in space and in time, and the effect of grid spacing and the interval length on the prediction-error variance will be evaluated for a square grid pattern in space, in a block-shaped universe  $\mathcal{S} \times \mathcal{T}$ .

From analysis of the prediction-error variance (15.36) it follows that for grid sampling the ratio  $\sigma_{\text{obk}}^2/\sigma^2$  with  $\sigma^2 = V[Z(\mathbf{s}, t)]$  can be represented by the following function  $r(\cdot)$ :

$$\frac{\sigma_{\text{obk}}^2}{\sigma^2} = r\left(n_s, n_t, \frac{a_s}{\sqrt{|\mathcal{S}|}}, \frac{a_t}{|\mathcal{T}|}\right), \quad (15.39)$$

where  $n_s$  and  $n_t$  are the number of sampling locations and sampling times, respectively. Figure 15.3 shows isolines of the ratio  $\sigma_{\text{obk}}^2/\sigma^2$  as a function of  $n_s$  and  $n_t$  for  $a_s/\sqrt{|\mathcal{S}|} = 1$  and  $a_t/|\mathcal{T}| = 1$ , using a spherical model (with zero nugget) for the variogram (see Appendix B). Appendix D shows similar figures for other combinations of  $a_s^2/\sqrt{|\mathcal{S}|}$  and  $a_t/|\mathcal{T}|$ . These figures can be used to determine the required grid spacing and interval length for grid sampling in



**Fig. 15.3.** Sampling on a centred space–time grid (square grid pattern in space) for predicting the spatio-temporal mean by space–time kriging. The figure shows the variance ratio  $\sigma_{\text{obk}}^2/\sigma^2$  for  $a_s/\sqrt{|\mathcal{S}|} = 1$  and  $a_t/|\mathcal{T}| = 1$  as a function of the number of sampling locations  $n_s$  and sampling times  $n_t$ . Figures for other combinations of  $a_s/\sqrt{|\mathcal{S}|}$  and  $a_t/|\mathcal{T}|$  are given in Appendix D.

space and time, given values of area  $|\mathcal{S}|$ , length of monitoring period  $|\mathcal{T}|$  and the statistical parameters  $\sigma^2$ ,  $a_s$  and  $a_t$ .

Suppose that the aim is to predict the spatio-temporal mean for a block-shaped universe, square in space, and that a variance reduction of 90 per cent is required, i.e.,  $\sigma_{\text{obk}}^2/\sigma^2 = 0.1$ . Further, suppose that  $a_s/\sqrt{|\mathcal{S}|} = 1$  and  $a_t/|\mathcal{T}| = 1$ , so that we can use Fig. 15.3. One possible combination of sample sizes in space and time is  $\log(\sqrt{n_s}) = 0.47$  and  $\log(n_t) = 0.82$ . Rounding fractions upwards to integers, this leads to 9 sampling locations and 7 sampling times. Alternatively, one could choose the combination  $\log(\sqrt{n_s}) = 0.70$  and  $\log(n_t) = 0.40$ , leading to 25 sampling locations and 3 sampling times. The number of sampling events is 63 for the first combination and 75 for the second. To determine which combination is preferable, a costs model can be used. If the total costs of sampling ( $c$ ) is dominated by the costs per event ( $c_o$ ), for instance due to lengthy observation times or an expensive method of

determination, then the total sample size is leading. This implies that taking a number of observations in space at a single time costs the same as taking the same number of observations at a single location at multiple times, i.e.,  $c = n_s n_t c_o$ . Given this costs model, the first combination is least expensive and therefore preferable.

Repeated sampling is often more expensive than taking the same number of observations in one sampling round. A linear costs model accounting for this effect is  $c = n_s n_t c_o + n_t c_t$ , where  $c_t$  is the fixed costs per sampling round. Given a required variance reduction, the optimal combination can be determined by evaluating this cost function for all combinations on the corresponding isoline in Fig. 15.3, and selecting the least expensive combination.

Alternatively, for quality optimization the aim is to find the sample size combination that results in the smallest prediction error variance for a given budget  $B$ , i.e.,  $n_s n_t c_o + n_t c_t \leq B$ . In this case the optimal combination can be found by plotting the line  $n_s n_t c_o + n_t c_t = B$  in Fig. 15.3. The point on this line for which the variance ratio is minimal is the optimal combination.

