Voronoi Cells, Probabilistic Bounds, and Hypothesis Testing in Mixed Integer Linear Models

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***Abstract*—Although real-valued linear models, whether or not of full rank, have been thoroughly investigated and are well documented, very little is known about statistical and probabilistic aspects of a mixed integer linear model, which arose from space geodesy and serves as the standard starting model for precise positioning using the global positioning system (GPS). Voronoi cells play a fundamental role in the least squares estimation of the integer unknowns of the model. In this paper, we first develop a method to construct Voronoi cells and study how to fit figures of simple shape to a Voronoi cell, both from inside and outside. We then derive a number of new lower and upper bounds on the probability that the integers of the model are correctly estimated. Finally, we discuss the tests of two hypotheses on the integer mean.**

***Index Terms*—Global positioning system (GPS), integer interval estimation, integer least squares, mixed integer linear models, nearest lattice point problem, probabilistic bounds, Voronoi cells.**

I. Introduction

CONSIDER the following mixed integer linear model:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{\beta} + \boldsymbol{B}\boldsymbol{z} + \boldsymbol{\epsilon} \tag{1}$$

where $\boldsymbol{y}$ is an n-dimensional vector of observations, $\boldsymbol{A}$ and $\boldsymbol{B}$ are $(n \times t)$ and $(n \times m)$ real-valued matrices of full column rank, respectively, $\boldsymbol{\beta}$ is a real-valued nonstochastic vector, i.e., $\boldsymbol{\beta} \in \mathbb{R}^t$, and $\boldsymbol{z}$ is an integer vector, i.e., $\boldsymbol{z} \in \mathbb{Z}^m$. Here $\mathbb{R}^t$ is defined as the t-dimensional real-valued space and $\mathbb{Z}^m$ as the m-dimensional integer space. $\boldsymbol{\epsilon}$ is the error vector of the observations $\boldsymbol{y}$. In this paper, we assume that the error vector $\boldsymbol{\epsilon}$ is normally distributed with mean zero and variance–covariance matrix $\boldsymbol{Q}_\epsilon(=\boldsymbol{P}^{-1}\sigma^2)$, namely, $\boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \boldsymbol{P}^{-1}\sigma^2)$. $\boldsymbol{P}$ is a given positive-definite matrix and σ^2 is an unknown positive scalar. Two special cases of (1) are: i) conventional (real-valued) linear models, if $\boldsymbol{B} = \boldsymbol{0}$; and ii) integer linear models, if $\boldsymbol{A} = \boldsymbol{0}$. If $\boldsymbol{z}$ is supposed to be Boolean, then (1) may also be called mixed **0–1** linear models. For more details about model classification, the reader is referred to [64] or [70].

The mixed integer linear model (1) was practically motivated directly by space geodetic techniques, or more precisely, the global positioning system (GPS), and has since become the standard starting basis for modern precise satellite-based positioning. More specifically, $\boldsymbol{y}$ is a collection of all the double-difference carrier phases between GPS receivers and satellites, $\boldsymbol{\beta}$ is the correction vector of baselines or relative coordinates, and $\boldsymbol{z}$ is the integer vector of double-difference numbers of full carrier wave cycles between receivers and satellites. $\boldsymbol{\epsilon}$ describes the residual observation errors of $\boldsymbol{y}$.

When (1) is referred to raw GPS phase observations between receivers and satellites, $\boldsymbol{\beta}$ includes many other (real-valued) parameters of biases such as satellite and receiver clock errors, ionospheric and tropospheric corrections, and orbit corrections, in addition to the coordinates to be sought. Given $\boldsymbol{z}$, it is a three-way classification model with a term of trend [41], [43]. The unwanted real-valued parameters of biases are often first eliminated by using the double-difference technique, which is mathematically justified by the equivalence theorem of Schaffrin and Grafarend [41] in the case of GPS or of Baksalary [4] in a general linear model. Since the equivalence theorem of Schaffrin and Grafarend [41] or Baksalary [4] holds true only for real-valued parameters and cannot be used to eliminate the integer parameters, (1) is the most general model one has to deal with, mathematically and practically, in order to compute the most precise coordinates from GPS. In fact, GPS has revolutionized almost all the areas of engineering and science that are related to positioning or positioning information, and certainly has had already great impact on our daily life. For the theory of GPS positioning, other satellite-based positioning systems developed, and/or under development, and some of their scientific and engineering applications, the reader is referred, for example, to [6], [24], [30], [32], [40], [44].

By the beginning of the 1990s, the parameter estimation in the model (1) has been treated as if the parameters $\boldsymbol{z}$ were not integral but real, and then aided by some tools of statistical hypothesis testings for real-valued linear models in order to validate the estimation of $\boldsymbol{z}$ [16]. The first attempt to rigorously estimate $\boldsymbol{z}$ mathematically from noisy GPS carrier phase measurements in geodesy was due to Teunissen [50]. He used the geometric approach of statistical estimation to solve the mixed integer least squares (LS) problem

$$\min_{\boldsymbol{\beta}\in\mathbb{R}^t,\ \boldsymbol{z}\in\mathbb{Z}^m} : \quad \mathrm{F} = (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{\beta} - \boldsymbol{B}\boldsymbol{z})^T\boldsymbol{P}(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{\beta} - \boldsymbol{B}\boldsymbol{z}). \tag{2}$$

Unlike the geometric approach of Teunissen [50], Xu *et al.* [68] provided an alternative two-step approach to solve (2). Since $\boldsymbol{z}$ is not continuous and cannot be differentiated, one cannot directly differentiate F with respect to $\boldsymbol{\beta}$ and $\boldsymbol{z}$, equate the differentials to zero, and then solve for the estimates of $\boldsymbol{\beta}$ and $\boldsymbol{z}$, as is usually done in (real-valued) linear models. Instead, they first differentiate F with respect to $\boldsymbol{\beta}$ and equate the differential to zero. Thus, the estimate of $\boldsymbol{\beta}$ can be expressed in terms of the

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estimate of $\boldsymbol{z}$. Then they substitute $\boldsymbol{\beta}$ of (2) with the newly derived relation and derive the following integer LS problem:

$$\min_{\boldsymbol{z}\in\mathbb{Z}^m}: \ \mathrm{F} = (\boldsymbol{z} - \hat{\boldsymbol{z}}_f)^T \boldsymbol{Q}_{\hat{z}_f}^{-1} (\boldsymbol{z} - \hat{\boldsymbol{z}}_f) \tag{3}$$

where $\hat{\boldsymbol{z}}_f$ is the floating solution of $\boldsymbol{z}$ and $\boldsymbol{Q}_{\hat{z}_f}$ is the (positive-definite) cofactor matrix of $\hat{\boldsymbol{z}}_f$ [69], [70]. The floating solution and its cofactor matrix are obtained by first treating the integers $\boldsymbol{z}$ as real-valued unknowns and then solving the real-valued version of (2), which results in the following equalities:

$$\begin{aligned} \hat{\boldsymbol{z}}_f &= \boldsymbol{Q}_{\hat{z}_f} \boldsymbol{B}^T \boldsymbol{PQPy} \\ \boldsymbol{Q}_{\hat{z}_f} &= (\boldsymbol{B}^T \boldsymbol{PQPB})^{-1} \\ \boldsymbol{Q} &= \boldsymbol{P}^{-1} - \boldsymbol{A}(\boldsymbol{A}^T \boldsymbol{PA})^{-1} \boldsymbol{A}^T \end{aligned}$$

(see [69], [70]). The LS estimator of the integer vector $\boldsymbol{z}$ can be represented as follows:

$$\hat{\boldsymbol{z}} = \sum_{\boldsymbol{z}\in\mathbb{Z}^m} \boldsymbol{z}\ \mathrm{I}(V(\boldsymbol{z}), \hat{\boldsymbol{z}}_f). \tag{4}$$

Here $\hat{\boldsymbol{z}}$ is the LS estimator of the integer vector $\boldsymbol{z}$, and $\mathrm{I}(V(\boldsymbol{z}), \hat{\boldsymbol{z}}_f)$ is the indicator function

$$\mathrm{I}(V(\boldsymbol{z}), \hat{\boldsymbol{z}}_f) = \begin{cases} 1, & \text{if } \hat{\boldsymbol{z}}_f \in V(\boldsymbol{z}) \\ 0, & \text{otherwise} \end{cases}$$

where $V(\boldsymbol{z})$ is the Voronoi cell centered at the point $\boldsymbol{z}$ and will be precisely defined and constructed in Section II. If $\boldsymbol{z} = \boldsymbol{0}$, the corresponding Voronoi cell is denoted by V_0. Actually, the estimator $\hat{\boldsymbol{z}}$ can be inferred from Hassibi and Boyd [23] and is explicitly followed by Teunissen [57]–[60].

The integer LS problem (3) has been often encountered in many areas of science and engineering, for example, integer programming, the geometry of numbers, communication theory, and cryptography. Although (3) is called the integer LS problem here, it is better known as the closest point problem or nearest lattice point problem and is known to be NP-hard [1], [11], [19]. Efficient algorithms to solve (3) can be found in [1], [42]. Applications of integer programming to GPS positioning can be found in [64], [69], [70]. Based on the isotropic probabilistic models of Xu [66], Xu [65] has shown by simulations that if the dimension of $\boldsymbol{z}$ is not too large, then GPS integer decorrelation methods (see, e.g., [18], [23], [51]–[53], [61], [65], [67], [69], [70]) can be used to speed up estimating $\boldsymbol{z}$.

Quality control and hypothesis testing in linear real-valued models have been well documented [29], [31], [43], [46], [48]. However, as far as the mixed integer linear model (1) is concerned, a theory for rigorous quality control and hypothesis testing is not available and can be very difficult, unless $\boldsymbol{Q}_{\hat{z}_f}$ is diagonal. Unlike real-valued linear models, the extent of ease (or difficulty) to deal with the cases of known or unknown σ^2 in connection with (1) can be substantially different. We assume that σ^2 is known and thus can be ignored hereafter.

Even after σ^2 is assumed to be given, statistical results for the mixed integer linear model (1) are rather limited and hardly applicable in practice. Up to the present, the only results have been concerned with the computation of the probabilities of correctly estimating the integers $\hat{\boldsymbol{z}}$, their residuals, and the baseline vectors [22], [23], [56]–[60]. Unfortunately, the probability of correctly estimating the integers can hardly be computed precisely due to the complexity of Voronoi cells, particularly if the dimension of $\boldsymbol{z}$ is sufficiently large, unless $\boldsymbol{Q}_{\hat{z}_f}$ is diagonal. Thus, almost all efforts have been focused on finding the lower and upper bounds for the probability of error in communication theory and lattice theory [11], [45], [62] and in GPS applications [22], [23], [55]–[57], [59]. The best upper probabilistic bound was given by Shannon [45], while the best lower probabilistic bound can be found in [22], [23], [55], [57], [59], [62]. The latter depends, however, on the solution of the shortest lattice vector problem. In order to avoid solving this new integer optimization problem, Teunissen [55] also gave some alternative lower bounds, though worse than the best possible one. Teunissen [54]–[56] also discussed the probabilistic bounds for the simple rounding solution and the integer bootstrapped estimator. The probability and accordingly the lower probabilistic bound of the bootstrapped integer estimator will be shown to be incorrect, however.