Figures D.1 to D.4 in Appendix D show that if  $a_s/\sqrt{|\mathcal{S}|}$  and  $a_t/|\mathcal{T}|$  are similar in magnitude, then the lines run roughly diagonal with a slope of approximately -2. Note that if we would have plotted  $\log(n_s)$  instead of  $\log(\sqrt{n_s})$  the slope would have been -1, indicating that the effect on the prediction error variance of adding one sampling location with  $n_t$  observations is equal to the effect of adding one sampling time at which  $n_s = n_t$  locations are observed. In case  $a_s/\sqrt{|\mathcal{S}|} \ll a_t/|\mathcal{T}|$ , the lines run roughly vertical (bottom diagrams in Fig. D.1), showing that much more can be gained by adding sampling locations, while for  $a_s/\sqrt{|\mathcal{S}|} \gg a_t/|\mathcal{T}|$  (upper left diagram in Fig. D.4) adding sampling times is much more efficient.

Although Figs. D.1 to D.4 are based on a square area, these figures can also be used to obtain rough estimates for irregularly shaped areas. Note that for such areas the number of sampling locations is not restricted to squares of integers (4, 9, 16, 25 etc.), but can be any integer. For irregularly shaped areas a regular grid can be too restrictive. Alternatives are a spatial coverage pattern type (Sect. 8.3.3) or a geostatistical pattern type (Sect. 8.3.4).

Figures D.1 to D.4 are based on variograms without nugget. For variograms with nugget a different set of figures is required. First, substituting part of the structured variance by unstructured variance (nugget variance) leads to smaller variance ratios  $\sigma_{\text{obk}}^2/\sigma^2$ . The larger the nugget-to-sill ratio, the smaller the ratio  $\sigma_{\text{obk}}^2/\sigma^2$ , i.e., the stronger the variance reduction. This implies that less observations are required to achieve the same variance reduction as depicted in these figures.

Second, it turns out that the nugget has an effect on the optimal sample-size combination, i.e., the optimal grid spacing and interval length. The larger the nugget-to-sill ratio, the smaller the difference between the number of sampling locations per spatial correlation length and the number of sampling times per temporal correlation length.

In case the universe  $\mathcal{S} \times \mathcal{T}$  is irregular or observations have already been made, other spatial patterns such as those of spatial coverage samples may be preferable. Even a different type of space–time pattern, such as interpenetrating space–time grids, could be in order.

A standard reference in model-based sampling design for spatio-temporal means is the paper by Rodríguez-Iturbe and Mejía (1974) on the design of rainfall networks. Here, the target is the long term spatial mean ( $|\mathcal{T}| \rightarrow \infty$ ) and the sampling is exhaustive in time (rainfall is measured as cumulative amounts) such that the length of the monitoring period and the number of rain gauges are the variables to be optimized.

### 15.3.5 Space–Time Kriging Current Means

The previous section treats the design of space–time samples for the whole monitoring period, simultaneously for all sampling times. This section deals with the situation where a spatial sample is designed for the next sampling time only, in other words *spatial* samples are designed sequentially.

As with co-kriging, static-synchronous patterns such as space–time grids is a good choice only when the spatial autocorrelation strongly dominates the temporal autocorrelation. In this case the sampling problem can be treated as one of sampling in space, see Sect. 7.3.

In the reverse case, there are two simple solutions. The first solution is an interpenetrating space–time grid. The required spacing of the grids at each sampling time might be approximated by calculating the space–time block-kriging variance for a range of grid spacings. The second solution is to design a spatial infill sample with k-means, using the locations of all sampling times that are temporally autocorrelated as prior locations (Sect. 8.3.3).

If neither the temporal nor the spatial autocorrelation is dominant, then the pattern of the locations might be optimized with simulated annealing, using the previous sampling events as prior data. The quality measure to be minimized is the block-kriging variance of the predicted current mean.

### 15.3.6 Kriging the Spatial Mean Temporal Trend

A question such as ‘has the surface temperature increased over the last 30 years?’ is quite common in environmental research. Usually such a question has to be answered based on a small number of time series of the variable involved (e.g. temperature) scattered around the area of interest. If the time series are long enough it is possible to estimate a trend at each sampling location, see Sect. 13.4.1. Of course, the magnitude and sign of the trend may be different at different locations, so that the question whether the average temperature has increased in a certain area cannot be answered by looking at time series only. The real question to be answered is therefore whether the spatial mean of the temporal trend in temperature is positive and significantly different from zero. Consequently, the goal of this section is sampling for



predicting spatial mean temporal trends. A general space–time model for this purpose has been developed by Sølna and Switzer (1996). Here we will use a much simpler model for designing a sample in space–time.