The purpose of this paper is threefold: i) we will develop a method to construct Voronoi cells and systematically study the fitting of the Voronoi cell V_0 from inside and outside. Fitting V_0 from inside is defined as the problem of using a point set with a simple shape, say $\underline{V_0}$, to approximate V_0 in a certain sense of optimality under the condition $\underline{V_0} \subseteq V_0$. Similarly, fitting V_0 from outside consists of using a point set, again with a simple shape, say $\overline{V_0}$, to best approximate V_0 under the condition $V_0 \subseteq \overline{V_0}$; ii) we provide a number of new lower and upper bounds for the probability that the integers $\hat{\boldsymbol{z}}$ are correctly estimated; and iii) we will discuss and apply these bounds to testing hypotheses on the integers of the model (1). In this paper, we will focus on the integer LS estimate. Simple rounding and other (suboptimal) solutions, which can be found in Teunissen [55] or Grafarend [18], for example, will not be investigated here. The paper is organized as follows. Section II will discuss how to construct the Voronoi cell V_0 by finding all the vertices of a polytope, which is the starting point for all the computations of probability. In Section III, we will discuss the problem of best fitting a Voronoi cell from inside and outside from the optimization point of view. Based on the results in Sections II and III, we will then provide in Section IV some new lower and upper bounds for the probability of correctly estimating the integers. Finally, in Section V, we will discuss the issue of testing hypotheses in mixed integer linear models.

II. Construction of Voronoi Cells

A. *Defining Voronoi Cells*

Although the global optimal integer LS estimate $\hat{\boldsymbol{z}}$ of (3) can be numerically obtained by using integer programming techniques [19], [38], [49], we must represent $\hat{\boldsymbol{z}}$, as given by (4), in terms of Voronoi cells in order to study its statistical and probabilistic aspects [22], [23], [55], [57], [59]. The Voronoi cell of $\hat{\boldsymbol{z}}$ is defined as the subset $V(\hat{\boldsymbol{z}})$ of $\mathbb{R}^m$ which contains all the points $\hat{\boldsymbol{z}}_f$ according to (3) or (4) and results in the same integer estimate $\hat{\boldsymbol{z}}$. In other words, all the points in $V(\hat{\boldsymbol{z}})$ are closer to $\hat{\boldsymbol{z}}$ than any $\boldsymbol{z}$ different from $\hat{\boldsymbol{z}}$. For convenience of discussions and brevity of notations in this and the following sections, we will rewrite (3) as

$$\min:\ \mathrm{F} = (\boldsymbol{z}-\boldsymbol{x})^T \boldsymbol{P}_x (\boldsymbol{z}-\boldsymbol{x}) \tag{5}$$

where $\boldsymbol{z} \in \mathbb{Z}^m$, $\boldsymbol{x} \in \mathbb{R}^m$, and $\boldsymbol{P}_x$ is positive definite.

By definition, finding the subset $V(\hat{\boldsymbol{z}})$ is equivalent to finding all $\boldsymbol{x}$ that satisfy

$$(\hat{\boldsymbol{z}}-\boldsymbol{x})^T \boldsymbol{P}_x (\hat{\boldsymbol{z}}-\boldsymbol{x}) \le (\boldsymbol{z}-\boldsymbol{x})^T \boldsymbol{P}_x (\boldsymbol{z}-\boldsymbol{x}) \tag{6}$$

for all $\boldsymbol{z} \in \mathbb{Z}^m$ and $\boldsymbol{z} \neq \hat{\boldsymbol{z}}$. The inequality (6) is actually the definition of the Voronoi cell of the integer lattice $\mathbb{Z}^m$ [9], [11], [20]. Some basic properties of the Voronoi cell $V(\hat{\boldsymbol{z}})$ are summarized as follows: i) it is symmetric with respect to $\hat{\boldsymbol{z}}$ and convex; ii) it is translation-invariant; iii) given $V(\boldsymbol{z}_1)$ and $V(\boldsymbol{z}_2)$ $(\boldsymbol{z}_1, \boldsymbol{z}_2 \in \mathbb{Z}^m)$, if $\boldsymbol{z}_1 \neq \boldsymbol{z}_2$, then the interiors of $V(\boldsymbol{z}_1)$ and $V(\boldsymbol{z}_2)$ are disjoint; iv) $\bigcup V(\boldsymbol{z}) = \mathbb{R}^m, \forall \boldsymbol{z} \in \mathbb{Z}^m$; and v) the volume of the Voronoi cell is equal to the determinant of the lattice.

We should note: i) that these properties hold for all lattices; and ii) that Conway and Sloane [11] use the Gram matrix to define the determinant of a lattice, and as a result, they define the determinant of a lattice as the square of the volume of the Voronoi region. For our integer lattice $\mathbb{Z}^m$, the volume of $V(\hat{\boldsymbol{z}})$ is exactly equal to unity. In the context of GPS applications, Hassibi and Boyd [22], [23] decomposed $\boldsymbol{P}_x$ into $\boldsymbol{G}^T\boldsymbol{G}$ and focused on the lattice generated by the matrix $\boldsymbol{G}$. As a consequence, the corresponding Voronoi cell has the volume of $[\det\{\boldsymbol{P}_x\}]^{1/2}$, where $\det\{\boldsymbol{A}\}$ stands for the determinant of the matrix $\boldsymbol{A}$. $V(\hat{\boldsymbol{z}})$ is also called a *pull-in region* by Teunissen [55]–[57]. In this paper, we shall call it a *Voronoi cell*. Since $\hat{\boldsymbol{z}}$ is free, without loss of generality, we can impose $\hat{\boldsymbol{z}} = \boldsymbol{0}$ in (6) and obtain the Voronoi cell V_0 as follows:

$$V_0 = \{\boldsymbol{x} \,|\, \boldsymbol{z}^T \boldsymbol{P}_x \boldsymbol{x} \le \boldsymbol{z}^T \boldsymbol{P}_x \boldsymbol{z}/2, \forall \boldsymbol{z} \in \mathbb{Z}^m \text{ and } \boldsymbol{z} \neq \boldsymbol{0}\}. \tag{7}$$

If $\hat{\boldsymbol{z}}$ and $\boldsymbol{z}$ in (6) are not lattice points, but belong instead to a finite set of k (arbitrarily) given points, then we have k Voronoi cells. Given k distinct points in m-dimensional space, a number of algorithms have been proposed to find the corresponding Voronoi cells [7], [8], [12], [14], [63]. However, when the number of points tends to infinity so that they form a lattice, finding the Voronoi cell becomes difficult. If $\boldsymbol{P}_x$ has some special structure, then the Voronoi cell can be computed analytically [10], [11]. For a general positive-definite matrix $\boldsymbol{P}_x$, Viterbo and Biglieri [62] proposed a diamond-cutting algorithm to approximate the Voronoi cell at a predetermined accuracy. They start from a parallelotope, introduce one hyperplane at each iteration to cut the polytope, and finally terminate the computation when the volume of the most recent polytope is equal to the determinant of the lattice within the tolerance of a predetermined error. Because of the tolerance error, the number of vertices produced could be different from that of the exact Voronoi cell. Thus, we will propose an alternative method to compute the Voronoi cell V_0 in the remainder of this section.

B. Finding a Finite Number of Hyperplanes for Constructing the Voronoi Cell V_0

The Voronoi cell V_0 of (7) has been seemingly limited by an infinite number of hyperplanes. No optimization methods can deal with an infinite number of constraints. According to Minkowski, however, V_0 can be completely determined by at most $(2^m - 1)$ pairs of hyperplanes [9], [20]. If the covering radius R_c of the Voronoi cell is known, then it is sufficient to use all the integer points inside the sphere of radius $2R_c$ [62]. Unfortunately, finding R_c is known to be NP-hard [11], and it is not practically feasible to use the covering radius to constrain the Voronoi cell. As a result, Viterbo and Biglieri [62] suggested a more or less arbitrary number for R_c. If such a number is found too small, then it is increased. A safe and easy method is to use an upper bound of R_c in order to obtain a finite number of potentially constraining hyperplanes. Indeed, although finding R_c is NP-hard, Babai [3] obtained $2^{m/2-1}\|\boldsymbol{b}_m^*\|$ as an upper bound of R_c in polynomial time by using the Lenstra–Lenstra–Lovász (LLL) algorithm of Lenstra *et al.* [33], where $\|\boldsymbol{b}_m^*\|$ is the length of the last basis vector of the reduced basis. Since the upper bound of the covering radius by Babai [3] increases exponentially, and since the knowledge on the Voronoi cell V_0 is of basic importance for quality control and statistical testing on (1), we will develop an alternative method by combining interval mathematics with the active set method of linear programming in order to first eliminate an infinite number of redundant hyperplanes, find all the vertices of V_0, and, as a result, solve the problem of constructing V_0.

As a key step, we will have to first find a finite number of hyperplanes. We will then prove that only these hyperplanes may contribute to the construction of V_0. In other words, the other (infinitely many) constraints are redundant or automatically satisfied. Since the inequality in (7)

$$\boldsymbol{z}^T \boldsymbol{P}_x \boldsymbol{x} \le \boldsymbol{z}^T \boldsymbol{P}_x \boldsymbol{z}/2 \tag{8}$$

must hold true for all $\boldsymbol{z} \in \mathbb{Z}^m$ and $\boldsymbol{z} \neq \boldsymbol{0}$, we can substitute $\boldsymbol{z}$ by $\boldsymbol{e}_1 = (1, 0, \dots, 0)^T$ in (8) and obtain

$$\boldsymbol{p}_1 \boldsymbol{x} \le p_{11}/2 \tag{9a}$$

where $\boldsymbol{p}_1$ is the first row vector of $\boldsymbol{P}_x$ and p_{11} is the first diagonal element of $\boldsymbol{P}_x$. As in deriving (9a), we substitute $\boldsymbol{z}$ by $-\boldsymbol{e}_1$ in (8) and obtain the second linear inequality constraint

$$\boldsymbol{p}_1 \boldsymbol{x} \ge -p_{11}/2. \tag{9b}$$

The linear constraints (9a) and (9b) can be summarized as

$$-p_{11}/2 \le \boldsymbol{p}_1 \boldsymbol{x} \le p_{11}/2. \tag{10a}$$

Similarly, we can replace $\boldsymbol{z}$ in (8) with $\boldsymbol{e}_i$ and $-\boldsymbol{e}_i$ to derive the linear constraints

$$-p_{ii}/2 \le \boldsymbol{p}_i \boldsymbol{x} \le p_{ii}/2 \qquad (i = 2, 3, \dots, m) \tag{10b}$$

where all the elements of the vector $\boldsymbol{e}_i$ equal zero except for its ith element being unity, p_{ii} is the ith diagonal element of $\boldsymbol{P}_x$, and $\boldsymbol{p}_i$ is the ith row vector of $\boldsymbol{P}_x$.

Collecting all the linear inequalities (10a) and (10b) together in the notation of interval mathematics, we have

$$\boldsymbol{P}_x\boldsymbol{x} = \mathbb{U} \tag{11}$$

where

$$\mathbb{U} = \begin{bmatrix} -p_{11}/2 & p_{11}/2 \\ -p_{22}/2 & p_{22}/2 \\ \vdots & \vdots \\ -p_{mm}/2 & p_{mm}/2 \end{bmatrix}.$$

By the solutions to the linear interval equations (11), we mean the point set $\{\boldsymbol{x}|\boldsymbol{P}_x\boldsymbol{x} = \boldsymbol{u}, \boldsymbol{u} \in \mathbb{U}\}$ (see, e.g., [21], [37], [39]). The tightest bounding box of the solution set is denoted by $\mathbb{X}$ and simply given as follows:

$$\mathbb{X} = \boldsymbol{P}_x^{-1}\mathbb{U}. \tag{12}$$

By the solution (12) we mean the point set

$$\mathbb{X} = \{\boldsymbol{x}|\boldsymbol{P}_x\boldsymbol{x} = \boldsymbol{u},\ \boldsymbol{u} \in \mathbb{U}\}$$

(see, e.g., [21], [37], [39]).

We can now use the bounding box $\mathbb{X}$ of $\boldsymbol{x}$ to find the upper bound of the objective function F over V_0, which is denoted by $\overline{F}_0$. Since V_0 is a subset of $\mathbb{X}$, $\overline{F}_0$ is also the upper bound of F within V_0. We may use two methods to find $\overline{F}_0$. The first method is to directly substitute the bounding box $\mathbb{X}$ into $\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x}$ and then use interval mathematics to compute $\overline{F}_0$. This method is easy to implement but would produce a larger upper bound, unless $\boldsymbol{P}_x$ is diagonal. The second method is to solve the following maximization problem:

$$\max : \mathrm{F} = \boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x} \tag{13}$$

subject to the bounding constraints

$$\boldsymbol{x} \in \mathbb{X}.$$

It is trivial to prove that the solution to (13) is one of the corner points of the bounding box $\mathbb{X}$, since F is quadratically concave and $\mathbb{X}$ is convex. Obviously, the optimal value is also the tightest upper bound of $\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x}$ over $\mathbb{X}$.

With the upper bound $\overline{F}_0$ over V_0, we construct the ellipsoid

$$\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x} = \overline{F}_0$$

from which we can further compute the length of the major axis of the ellipsoid

$$l_p = \sqrt{\overline{F}_0/\lambda_{\min}} \tag{14}$$

where $\lambda_{\min}$ is the minimum eigenvalue of $\boldsymbol{P}_x$. Since $\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x}$ attains its maximum value $\overline{F}_0$ at the boundary of the ellipsoid, then for any $\boldsymbol{y}$ satisfying $\|\boldsymbol{y}\| > l_p$, we must have

$$\boldsymbol{y}^T\boldsymbol{P}_x\boldsymbol{y} > \overline{F}_0. \tag{15}$$

It is trivial to prove that if

$$\|\boldsymbol{z}\| > 2l_p \tag{16}$$

then we always have

$$\|\boldsymbol{z}\| - \|\boldsymbol{x}\| > l_p$$

for any point $\boldsymbol{x}$ inside the hypersphere with radius l_p, namely, $\|\boldsymbol{x}\| \leq l_p$. Using the triangle inequality of vector inner product

$$\|(\boldsymbol{z}-\boldsymbol{x}) + \boldsymbol{x}\| \leq \|\boldsymbol{z}-\boldsymbol{x}\| + \|\boldsymbol{x}\|$$

we can readily prove

$$\|\boldsymbol{z}-\boldsymbol{x}\| > l_p.$$

Thus, for any $\boldsymbol{z}$ satisfying (16) and any $\boldsymbol{x}$ in V_0, we immediately obtain

$$(\boldsymbol{z}-\boldsymbol{x})^T\boldsymbol{P}_x(\boldsymbol{z}-\boldsymbol{x}) > \overline{F}_0 \tag{17}$$

according to (15).

The inequality (17) clearly implies that if $\boldsymbol{z}$ satisfies (16), then (8) is automatically satisfied. In other words, all the integer points satisfying (16) do not constrain V_0 at all and can be eliminated. As a consequence, we successfully eliminate an infinite number of redundant hyperplanes by using a sphere to enclose V_0.

Similarly, we can also use an ellipsoid to enclose V_0. In order to do so, we can first transform $\boldsymbol{y} = \boldsymbol{U}\boldsymbol{x}$, where $\boldsymbol{U}$ is the matrix of eigenvectors of $\boldsymbol{P}_x$, determine the bounds $\mathbb{Y}$ of $\boldsymbol{y}$, and then find the new upper bound for $\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x}$ as follows:

$$\overline{F}_0 = \sum_{i=1}^{m} \lambda_i \left\{\max(|\underline{y}_i|,\ |\overline{y}_i|)\right\}^2 \tag{18}$$

where $\{\lambda_i\}$ is the set of all the eigenvalues of $\boldsymbol{P}_x$. $\underline{y}_i$ and $\overline{y}_i$ are the lower and upper bounds of y_i, respectively, and are given by $\mathbb{Y}$. Furthermore, given the quadratic constraints

$$\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x} \leq \overline{F}_0 \tag{19a}$$

$$\boldsymbol{y}^T\boldsymbol{P}_x\boldsymbol{y} > 4\overline{F}_0 \tag{19b}$$

we can readily prove

$$(\boldsymbol{y}-\boldsymbol{x})^T\boldsymbol{P}_x(\boldsymbol{y}-\boldsymbol{x}) > \overline{F}_0. \tag{19c}$$

The inequality (19c) clearly implies that all the integer points outside the ellipsoid $\boldsymbol{y}^T\boldsymbol{P}_x\boldsymbol{y} = 4\overline{F}_0$ impose no constraints on V_0 and can be automatically eliminated.

To summarize, we can state the following theorem.

Theorem 1: Given a positive-definite matrix $\boldsymbol{P}_x$, and the corresponding integer least squares problem (5), the Voronoi cell V_0 associated with its solution is defined either by

$$V_0 = \{\boldsymbol{x} \mid \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{x} \leq \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{z}/2, \\ \forall \boldsymbol{z} \in \mathbb{Z}^m,\ \boldsymbol{z} \neq \mathbf{0} \text{ and } \|\boldsymbol{z}\| \leq 2l_p\} \tag{20a}$$

in the case of spherical enclosure, or alternatively, by

$$V_0 = \{\boldsymbol{x} \mid \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{x} \leq \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{z}/2, \forall \boldsymbol{z} \in \mathbb{Z}^m, \\ \boldsymbol{z} \neq \mathbf{0} \text{ and } \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{z} \leq 4\overline{F}_0\} \tag{20b}$$

in the case of ellipsoidal enclosure.

C. Constructing the Voronoi Cell V_0

For a general positive-definite matrix $\boldsymbol{P}_x$, it is unlikely that all the integer points inside the sphere $\mathcal{S} = \{\boldsymbol{x} \mid \|\boldsymbol{x}\| \leq 2l_p\}$ or the ellipsoid $\mathcal{S} = \{\boldsymbol{x} \mid \boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x} \leq 4\overline{F}_0\}$ would actively constrain on V_0; some of these points are redundant and can thus also be eliminated. In this subsection, we will first discuss the identification of redundant constraints for V_0 and then use the active set method of linear programming to find all the vertices of V_0. Therefore, we construct the Voronoi cell V_0.

It is trivial to show that given the two integer vectors $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$ in $\mathcal{S}$, if $\boldsymbol{z}_2 = \alpha\boldsymbol{z}_1$, then $\boldsymbol{z}_2$ is redundant, where α is an integer. Thus, all the integer points $\alpha\boldsymbol{e}_i$ ($|\alpha| > 1$) inside $\mathcal{S}$ are redundant. Similarly, the integer points $\alpha\sum\boldsymbol{e}_i$ ($|\alpha| > 1$) inside $\mathcal{S}$ are also redundant. By inserting each of the integer points inside $\mathcal{S}$, except for the obviously redundant ones, into the linear inequality $\boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{x} \leq \boldsymbol{z}^T\boldsymbol{P}_x\boldsymbol{z}/2$, and then collecting them together, we have the linear inequality constraints

$$\boldsymbol{G}\boldsymbol{x} \leq \boldsymbol{b} \tag{21}$$

where $\boldsymbol{G}$ is a $(q \times m)$ real-valued matrix. Still, not every hyperplane of (21) constrains on V_0, although (21) uniquely defines the Voronoi cell.

Constructing the Voronoi cell V_0 is now mathematically equivalent to finding all the vertices of the polytope or polyhedron defined by (21), each of which is a solution of a fundamental subsystem of (21) [5]. Since V_0 is symmetric, we only need to find half the number of vertices on and above a certain hyperplane $x_i = 0$. An inequality of (21) is said to be *redundant* or *irrelevant* if it is automatically satisfied or if it does not contribute one face to the Voronoi cell V_0.

The redundant constraints of (21) always involve extra computational work in enumerating the vertices of V_0. There are two approaches to dealing with redundant constraints. One approach is to first find these redundant constraints, discard them, and then systematically solve for all the fundamental subsystems of (21) by using techniques of linear programming. To check whether any constraint of (21) is redundant, we have to solve

$$\min : \boldsymbol{g}_i\boldsymbol{x} \tag{22}$$

subject to the linear constraints (21), where $\boldsymbol{g}_i$ is the ith-row vector of $\boldsymbol{G}$. If the minimum of $\boldsymbol{g}_i\boldsymbol{x}$ is smaller than b_i, then the ith constraint of (21) is redundant [17]. To check through all the constraints of (21), we have to solve $q/2$ linear programming problems, due to the symmetry of V_0, which can be computationally quite prohibitive in its own right. It should be noted that a constraint found to be nonredundant through (22) may still be redundant or irrelevant, if it does not contribute a face of dimension $(m-1)$ to the polytope V_0.

The second and most often used approach is to directly construct V_0 by finding all its vertices, and as a by-product of this procedure, to identify and eliminate all the redundant constraints that do not form a face of dimension $(m-1)$ for V_0 from (21). Most methods of this kind have been based on the simplex method of linear programming [5], [26], [34], [35]. A basic strategy for the enumeration of vertices of a polytope is thus to repeatedly perform pivotal operations in a simplex tableau. For other types of techniques for enumerating the vertices of a polytope, the reader is referred to [28], [71].

In this paper, we will modify the pivoting algorithm of Mañas and Nedoma [34] to find all the vertices of V_0. For the linear inequalities (21) for the construction of V_0, we always have much more inequalities than variables ($q \geq 2m$). From the computational point of view, the simplex method is less efficient than the active set method, since the former has to update a matrix of order $(q \times q)$ at each iteration, while the latter needs only updating a matrix of order $(m \times m)$ [15]. Thus, as a first modification, we will implement the active set method in our algorithm to find all the vertices of the Voronoi cell V_0. The second modification is to replace the neighboring set of nodes with the set of edges, and thus avoid repeating the computation of the vertices found. Because V_0 is symmetrical, the computation work can be halved by only finding the vertices on one side of the hyperplane $x_i = 0$.

Before we present the algorithm to enumerate all the vertices of V_0, we have some notations to explicate. Two vertices of a polytope are said to have an edge if they have the same $(m-1)$ bases. Denote the vertex set of V_0 by $\mathcal{V}$ and the corresponding edge set by $\mathcal{E}$. Then the algorithm can be outlined as follows.