This model has the following form:

$$Z(\mathbf{s}, t) = \alpha(\mathbf{s}) + \beta(\mathbf{s}) \cdot (t - t_0) + \epsilon(\mathbf{s}, t), \tag{15.40}$$

where  $\alpha(\mathbf{s})$  and  $\beta(\mathbf{s})$  are level and trend coefficients respectively, that are Stochastic Functions of location in space and, for a given location  $\mathbf{s}$ , parameters in time,  $t_0$  is the initial time and  $\epsilon(\mathbf{s}, t)$  is a zero-mean residual which is assumed to have the following properties:

$$E[\epsilon(\mathbf{s}_1, t_1) \cdot \epsilon(\mathbf{s}_2, t_2)] = \begin{cases} \sigma_\epsilon^2 \exp(-|t_2 - t_1|/a_t) & \text{if } \mathbf{s}_1 = \mathbf{s}_2 \\ 0 & \text{if } \mathbf{s}_1 \neq \mathbf{s}_2 \end{cases} \tag{15.41}$$

In words, we assume that the residuals are correlated in time, but are uncorrelated in space.

Equation (15.40) can be reformulated in matrix–vector form as:

$$\mathbf{z}(\mathbf{s}) = \begin{bmatrix} z(\mathbf{s}, t_1) \\ z(\mathbf{s}, t_2) \\ \vdots \\ z(\mathbf{s}, t_{n_t}) \end{bmatrix} \quad \boldsymbol{\beta}(\mathbf{s}) = \begin{bmatrix} \alpha(\mathbf{s}) \\ \beta(\mathbf{s}) \end{bmatrix}$$

$$\mathbf{T}(\mathbf{s}) = \begin{bmatrix} 1 & t_1 - t_0 \\ 1 & t_2 - t_0 \\ \vdots & \vdots \\ 1 & t_{n_t} - t_0 \end{bmatrix} \quad \boldsymbol{\epsilon}(\mathbf{s}) = \begin{bmatrix} \epsilon(\mathbf{s}, t_1) \\ \epsilon(\mathbf{s}, t_2) \\ \vdots \\ \epsilon(\mathbf{s}, t_{n_t}) \end{bmatrix},$$

so that

$$\mathbf{z}(\mathbf{s}) = \mathbf{T}(\mathbf{s}) \cdot \boldsymbol{\beta}(\mathbf{s}) + \boldsymbol{\epsilon}(\mathbf{s}). \tag{15.42}$$

Using (15.41) the covariance matrix  $\mathbf{C}(\mathbf{s}) = \boldsymbol{\epsilon}(\mathbf{s}) \cdot \boldsymbol{\epsilon}(\mathbf{s})'$  can be constructed. With the help of this covariance matrix and the above matrix–vector definitions the Generalized Least Squares estimate of  $\boldsymbol{\beta}(\mathbf{s})$  can be obtained as (Cressie, 1993):

$$\widehat{\boldsymbol{\beta}}(\mathbf{s}) = [\mathbf{T}'(\mathbf{s}) \cdot \mathbf{C}^{-1}(\mathbf{s}) \cdot \mathbf{T}(\mathbf{s})]^{-1} \cdot \mathbf{T}'(\mathbf{s}) \cdot \mathbf{z}(\mathbf{s}), \tag{15.43}$$

and the estimation covariance matrix as

$$\mathbf{V}[\widehat{\boldsymbol{\beta}}(\mathbf{s})] = [\mathbf{T}'(\mathbf{s}) \cdot \mathbf{C}^{-1}(\mathbf{s}) \cdot \mathbf{T}(\mathbf{s})]^{-1}. \tag{15.44}$$

From application of (15.43) and (15.44) to all  $n_s$  locations one obtains estimates of trends  $\widehat{\boldsymbol{\beta}}(\mathbf{s}_i)$  and the variances of the estimation errors  $V[\widehat{\boldsymbol{\beta}}(\mathbf{s}_i)]$ .