Algorithm for enumerating the vertices of V_0

i) Given an initial vertex of V_0, say v_0, compute the edges $e_{01}, e_{02}, \ldots, e_{0k_0}$ that originate from v_0. k_0 takes its minimum m if v_0 is not degenerate. Assign v_0 to $\mathcal{V}$ and all the edges $e_{01}, e_{02}, \ldots, e_{0k_0}$ to a temporary working set $\mathcal{W}$ of edges, namely, $\mathcal{V} = \{v_0\}$, $\mathcal{E} = \emptyset$, and $\mathcal{W} = \{e_{01}, e_{02}, \ldots, e_{0k_0}\}$;

ii) If $\mathcal{W}$ is empty, terminate. Take one element e_{jh} from $\mathcal{W}$ and use the active set method to find the next vertex v_i. If the vertex is below a predetermined hyperplane, repeat this step; or if $v_i \in \mathcal{V}$, store the edge in $\mathcal{E}$, eliminate the corresponding edge data from $\mathcal{W}$, and then repeat this step;

iii) Add the vertex to $\mathcal{V}$ and the edge with the two vertices as its end points to $\mathcal{E}$. Compute the new edges of v_i other than e_{jh} and store them into $\mathcal{W}$. Go to Step ii).

After all the vertices and the edges of V_0 are found, we can then construct and visualize V_0 in the case of low dimensions.

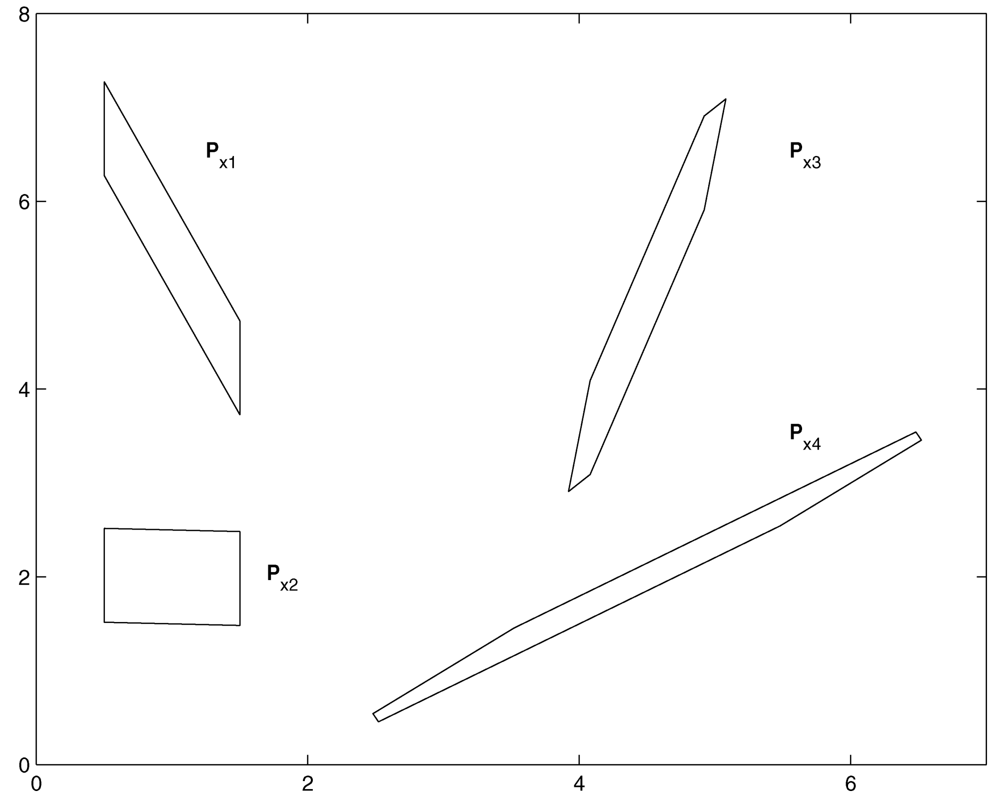

Fig. 1. The orientations, shapes and actual sizes of the four Voronoi cells.

TABLE I
THE AZIMUTHS OF THE MAJOR AXES OF THE FOUR ELLIPSES AND THEIR CORRESPONDING CONDITION NUMBERS, WHICH DEFINE THE EIGENVECTORS AND THE SHAPES OF THE MATRICES, RESPECTIVELY

matrices	$\mathbf{P}_{x1}$	$\mathbf{P}_{x2}$	$\mathbf{P}_{x3}$	$\mathbf{P}_{x4}$
azimuths	$-1^o25'46.5''$	$-0^o01'42.1''$	$14^o57'01.1''$	$53^o04'32.5''$
condition numbers	110.286909	69.007459	128.385902	228.729906

Thus, all the irrelevant constraints of (21) are automatically eliminated, and (21) can now be rewritten as follows:

$$\boldsymbol{G}_1\boldsymbol{x} \leq \boldsymbol{b}_1. \tag{23}$$

Here each of the constraints (23) contributes one face of dimension $(m-1)$ to V_0.

We should note, however, that constructing the lattice Voronoi cell could not be completed in polynomial time. The computational complexity can be attributed to two exponential numbers: i) the Voronoi cell can be actively constrained by, at most, the exponential number of $2(2^m-1)$ hyperplanes according to a theorem of Minkowski [9], [20]. This implies that the active set method would take exponential time to find the step length along all the searching directions in order to compute a new vertex of V_0. Since the system of inequalities (21) was derived by using an upper bound of V_0, the total number of inequalities in (21) will generally even be larger than that of the active constraints of V_0 and, as a result, further complicates the computation of the vertices of V_0; and ii) as a direct consequence of i), V_0 will have an exponential number of vertices, which demand exponential time to compute.

D. Examples

In order to demonstrate the method of constructing the Voronoi cell V_0 and have an impression on it, we use isotropic probabilistic models of Xu [66] and uniform distributions to generate the eigenvectors and eigenvalues of $\boldsymbol{P}_x$, respectively. One may use other distributions to generate the eigenvalues of $\boldsymbol{P}_x$ [2]. Although our method is applicable to problems of any dimension, we will limit ourselves to two- and three-dimensional matrices $\boldsymbol{P}_x$ for ease of visualization. Of many randomly generated examples, we select the following four matrices:

$$\boldsymbol{P}_{x1} = \begin{bmatrix} 110.218887 & 2.725671 \\ 2.725671 & 1.068022 \end{bmatrix}$$
$$\boldsymbol{P}_{x2} = \begin{bmatrix} 69.007442 & 0.033671 \\ 0.033671 & 1.000017 \end{bmatrix}$$
$$\boldsymbol{P}_{x3} = \begin{bmatrix} 119.907837 & -31.750722 \\ -31.750722 & 9.478065 \end{bmatrix}$$
$$\boldsymbol{P}_{x4} = \begin{bmatrix} 83.190475 & -109.370723 \\ -109.370723 & 146.539431 \end{bmatrix}$$

to illustrate the change in the shape of the Voronoi cell with the orientation and shape of the ellipse defined by $\boldsymbol{P}_x$.

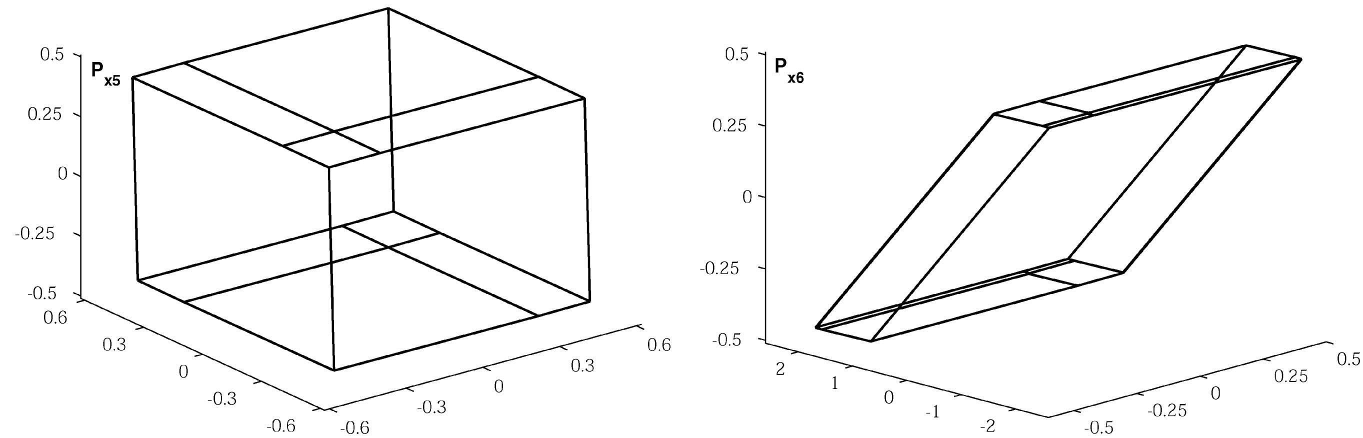

Fig. 2. The orientations, shapes, and actual sizes of the two three-dimensional Voronoi cells.

The four Voronoi cells V_0 are shown in Fig. 1. To see how the orientation and shape of V_0 are related to the eigenvectors and eigenvalues of $\boldsymbol{P}_x$, we also list the azimuths of the major axes of the four ellipses and the condition numbers of the four matrices in Table I. By comparing Fig. 1 with Table I, we see that i) the elongation of V_0 is generally in agreement with the condition number of $\boldsymbol{P}_x$ if the orientations of the ellipse are significantly different from the original coordinate axes; and ii) the orientation of V_0 is also generally in agreement with one of the eigenvectors of $\boldsymbol{P}_x$. Slight changes in the eigenvectors and/or eigenvalues of $\boldsymbol{P}_x$ can significantly affect the shape of V_0 (compare the Voronoi cells of $\boldsymbol{P}_{x1}$ and $\boldsymbol{P}_{x2}$ in Fig. 1), however. In order to further demonstrate this last point, we also plot the Voronoi cells of the following three-dimensional positive-definite matrices:

$$\boldsymbol{P}_{x5} = \begin{bmatrix} 1.890259 & 0.000224 & 0.380390 \\ 0.000224 & 1.102245 & 0.259348 \\ 0.380390 & 0.259348 & 103.263640 \end{bmatrix}$$
$$\boldsymbol{P}_{x6} = \begin{bmatrix} 1.957732 & 0.012075 & 0.403347 \\ 0.012075 & 1.372931 & 5.664388 \\ 0.403347 & 5.664388 & 143.269738 \end{bmatrix}$$

in Fig. 2, both consisting of 24 vertices and 14 planes. Although the two matrices $\boldsymbol{P}_{x5}$ and $\boldsymbol{P}_{x6}$ are only slightly different in terms of the eigendirections, the shapes of their Voronoi cells are significantly different. Note, however, that some of the planes are too small to be visible in Fig. 2.

III. Fitting the Voronoi Cell V_0

For a general positive definite $\boldsymbol{P}_x$, in particular, if its dimension is also high, then the shape of V_0 has to be represented by a very large number of vertices, together with the corresponding set of faces of V_0. The complexity of V_0 will make any further mathematical operations on it, for example, probabilistic computation over V_0, very difficult. Although an upper bound of the probability of correctly estimating the integers can be derived based on the well-known results of Shannon [45] in a Gaussian channel (see also [11], [22], [23], [62]), or more generally, a channel with a symmetrically elliptical distribution, such a simple and elegant probabilistic bound is not valid if the probability distributions of data are asymmetric. Thus, it is highly desirable to find some lower and upper bounds to approximate V_0. A lower bound was given by Hassibi and Boyd [22], [23] in the context of GPS applications, based on the concept of lattice packing [11], [20]. Teunissen [55], [59] also provided lower and upper bounds for V_0 recently. His upper bound is defined by two parallel hyperplanes and his best possible lower bound is the same as that of Hassibi and Boyd [23] and depends on the solution to an integer distance or shortest lattice vector problem by definition. To avoid this new integer optimization problem, Teunissen [55] provided some smaller lower bounds as well.

We may note that a rough upper bound of V_0 is a rectangular box and has actually already been given by (12). In this section, we will find new bounds that would best approximate V_0 from inside and outside in a certain sense of optimality. More specifically, we will find rectangles, spheres, and ellipsoids to best fit V_0. If all the vertices of V_0 have been found, then we can readily use this data set to derive the smallest possible rectangle, sphere, and ellipsoid that bound V_0 from outside. Similarly, we can find the largest possible rectangle, sphere, and ellipsoid that bound V_0 from inside. Because of the complexity of V_0, it is also important to find the lower and upper bounds without first enumerating all the vertices and faces of V_0, which will be investigated in the following.

A. Lower and Upper Bounds of Rectangular Type for V_0

If $\boldsymbol{P}_x$ is diagonal, then (12) is actually the best possible rectangle to bound V_0 from outside. For a general positive-definite matrix $\boldsymbol{P}_x$, the lower and upper bounds of rectangular type for V_0 have to be derived based on the inequality constraints (21). A rectangle symmetric with respect to the origin can always be represented by

$$-\boldsymbol{d} \leq \boldsymbol{R}\boldsymbol{x} \leq \boldsymbol{d} \tag{24}$$

where $\boldsymbol{R}$ is a rotation matrix and $\boldsymbol{d} > \boldsymbol{0}$.

By using the transformation $\boldsymbol{x}_r = \boldsymbol{R}\boldsymbol{x}$, we can rewrite (21) and (24) as follows:

$$\boldsymbol{G}\boldsymbol{R}^T\boldsymbol{x}_r \leq \boldsymbol{b} \tag{25a}$$
$$-\boldsymbol{d} \leq \boldsymbol{x}_r \leq \boldsymbol{d}. \tag{25b}$$

Finding a minimum rectangular upper bound of V_0 is equivalent to finding the smallest positive vector $\boldsymbol{d}$ such that V_0 is a subset defined by (25b). As a result, we must have $d_i = x_{ri}^{\max}(\boldsymbol{R})$. Given $\boldsymbol{R}$, each $x_{ri}^{\max}(\boldsymbol{R})$ is defined by the linear programming problem:

$$\max : x_{ri} \tag{26}$$

subject to the linear constraints (25a), where x_{ri} is the ith component of $\boldsymbol{x}_r$. Thus, the minimum upper bound of rectangular type can be obtained by solving the following optimization problem:

$$\min : \mathrm{F}_1 = \prod_{i=1}^{m} x_{ri}^{\max}(\boldsymbol{R}) \tag{27a}$$

in terms of minimum volume, or alternatively

$$\min : \mathrm{F}_2 = \sum_{i=1}^{m} x_{ri}^{\max}(\boldsymbol{R}) \tag{27b}$$

in terms of minimum total length of edges. F_1 and/or F_2 must be minimized with respect to the independent elements of the rotation matrix $\boldsymbol{R}$.

In particular, if no rotation is applied, we only need to solve the linear programming problem

$$\max : x_i \tag{28}$$

subject to the linear constraints (21) for each $i \in \{1, 2, \ldots, m\}$. Because (21) defines a bounded polytope, namely, the Voronoi cell V_0, all the linear programming problems (28) have unique maximum objective values, say $x_i^{\max}$ $(i = 1, 2, \ldots, m)$. By the symmetry of V_0, we know immediately that the least value for each component of $\boldsymbol{x}$ is $-x_i^{\max}$ $(i = 1, 2, \ldots, m)$. Thus, the smallest rectangle that most tightly bounds V_0 from outside in this special case is given by

$$\mathbb{X}_{\max} = \begin{bmatrix} -x_1^{\max} & x_1^{\max} \\ -x_2^{\max} & x_2^{\max} \\ \vdots & \vdots \\ -x_m^{\max} & x_m^{\max} \end{bmatrix}. \tag{29}$$

In a similar manner to (27a), the maximum lower bound of rectangular type to fit the Voronoi cell from inside can be found by maximizing

$$\max : \mathrm{F}_1 = \prod_{i=1}^{m} d_i \tag{30}$$

subject to two conditions of constraints: i) the inequality constraints (25a), and ii) that any of the vertices of the rectangle defined by (25b) must not be outside V_0. In fact, these two conditions are equivalent to requiring that all the vertices of (25b) satisfy (25a).

If no rotation is applied and if one would use a cube to approximate V_0 from inside by using the criterion of maximum length of edges, then the fitting model can be simplified as follows:

$$\max : \mathrm{F} = \sum_{i=1}^{m} x_i \tag{31a}$$

subject to (21), and

$$x_1 = x_2 = \cdots = x_m (= x), x > 0 \tag{31b}$$

$$\{\boldsymbol{x} | x_i = (-1)^j x; i \in \{1, 2, \ldots, m\}; j \in \{0, 1\}\} \subset V_0. \tag{31c}$$

The constraint (31c) implies that all the 2^m vertices of the cube must not be outside V_0. The solution of (31) can then be directly determined as follows:

$$x = \min : \{x \mid x \sum_{j=1}^{m} g_{ij}(-1)^{k_j} = b_i, \quad x > 0, \ k_j \in \{0, 1\}, \ i \in \{1, 2, \ldots, q\}\} \tag{32}$$

where g_{ij} are the elements of $\boldsymbol{G}$. In other words, the side of the cube is equal to the maximum positive number that satisfies all the $(q\,2^m)$ inequalities of the kind $ax \leq b$, where a and b can be derived from the inequalities of (21), (31b), and (31c), which can be shown to be equivalent to the minimum positive number of (32).

B. Lower Bounds of Ellipsoidal Type for V_0

An arbitrary ellipsoid with its center at the origin of coordinate system can always be represented by

$$\boldsymbol{x}^T \boldsymbol{E}^{-1} \boldsymbol{x} = 1 \tag{33}$$

where $\boldsymbol{E}$ is positive definite. By decomposing $\boldsymbol{E}$ into $\boldsymbol{L}\boldsymbol{L}^T$ and making the transformation $\boldsymbol{x} = \boldsymbol{L}\boldsymbol{x}_e$, we can rewrite the ellipsoid (33) as follows:

$$\boldsymbol{x} = \boldsymbol{L}\boldsymbol{x}_e \tag{34a}$$

$$\boldsymbol{x}_e^T \boldsymbol{x}_e = 1 \tag{34b}$$

where $\boldsymbol{L}$ is lower triangular with all its diagonal elements l_{ii} being positive. Thus, the best approach to bounding V_0 from inside is to find the largest ellipsoid (33) or (34), in the sense of maximum volume, such that it is completely inscribed inside V_0. Since the volume of the ellipsoid (33) is proportional to the product of the diagonal elements of $\boldsymbol{L}$, we only need to solve the following optimization problem:

$$\max : \mathrm{F}_1 = \prod_{i=1}^{m} l_{ii} \tag{35a}$$

subject to

$$\boldsymbol{G}\boldsymbol{L}\boldsymbol{x}_e \leq \boldsymbol{b}, \tag{35b}$$

the unit constraint (34b), and the positive constraints $l_{ii} > 0$ $(i = 1, 2, \ldots, m)$. In order for the ellipsoid (33) to lie inside V_0, each inequality constraint of (35b) must be true for all unit vectors $\boldsymbol{x}_e$, if and only if $\boldsymbol{x}_e = (\boldsymbol{g}_i\boldsymbol{L})^T / ||\boldsymbol{g}_i\boldsymbol{L}||$ for all i. Thus, we can replace (35b) and (34b) by

$$\boldsymbol{g}_i \boldsymbol{L}\boldsymbol{L}^T \boldsymbol{g}_i^T \leq b_i^2, \qquad i = 1, 2, \ldots, q. \tag{36}$$

In fact, the optimization model (35a) under the constraints (36) has been known as the problem of finding the maximal inscribed ellipsoid for a polytope [27]. Unlike Khachiyan and Todd [27], we work directly on the lower triangular matrix $\boldsymbol{L}$ such that the positive-definiteness of $\boldsymbol{E}$ is automatically satisfied. In addition, we implement the hybrid global optimization algorithm proposed by Xu [68] to ensure finding the global optimal solution.

In particular, if the shape of the ellipsoid is predetermined on the basis of $\boldsymbol{P}_x$, the problem can be mathematically simplified as follows:

$$\max : \mathrm{F} = \boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} \tag{37a}$$

subject to

$$\boldsymbol{G}\boldsymbol{x} \leq \boldsymbol{b} \tag{37b}$$

and

$$\{\boldsymbol{y} \mid \boldsymbol{y}^T \boldsymbol{P}_x \boldsymbol{y} = \boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x},\ \boldsymbol{y} \in \mathbb{R}^m\} \subset V_0. \tag{37c}$$

The constraint (37c) is important in that it imposes all the points on the found ellipsoid to lie inside V_0. Therefore, the solution to (37) is exactly the maximum ellipsoid which is completely inscribed in V_0 and is the best lower bound of ellipsoidal type as defined in the sense of (37a).

Obviously, (37) is a convex programming problem, and thus the maximum objective value must be unique. The solutions will not be unique, however, since V_0 is symmetrically constructed by a number of hyperplanes. This nonuniqueness of solutions does not disturb us at all, since all that we need is the equation of the ellipsoid that best approximates V_0 from inside.

It can be proved that (37) is mathematically equivalent to finding $\boldsymbol{x}$ such that

$$\min : \{f^i_{\min}\} \tag{38a}$$

where $f^i_{\min}$ is the minimum objective value of the following optimization problem:

$$\min : \mathrm{F} = \boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} \tag{38b}$$

subject to

$$\boldsymbol{g}_i \boldsymbol{x} = b_i \tag{38c}$$

for each $i \in \{1, 2, \ldots q\}$, b_i is the ith element of $\boldsymbol{b}$.

In fact, the equivalence between (37) and (38) can be established as follows. Denote the minimum objective value of (38) by $F^{\text{ell}}_{\min}$. Then, the corresponding solution(s) will automatically satisfy (37b). As a consequence, the ellipsoid

$$\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} = F^{\text{ell}}_{\min} \tag{39}$$

is completely inscribed inside the region defined by (37b), namely, V_0. Thus, (37c) is satisfied. For any $f > F^{\text{ell}}_{\min}$, part of the ellipsoid $\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} = f$ will go beyond, at least, one constraint $\boldsymbol{g}_i \boldsymbol{x} \leq b_i$, and thus violates the constraint (37c).