Next, the spatial average  $\bar{\boldsymbol{\beta}}$  can be predicted using block-kriging of the  $\widehat{\boldsymbol{\beta}}(\mathbf{s}_i)$ , where the estimation errors  $\widehat{\boldsymbol{\beta}}(\mathbf{s}_i) - \boldsymbol{\beta}(\mathbf{s}_i)$  of the temporal estimation

problem are now treated as ‘observation’ errors in a spatial context. Thus, ordinary block-kriging with uncertain data is used (de Marsily, 1986). The prediction and prediction-error variance have the same form as with the regular ordinary kriging system:

$$\tilde{\beta} = \sum_{i=1}^{n_s} \lambda_i \hat{\beta}(\mathbf{s}_i) \tag{15.45}$$

$$V(\tilde{\beta} - \bar{\beta}) = \sum_{i=1}^{n_s} \lambda_i \gamma_{\beta}(\mathbf{s}_i, \mathcal{S}) + \nu - \gamma_{\beta}(\mathcal{U}, \mathcal{U}), \tag{15.46}$$

but the normal equations to obtain the weights and the value of the Lagrange multiplier have additional terms containing the estimation variances:  $V[\hat{\beta}(\mathbf{s}_i)]$ :

$$\sum_{j=1}^{n_s} \lambda_j \gamma_{\beta}(\mathbf{h}_{ij}) - \lambda_i V[\hat{\beta}(\mathbf{s}_i)] + \nu = \gamma_{\beta}(\mathbf{s}_i, \mathcal{S}) \quad i = 1, \dots, n_s \tag{15.47}$$

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

The function  $\gamma_{\beta}(\mathbf{h}_{ij})$  is the variogram of the real trend coefficients  $\beta$ . Of course this is unknown. What can be estimated from the estimates  $\hat{\beta}(\mathbf{s}_i)$  at the sampling locations is the variogram  $\gamma_{\hat{\beta}}(\mathbf{h}_{ij})$ . An approximation of the true variogram  $\gamma_{\beta}(\mathbf{h}_{ij})$  may be obtained as follows ( $n_{ti}$  is the number of sampling times at sampling location  $i$ ; the sampling interval length is assumed to be constant and equal for all sampling locations):

$$\gamma_{\beta}(\mathbf{h}_{ij}) \approx \gamma_{\hat{\beta}}(\mathbf{h}_{ij}) - \frac{\sum_{i=1}^{n_s} n_{ti} V[\hat{\beta}(\mathbf{s}_i)]}{\sum_{i=1}^{n_s} n_{ti}}. \tag{15.48}$$

In practice, the prediction of the spatial mean temporal trend consists of the following steps:

1. perform a Generalized Least Squares estimate of the trend parameter at each location with a time series. This entails:
  - a) start with an Ordinary Least Squares regression of  $\alpha + \beta(t - t_0)$  to the time series;
  - b) calculate the residuals  $\epsilon_t$ ;
  - c) estimate the covariance of the residuals (using the variogram estimator if observations are not equally spaced in time; see Chap. 9);
  - d) fit relation (15.41) to the estimated covariance function;
  - e) build the covariance matrix  $\mathbf{C}$  with (15.42) and perform the Generalized Least Squares estimate with (15.43);
  - f) repeat steps b to e until the estimate  $\hat{\beta}(\mathbf{s}_i)$  converges;

- g) evaluate (15.44) to obtain the estimation variance  $V[\widehat{\beta}(\mathbf{s}_i)]$ ;
- 2. estimate the variogram  $\gamma_{\widehat{\beta}}(\mathbf{s}_i - \mathbf{s}_j)$  from the estimated trend coefficients  $\widehat{\beta}(\mathbf{s}_i)$  at the locations and fit a permissible variogram function (see Chap. 9);
- 3. approximate the true variogram  $\gamma_{\beta}(\mathbf{h}_{ij})$  with (15.48), making sure that  $\gamma_{\beta}(\mathbf{h}_{ij})$  is positive for all lags;
- 4. solve (15.47) and evaluate (15.45) and (15.46) to obtain the prediction  $\widetilde{\beta}$  and the prediction error variance  $V(\widetilde{\beta} - \overline{\beta})$ .

The prediction and the prediction-error variance can then be used to calculate a prediction interval for the spatial mean temporal trend  $\overline{\beta}$ . Assuming normality and a confidence level of 0.95, the interval equals  $\widetilde{\beta} \pm 1.96\sqrt{V(\widetilde{\beta} - \overline{\beta})}$ . If this interval does not include zero, one can conclude that a spatial mean temporal trend exists.