Since the number of optimization problems (38b) and (38c) is finite and since all of these optimization problems are convex and constrained on one hyperplane, the solution to each of (38b) and (38c) can be readily written as follows:

$$\boldsymbol{x}_i = \frac{b_i}{\boldsymbol{g}_i \boldsymbol{P}_x^{-1} \boldsymbol{g}_i^T} \boldsymbol{P}_x^{-1} \boldsymbol{g}_i^T, \qquad i = 1, 2, \ldots, q$$

from which we can easily obtain $F^{\text{ell}}_{\min}$ of (39). Therefore, the largest possible ellipsoid that best fits V_0 from inside is represented in this case by

$$\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} = \min : \left\{ \frac{b_i^2}{\boldsymbol{g}_i \boldsymbol{P}_x^{-1} \boldsymbol{g}_i^T};\ i = 1, 2, \ldots, q \right\}. \tag{40}$$

Substituting $\boldsymbol{g}_i$ and b_i into (40), we have

$$\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} = \min : \left\{ \frac{1}{4} \boldsymbol{z}_i^T \boldsymbol{P}_x \boldsymbol{z}_i;\ i = 1, 2, \ldots, q \right\}$$

which is equivalent to:

$$\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} = \frac{1}{4}\ \boldsymbol{z}_{\min}^T \boldsymbol{P}_x \boldsymbol{z}_{\min}. \tag{41}$$

Here $\boldsymbol{z}_{\min}$ is a solution of minimizing $\boldsymbol{z}^T \boldsymbol{P}_x \boldsymbol{z}$ for all $\boldsymbol{z} \in \mathbb{Z}^m$ and $\boldsymbol{z} \neq \boldsymbol{0}$. Equation (41) has shown that the lower bound of the ellipsoidal type for V_0 can be obtained either by computing a number of $b_i^2/(\boldsymbol{g}_i \boldsymbol{P}_x^{-1} \boldsymbol{g}_i^T)$ or by solving an integer distance problem.

Similarly, one can find the largest possible sphere to best fit V_0 from inside, which is simply given as follows:

$$\begin{aligned} \boldsymbol{x}^T \boldsymbol{x} &= \min : \left\{ \frac{b_i^2}{\boldsymbol{g}_i \boldsymbol{g}_i^T};\ i = 1, 2, \ldots, q \right\} \\ &= \min : \left\{ \frac{(\boldsymbol{z}_i^T \boldsymbol{P}_x \boldsymbol{z}_i)^2}{4\, \boldsymbol{z}_i^T \boldsymbol{P}_x^2 \boldsymbol{z}_i};\ i = 1, 2, \ldots, q \right\}. \end{aligned} \tag{42}$$

C. Upper Bounds of Ellipsoidal Type for V_0

Bounding V_0 from outside can be solved, whenever the shape of an ellipsoid is fixed. As in the determination of lower bounds of ellipsoidal type, one can use both the representation (33) and $\boldsymbol{P}_x$ to find the upper bounds of ellipsoidal type. Since the mathematical principle of determining the upper bound is identical, we will focus on $\boldsymbol{P}_x$, which can be formulated as the following optimization model:

$$\max : \mathrm{F} = \boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x}$$

subject to (21). Equivalently, we have the complete model

$$\min : \mathrm{F} = -\boldsymbol{x}^T \boldsymbol{P}_x \boldsymbol{x} \tag{43a}$$

subject to (21), or

$$\boldsymbol{G}\boldsymbol{x} \leq \boldsymbol{b}. \tag{43b}$$

The Kuhn–Tucker first-order conditions for (43) are

$$-\boldsymbol{P}_x\boldsymbol{x} + \boldsymbol{G}^T\boldsymbol{\lambda} = \boldsymbol{0} \tag{44a}$$
$$\boldsymbol{G}\boldsymbol{x} \le \boldsymbol{b} \tag{44b}$$
$$\boldsymbol{\lambda}^T(\boldsymbol{b} - \boldsymbol{G}\boldsymbol{x}) = 0, \qquad \boldsymbol{\lambda} \ge \boldsymbol{0} \tag{44c}$$

where $\boldsymbol{\lambda}$ is the vector of Lagrange multipliers.

From (44a), we have

$$\boldsymbol{x} = \boldsymbol{P}_x^{-1}\boldsymbol{G}^T\boldsymbol{\lambda}. \tag{45}$$

Denote

$$\boldsymbol{h} = \boldsymbol{b} - \boldsymbol{G}\boldsymbol{x} = \boldsymbol{b} - \boldsymbol{G}\boldsymbol{P}_x^{-1}\boldsymbol{G}^T\boldsymbol{\lambda} \ge \boldsymbol{0}.$$

Then the Kuhn-Tucker conditions (44) are equivalent to

$$\boldsymbol{G}\boldsymbol{P}_x^{-1}\boldsymbol{G}^T\boldsymbol{\lambda} + \boldsymbol{h} = \boldsymbol{b} \tag{46a}$$
$$\boldsymbol{\lambda}^T\boldsymbol{h} = 0, \qquad \boldsymbol{\lambda} \ge \boldsymbol{0},\ \ \boldsymbol{h} \ge \boldsymbol{0}. \tag{46b}$$

The conditions (46) are a standard linear complementarity problem. Since $\boldsymbol{G}\boldsymbol{P}_x^{-1}\boldsymbol{G}^T$ is semi-positive definite, the solution to (46) exists. After $\boldsymbol{\lambda}$ is obtained, we can then compute $\boldsymbol{x}$ through (45), and further the minimum value of F in (43a). We should note that because $\boldsymbol{G}\boldsymbol{P}_x^{-1}\boldsymbol{G}^T$ is only semi-positive definite, there may exist a number of solutions $\boldsymbol{\lambda}$. Although $\boldsymbol{\lambda}$ is likely not unique and would produce different $\boldsymbol{x}$, the minimum value of (43a) remains unchanged. In fact, since (43) is a convex programming problem, the optimal value of the objective function is mathematically unique, though $\boldsymbol{x}$ may not be unique. Geometrically, these nonunique $\boldsymbol{x}$, due to the symmetry of V_0, correspond to some vertices of V_0.

Now denote the minimum value of F by $-F_{\max}^{\text{ell}}$, where $F_{\max}^{\text{ell}} > 0$. Then we obtain the ellipsoid

$$\boldsymbol{x}^T\boldsymbol{P}_x\boldsymbol{x} = F_{\max}^{\text{ell}} \tag{47}$$

which is the minimum ellipsoid that completely encloses V_0. Thus, (47) is the minimum upper ellipsoid bounding V_0. By using exactly the same approach, we can also obtain the ellipsoid of type (47) by replacing $\boldsymbol{P}_x$ with $\boldsymbol{E}^{-1}$. It is omitted here, however.

Alternatively, one may seek a sphere to bound V_0 from outside. In this case, one can simply replace the matrix $\boldsymbol{P}_x$ from (43) to (46) with the identity matrix. Without loss of generality, denote the corresponding minimum objective value by $-F_{\max}^{\text{sph}}$, where $F_{\max}^{\text{sph}} > 0$. Then the minimum sphere that completely encloses V_0 is given as follows:

$$\boldsymbol{x}^T\boldsymbol{x} = F_{\max}^{\text{sph}}. \tag{48}$$

The radius of the sphere is the squared root of $F_{\max}^{\text{sph}}$.

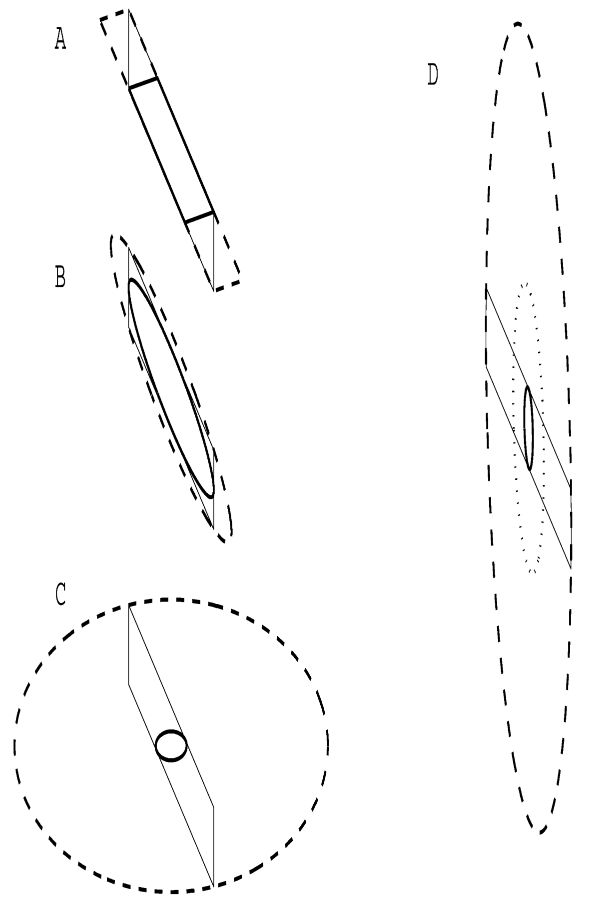

Fig. 3. Fitting the Voronoi cell V_0 by using the different types of figures: A—rectangular type; B—first ellipsoidal type with maximum volume; C—spherical type; and D—second ellipsoidal type with the shapes fixed by the matrix $\boldsymbol{P}_{x1}$. The Voronoi cell V_0 is shown in these fittings in solid line. Thick dashed and thick solid lines show the upper and lower bounds of the Voronoi cell V_0 for each type of fitting, respectively. Thick dotted line in subplot D shows the ellipse with the same area as that of the Voronoi cell.

Before finishing this section, we have to note that finding the lower and upper bounds for V_0 can also be computationally very difficult, since the total number of active constraints of V_0 can be exponential, again according to a theorem of Minkowski [9], [20]. However, it is less complex than constructing the Voronoi cell, since the second exponential number mentioned in Section II is of no concern at all here. In order to demonstrate the fittings of V_0 by the methods presented in this section, we implement the hybrid global optimization method proposed by Xu [68] to guarantee the global optimal solutions and show the lower and upper bounds of each type of fitting in Fig. 3 with the first example in Section II-D. The lower and upper bounds of rectangular type are obtained by solving the maximization problem (30) and the minimization problem (27a), respectively. For convenience of discussions, we will refer to the ellipsoidal type of fitting with maximum volume and the same type of fitting with the predetermined shape by using $\boldsymbol{P}_x$ as the first and second ellipsoidal types of fitting, respectively.

It is clear from Fig. 3 that the rectangles and ellipses of maximum area fit V_0 very well. The spherical type of fitting performs

TABLE II

THE LOWER AND UPPER BOUNDS OF AREA AND PROBABILITY FOR EACH TYPE OF FITTING: RECT—RECTANGULAR TYPE; MAXE —FIRST ELLIPSOIDAL TYPE WITH MAXIMUM VOLUME; SPHERE —SPHERICAL TYPE; AND FIXEDE—SECOND ELLIPSOIDAL TYPE WITH THE PREDETERMINED SHAPES BY $\boldsymbol{P}_{x1}$. ALSO LISTED ARE THE AREAS OF V_0 AND THE SHANNON'S TYPE OF ELLIPSE, AND THEIR CORRESPONDING PROBABILITIES. LOWERB AND UPPERB STAND FOR LOWER AND UPPER BOUNDS, RESPECTIVELY

Fitting Methods		Rect	MaxE	Sphere	FixedE	Shannon's type	V_0
Areas	LowerB	0.6578	0.7870	0.1045	0.0799	1.0000	1.0000
	UpperB	1.3371	1.5784	10.6545	7.7632		
Probabilities	LowerB	0.4242	0.4220	0.1360	0.1476	0.8647	0.4284
	UpperB	0.4284	0.5732	0.9565	1.0000		

TABLE III

. THE LOWER AND UPPER BOUNDS OF AREA AND PROBABILITY FOR EACH TYPE OF FITTING: RECT —RECTANGULAR TYPE; MAXE— FIRST ELLIPSOIDAL TYPE WITH MAXIMUM VOLUME; SPHERE—SPHERICAL TYPE; AND FIXEDE —SECOND ELLIPSOIDAL TYPE WITH THE PREDETERMINED SHAPES BY $\boldsymbol{P}_{x2}$. ALSO LISTED ARE THE AREAS OF V_0 AND THE SHANNON'S TYPE OF ELLIPSE, AND THEIR CORRESPONDING PROBABILITIES. LOWERB AND UPPERB STAND FOR LOWER AND UPPER BOUNDS, RESPECTIVELY

Fitting Methods		Rect	MaxE	Sphere	FixedE	Shannon's type	V_0
Areas	LowerB	0.9664	0.7854	0.7845	0.0945	1.0000	1.0000
	UpperB	1.0332	1.5701	1.6238	6.6126		
Probabilities	LowerB	0.4549	0.4537	0.4534	0.1723	0.8647	0.4618
	UpperB	0.4618	0.6112	0.6194	1.0000		

poorly, as can be seen in subplot C of Fig. 3. Unlike the first ellipsoidal type of fitting, the second ellipsoidal type of fitting results in rather poor lower and upper bounds (compare subplot D of Fig. 3). For the second ellipsoidal type of fitting, if the new condition that the area enclosed by the ellipse is equal to that of V_0 is imposed, the fitting does not perform well either, although the resulted upper bound, together with the lower bound of the second ellipsoidal type, has been often used in the literature [23], [57]–[59], [62]. The areas of all the lower and upper bounds, together with the corresponding lower and upper probabilistic bounds, are listed in Table II. It can be seen from this table, in terms of fitted areas, that the first ellipsoidal and rectangular types provide the best fitting performance from inside and outside, respectively. The spherical and second ellipsoidal types of fitting are worse than the first ellipsoidal and rectangular types of fitting by a maximum factor of 9.8 in lower bounds and by a maximum factor of almost 8.0 in upper bounds. In the case of the second example in Section II-D, except for the second ellipsoidal type of fitting, all the other three types of fitting produce rather satisfactory results (compare with Table III). In particular, the rectangular type of fitting produces the tightest lower and upper bounds, and outperforms all the other three types of fitting significantly, in both lower and upper bounds. The second example also demonstrates that the spherical type of fitting can work well in some cases.

IV. LOWER AND UPPER PROBABILISTIC BOUNDS

For statistical inference and quality control on the estimated integers $\hat{\boldsymbol{z}}$ from the observations $\boldsymbol{y}$, we often have to compute the probability that $\hat{\boldsymbol{z}}$ is correctly estimated. This probability is denoted by $P(\hat{\boldsymbol{z}})$. In general, we can assume a probability density function $f(\boldsymbol{x})$ for the real-valued random vector $\hat{\boldsymbol{z}}_f$ of (3) and then compute $P(\hat{\boldsymbol{z}})$. Since $\boldsymbol{\epsilon}$ has been assumed to be normally distributed with zero mean and variance $\boldsymbol{P}^{-1}\sigma^2$, $\hat{\boldsymbol{z}}_f$ is also normally distributed with mean $\boldsymbol{z}$ and variance $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2$, namely, $\hat{\boldsymbol{z}}_f \sim N(\boldsymbol{z},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)$, where σ^2 has been assumed to be known.

The probability $P(\hat{\boldsymbol{z}})$ can now be computed as follows:

$$\begin{aligned} P(\hat{\boldsymbol{z}}) &= P(\hat{\boldsymbol{z}}_f \in V_0 + \hat{\boldsymbol{z}}) = \int_{V_0+\hat{\boldsymbol{z}}} N(\boldsymbol{z},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \\ &= \int_{V_0} N(\boldsymbol{z}-\hat{\boldsymbol{z}},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \end{aligned} \tag{49}$$

where $d\boldsymbol{x} = dx_1 dx_2 \ldots dx_m$. If $\hat{\boldsymbol{z}}$ is assumed to be equal to the unknown true integer vector $\boldsymbol{z}$, then (49) becomes

$$P(\hat{\boldsymbol{z}}) = \int_{V_0} N(\boldsymbol{0},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \tag{50}$$

which is independent of the integer LS estimate and was given by Hassibi and Boyd [22], [23], and Teunissen [55]. However, the interpretations of (49) and (50) are different. The equality (49) describes the probability for any given or known event, since the elements of $\hat{\boldsymbol{z}}$ are integer random variables. The equality (50) calculates the probability for the unknown event that the integer LS estimate is equal to its true integer vector. Neither of these two interpretations could be practically satisfactory. We will re-interpret (49) in terms of integer interval estimation at the end of this section.

Since V_0 can be very complex for a general positive-definite matrix $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}$, precise computation of $P(\hat{\boldsymbol{z}})$ can be very difficult, though not impossible. Finding lower and upper bounds for $P(\hat{\boldsymbol{z}})$ could thus become even more important than directly computing it. Given a set of codewords of finite length, Shannon [45] studied the probability of error of decoding in a white Gaussian channel and obtained an elegant, well-known formula to compute a lower bound of probability of error. It can be directly applied to derive the corresponding lower bound of probability of error in the most general context of the Voronoi cell of a lattice [62]. Upper bounds of probability of error can be derived either by using Boole's inequality of probability or the packing radius of a lattice [11], [62]. In the case of GPS applications, one is more interested in computing the probability $P(\hat{\boldsymbol{z}})$ of correctly estimating the integers of the model than the probability of error $(1 - P(\hat{\boldsymbol{z}}))$. Thus, the lower bound of $(1 - P(\hat{\boldsymbol{z}}))$ is equivalent to the upper bound of $P(\hat{\boldsymbol{z}})$, which is given as follows:

$$P(\hat{\boldsymbol{z}}) = \int_{V_0} N(\mathbf{0},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \leq \int_{E_0} N(\mathbf{0},\ \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \quad (51)$$

where

$$E_0 = \{\boldsymbol{x} \,|\, \boldsymbol{x}^T\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}\boldsymbol{x}/\sigma^2 \leq \rho_0^2\}$$

and the positive constant ρ_0^2 satisfies the condition that the defined ellipsoid is of unit volume. The probabilistic inequality (51) was first given by Hassibi and Boyd [22], [23] for GPS applications, though, in a different form. It will be referred to as the upper probabilistic bound of Shannon's type in the remainder of this paper. The most attractive features of (51) are twofold: i) that it does not require an upper bound of V_0 and is easy to compute; and ii) it will become clear later that it is the best upper probabilistic bound of ellipsoidal type if the shape of the ellipsoid is predetermined by using $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}$. However, we have to note that it is not valid any more if the probability distributions of data are not symmetrical.

In this paper, we will derive other lower and upper probabilistic bounds for $P(\hat{\boldsymbol{z}})$ by finding lower and upper bounds of the Voronoi cell V_0, which are denoted by $\underline{V_0}$ and $\overline{V_0}$, respectively. Then we have

$$\underline{P(\hat{\boldsymbol{z}})} \leq P(\hat{\boldsymbol{z}}) \leq \overline{P(\hat{\boldsymbol{z}})} \quad (52)$$

where $\underline{P(\hat{\boldsymbol{z}})}$ and $\overline{P(\hat{\boldsymbol{z}})}$ are the lower and upper probabilistic bounds, respectively, and

$$\underline{P(\hat{\boldsymbol{z}})} = \int_{\underline{V_0}} N(\mathbf{0}, \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x} \quad (53a)$$

and

$$\overline{P(\hat{\boldsymbol{z}})} = \int_{\overline{V_0}} N(\mathbf{0}, \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2)d\boldsymbol{x}. \quad (53b)$$

The first results on lower and upper bounds for $P(\hat{\boldsymbol{z}})$ were given by Hassibi and Boyd [22], [23] and Viterbo and Biglieri [62]. Since their upper probabilistic bound for $P(\hat{\boldsymbol{z}})$ is essentially derived on the basis of Shannon [45], it is the best possible so far if the probability distributions of data are elliptically symmetric. The lower bound was also rederived by Teunissen [55], [59]. In terms of $\underline{V_0}$ and $\overline{V_0}$, the best possible values are reproduced as follows:

$$\underline{V_0} = \{\boldsymbol{x} \mid \boldsymbol{x}^T\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}\boldsymbol{x} \leq F_{\min}/4,\ \boldsymbol{x} \in \mathbb{R}^m\} \quad (54a)$$

$$\overline{V_0} = \{\boldsymbol{x} \mid |\boldsymbol{h}^T\boldsymbol{x}| \leq 1/2,\ \boldsymbol{x} \in \mathbb{R}^m\} \quad (54b)$$

$$\boldsymbol{h} = \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}\boldsymbol{z}_{\min}/\boldsymbol{z}_{\min}^T\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}\boldsymbol{z}_{\min}. \quad (54c)$$

The lower bound $\underline{V_0}$ of (54a) can be found in [22], [23], [55], [59], and the upper bound $\overline{V_0}$ of (54b) in [59]. Here $\boldsymbol{z}_{\min}$ and $F_{\min}$ are a solution to the shortest lattice vector problem

$$\min : \mathrm{F} = \boldsymbol{z}^T\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}\boldsymbol{z} \quad (54d)$$

for all $\boldsymbol{z} \in \mathbb{Z}^m$ and $\boldsymbol{z} \neq \mathbf{0}$. Solving (54d) is conjectured to be NP-hard, though not completely proved yet [11], [19]. If solving (54d) is not desirable, one can find alternative lower bounds in [55], though they are worse than (54a).

We have investigated the construction of the Voronoi cell in Section II and in Section III developed the methods to find the lower and upper bounds of V_0 by systematically recasting the problems of bounding V_0 as optimization models. Based on these bounding results, which can be straightforwardly available by replacing $\boldsymbol{P}_x$ with $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}$, we can readily obtain the corresponding lower and upper probabilistic bounds of $P(\hat{\boldsymbol{z}})$.

Comparing our results with those of Hassibi and Boyd [22], [23], Viterbo and Biglieri [62] and Teunissen [55], [59], we can see that their lower probabilistic bound corresponds exactly to our $\underline{V_0}$ of second ellipsoidal type given by (40), although the derivations are different. It is the largest possible lower bound of ellipsoidal type if $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}$ is used to define the ellipsoid. In practice, if all these lower and upper bounds are computed, then the best lower and upper probabilistic bounds are the largest lower bound and the smallest upper bound among the rectangular, ellipsoidal, and spherical types of bounds, respectively. Since these three types of bounds are mathematically very simple, one can then use approximation techniques of multiple integrals [47] to compute the probabilistic bounds.