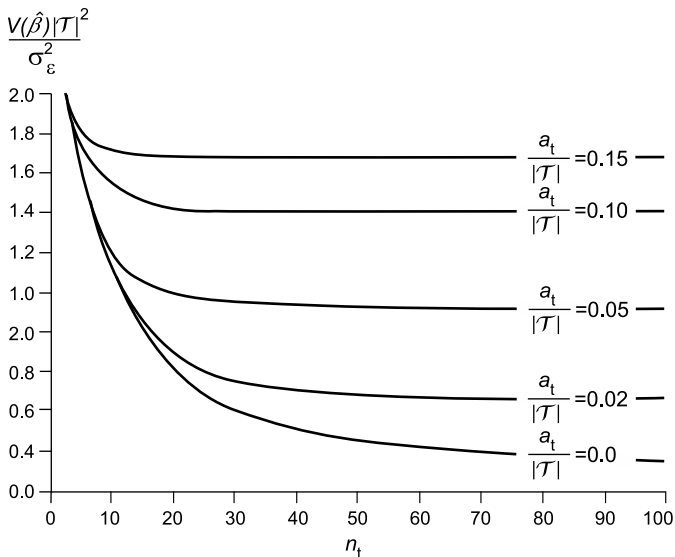
In this context, the smallest relevant trend  $\beta_{\min}$  that can still be detected, can be used to assess the sample size needed. To this end, a quality requirement related to the half-width of the 95% prediction interval can be used:

$$V(\widetilde{\beta} - \overline{\beta}) \leq \left(\frac{\beta_{\min}}{1.96}\right)^2. \tag{15.49}$$

The sampling problem is then to assess the required length of the time series, and the number and locations of these time series to make sure that the quality requirement (15.49) is met.

In the following we consider the case of sampling on a space–time grid, with a square grid pattern in space. Some figures are presented that can be used to determine the optimal interval length and grid spacing required to estimate the spatial mean temporal trend with prescribed precision. The assumptions are that the temporal covariance parameters in (15.41) are equal for all locations, and that the variogram  $\gamma_{\beta}(\mathbf{h}_{ij})$  is of spherical form with zero nugget. Given these assumptions, the parameters that must be known are: length of the time series  $|\mathcal{T}|$ , size of the area  $|\mathcal{S}|$ , temporal covariance parameters  $\sigma_{\epsilon}^2$  and  $a_t$  and semivariance parameters  $\sigma_{\beta}^2$  and  $a_s$ .

Figure 15.4 shows the relation between the ratio  $V(\widehat{\beta})|\mathcal{T}|^2/\sigma_{\epsilon}^2$  and the number of sampling times  $n_t$ , for several ratios  $a_t/|\mathcal{T}|$ . Note that the trend estimation variance has been normalized both by the residual variance as well as by the length of the monitoring period to obtain a dimensionless parameter. Given the residual variance  $\sigma_{\epsilon}^2$  and the length of monitoring period  $|\mathcal{T}|$ , the estimation variance  $V(\widehat{\beta})$  decreases with the number of sampling times  $n_t$ . The smaller temporal autocorrelation length, the stronger this sampling-frequency effect is. Figure 15.5 shows isolines of the variance ratio  $V(\widetilde{\beta} - \overline{\beta})/\sigma_{\beta}^2$  for combinations of the ratio  $V(\widehat{\beta})/\sigma_{\beta}^2$  and the number of sampling locations  $n_s$ , for  $a_s/\sqrt{|\mathcal{S}|} = 0.1, 0.5, 1.0, 2.0$  ( $\sigma_{\beta}^2$  is the sill of the variogram of the real



**Fig. 15.4.** Systematic sampling for estimating the temporal trend at a given location with Generalized Least Squares, assuming an exponential temporal covariance of the residuals. The figure shows the relationship between the dimensionless estimation variance  $V(\hat{\beta})|\mathcal{T}|^2/\sigma_\epsilon^2$  and the number of sampling times  $n_t$ , for five ratios  $a_t/|\mathcal{T}|$ .

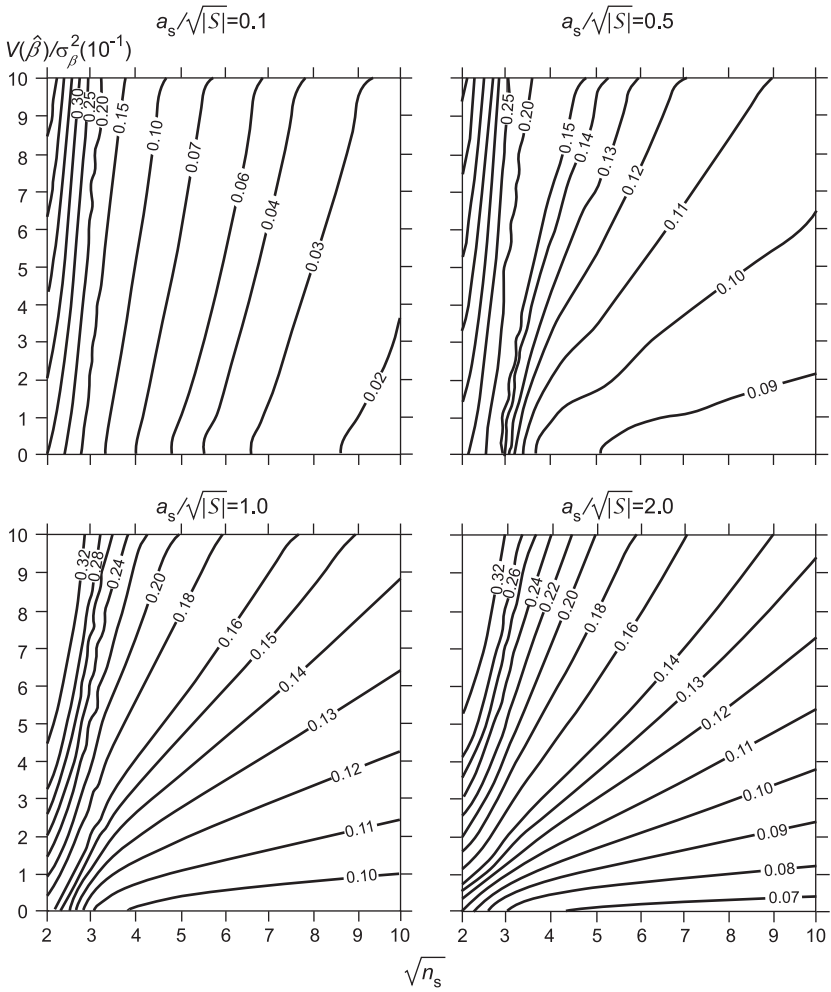
trend coefficient). Figures 15.4 and 15.5 can be used to evaluate the effect of the number of sampling times and the number of sampling locations on the prediction-error variance  $V(\tilde{\beta} - \bar{\beta})$ . First, for a proposed  $n_t$  the value of  $V(\hat{\beta})$  is determined from Fig. 15.4. Next, using the value of  $V(\hat{\beta})$  to determine the ratio  $V(\hat{\beta})/\sigma_\beta^2$ , the variance ratio  $V(\tilde{\beta} - \bar{\beta})/\sigma_\beta^2$ , and thus  $V(\tilde{\beta} - \bar{\beta})$  can be obtained from Fig. 15.5 for a given number of sampling locations  $n_s$ . This way, combinations of numbers of sampling locations and sampling times can be sought that are in accordance with quality requirement (15.49).

Although space–time grids clearly have operational advantages, we would like to stress that for predicting spatial mean temporal trend this type of pattern will not always be optimal. In situations with a large temporal range of the variogram of the residuals, an  $r$ -period synchronous pattern may be more efficient.

The assumption that the spatio-temporal residual  $\epsilon(\mathbf{s}, t)$  is spatially independent, leading to spatially independent estimation errors  $\hat{\beta}(\mathbf{s}) - \beta(\mathbf{s})$  is rather strong. However, it leads to relatively simple equations and is therefore suitable for sampling design. If, after data have been collected, it turns out that these assumptions are not supported by the data, then a more general model for inference and prediction may be in order. One option is the statisti-

cal space–time model and prediction method described by Sølna and Switzer (1996).

A special case of a temporal trend is a step trend, a sudden change in the model mean due to an intervention, see Sect. 13.4.1. If one wants to account for changes in the model mean not related to the intervention, then one may also sample synchronously one or more purposively selected control sites outside the intervention area, and postulate a time model for the pairwise differences between the impact and control sites, see Sect. 15.2.6.



**Fig. 15.5.** Sampling on a centred space–time grid (square grid pattern in space) for predicting the spatial mean temporal trend by kriging with uncertain data, assuming a spherical spatial covariance model. The figure shows the ratio  $V(\hat{\beta})/\sigma_{\beta}^2$  as a function of the ratio  $V(\hat{\beta})/\sigma_{\beta}^2$  and the number of sampling locations  $n_s$ , for four different ratios  $a_s/\sqrt{|S|}$ .