Taking the first two Voronoi cells in Section II as examples, we knew, in terms of areas, that the lower and upper bounds of rectangular and first ellipsoidal types (with maximum volume) fit V_0 tightly, and that the second ellipsoidal type (with a predetermined shape) performed the worst, although it is most often used in the literature [23], [57]–[59], [62]. Here we will continue our discussion of these two examples in terms of lower and upper probabilistic bounds. To start our discussion, we assume that $\hat{\boldsymbol{z}}_f$ has the Gaussian distribution such that the thick dotted ellipse in subplot D of Fig. 3 corresponds to a probability of 0.8647, which is the upper probabilistic bound of Shannon's type and is actually equivalent to two times standard deviation. Accordingly, we computed the lower and upper probabilistic bounds of each type of fitting and listed the results in Tables II and III.

As can be clearly seen from these two tables, the rectangular type of fitting produces the tightest lower and upper probabilistic bounds, and almost reproduces the exact probability over V_0 under the assumption. The first ellipsoidal type of bounds of V_0 results in a rather fine lower bound of probability, but its upper probabilistic bound is overestimated by 33.8% in the first example and 32.4% in the second example, respectively. Even though the lower bound of first ellipsoidal type of fitting was shown to perform better than that of rectangular type of fitting in terms of area in the first example of Section III-C, the lower probabilistic bound of rectangular type is better in terms of probability. This is not surprising, since, in the first example,

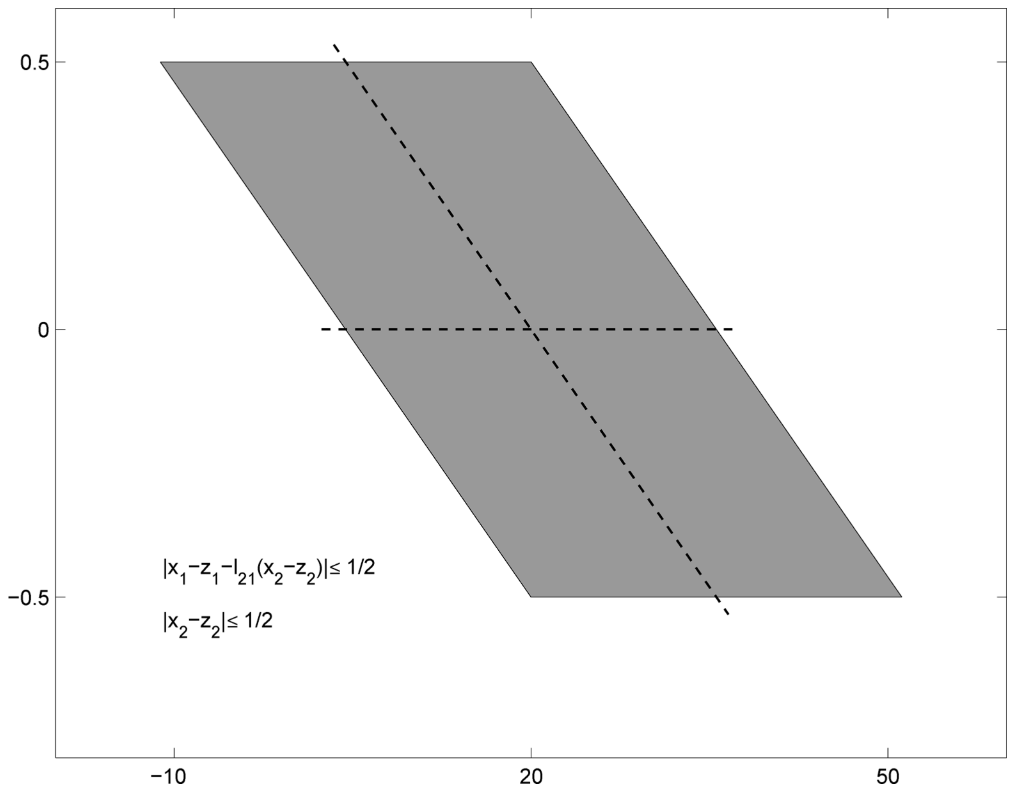

Fig. 4. Illustrated domain of integration used for computing the probability that the integer bootstrapped estimator correctly produces the integer vector $\boldsymbol{z}$ of the model.

the lower-bounded region of rectangular type is not completely covered by that of first ellipsoidal type, and since this uncovered region has much more weight than the lower-bounded region of first ellipsoidal type not covered by its rectangular counterpart. The lower and upper probabilistic bounds of second ellipsoidal type perform poorly in both examples, if the shapes of the ellipsoids are fixed by using $\boldsymbol{P}_x$. They are significantly different from the exact probability of correctly estimating the integers computed inside the Voronoi cell. Although the upper probabilistic bound of Shannon's type has been known to be the best, it is not comparable with that of either rectangular or first ellipsoidal type in both examples, and overestimates the probability by 101.8% in the first example and 87.2% in the second example, respectively. The probabilistic bounds of spherical type perform poorly in the first example but are reasonably good in the second example.

In addition to the integer LS estimate of $\boldsymbol{z}$, the so-called integer bootstrapped estimator has been substantially investigated by Teunissen [55]–[59]. The probability and its corresponding lower bound of correctly estimating the integers, given in [55], [56], [59], for example, are incorrect. Let us first remember that they are derived by simply multiplying the probability of each transformed new random variable over the interval $[-1/2,\, 1/2]$ due to the diagonal nature of the conditional variance–covariance matrix. Now assume a two-dimensional positive-definite matrix $\boldsymbol{P}_x$ of (5), whose corresponding domain of integration for the integer bootstrapped estimator is shown in Fig. 4. It is very clear that there can be, in general, many integer points inside the shaded area, which is the domain of integration. In other words, the probability and its lower bound for the integer bootstrapped estimator to correctly estimate the integer vector $\boldsymbol{z}$, as described above, correspond to all these integer points but certainly not just only one integer point. Since all the probabilistic results reported in [55]–[59] for the integer bootstrapped estimator are based on the claimed assumption that there is one and only one integer point inside the domain of integration, the counterexample illustrated here has clearly invalidated the assumption and, as a result, also the corresponding reported probabilistic results.

A few more words may be appropriate before finishing this section. Since the mean $\boldsymbol{z}$ is unknown, Hassibi and Boyd [22], [23] and Teunissen [55], [59] simply substituted the mean or unknown true integer vector $\boldsymbol{z}$ in (49) with the integer estimate $\hat{\boldsymbol{z}}$ to compute $P(\hat{\boldsymbol{z}})$ as if $\hat{\boldsymbol{z}}$ were the unknown true integer vector $\boldsymbol{z}$. Without this presumed substitution, we could not compute $P(\hat{\boldsymbol{z}})$. To statistically justify the substitution, the hypothesis that the LS estimate of $\boldsymbol{z}$ is equal to the unknown true integer vector has to be tested first. If it is accepted with a sufficiently large confidence level, then we could accept (50) as the probability that $\hat{\boldsymbol{z}}$ is correctly estimated. From this point of view, the corresponding probability should be more properly interpreted as a pre-test probability. As a consequence, we always obtain a largest possible probability for $P(\hat{\boldsymbol{z}})$. Since fixing GPS integer ambiguities incorrectly is practically disastrous for precise positioning, too optimistic an estimate for $P(\hat{\boldsymbol{z}})$ is highly undesirable. In fact, if $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2$ is sufficiently large, the integer points in the neighborhood of $\hat{\boldsymbol{z}}_f$ may all likely be an estimate of $\boldsymbol{z}$. To reflect this situation, we may substitute $\boldsymbol{z}$ with its real-valued estimate $\hat{\boldsymbol{z}}_f$. The corresponding probabilistic results could then be interpreted in terms of integer interval estimation.

For real-valued linear models, the interval estimate of the model parameters can have an arbitrarily given probability to cover the true (unknown) values, depending on the estimate of the parameters. In the case of mixed integer linear models, the size and shape of the Voronoi cell V_0 have been fixed. Accordingly, position, size, and shape for integer interval estimation have been fixed, and instead, the probability for the Voronoi cell to cover the true integer point cannot be predetermined.

V. Statistical Hypothesis Testing

Given a probability distribution for the observations $\boldsymbol{y}$, hypothesis testing has been well developed and documented in the literature of real-valued linear models [29], [31], [43], or equivalently the model (1) without the second term $\boldsymbol{Bz}$. In contrast with real-valued linear models, we know almost nothing about hypothesis testing in the mixed integer linear model (1), unless the unknown integer vector is treated as if it were real-valued [13]. Since $\boldsymbol{z}$ is discrete, the sum of squared residuals and the generalized likelihood-ratio statistic are not chi-square distributed nor F-distributed, respectively.

In a real-valued linear model, it always makes sense to test hypotheses of types $\boldsymbol{H\beta} = \boldsymbol{c}$. For the mixed integer linear model (1), $\boldsymbol{Hz} = \boldsymbol{c}$ can be incorrect in the first instance and no statistical testing is needed. For instance, given a (real-valued) nonsingular $(m \times m)$ matrix $\boldsymbol{H}$ and a (real-valued) vector $\boldsymbol{c}$, if $\boldsymbol{H}^{-1}\boldsymbol{c}$ is not integral, then we can immediately conclude that $\boldsymbol{Hz} = \boldsymbol{c}$ is wrongly formulated, since $\boldsymbol{z}$ must be integral. For an arbitrary set of $\boldsymbol{H}$ and $\boldsymbol{c}$ with $\mathrm{rank}(\boldsymbol{H}) < m$, proving that the corresponding hypothesis is incorrectly formulated can be very difficult or even more difficult than testing the hypothesis itself. In the following discussions, we assume that $\boldsymbol{H}$ and $\boldsymbol{c}$ make sense to construct hypotheses. We will formulate the equivalent hypotheses in terms of Voronoi cells. In the two-dimensional case, for example, testing $z_1 - z_2 = 0$ is equivalent to testing whether $\boldsymbol{z}$ is in the set $\{\, \boldsymbol{z} \,|\, z_1 - z_2 = 0, \forall z_1, z_2 \in \mathbb{Z}\}$ with an infinitely countable number of elements, and as a result, is dependent on the probability of error computed over the Voronoi cells of these integer lattice points.

Since the error vector $\boldsymbol{\epsilon}$ of (1) is assumed to be normally distributed, namely, $\boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \boldsymbol{P}^{-1}\sigma^2)$, and σ^2 is known or given, the floating solution $\hat{\boldsymbol{z}}_f$ of $\boldsymbol{z}$ is also normally distributed with variance–covariance matrix $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2$. We now discuss, in connection with precise GPS positioning, testing two hypotheses on the integers $\boldsymbol{z}$ in the mixed integer linear model (1): i) $\boldsymbol{z} = \boldsymbol{z}_0$ with $\boldsymbol{z}_0$ given; and ii) $\boldsymbol{z} \in \mathcal{Z}$ with $\mathcal{Z}$ being a given subset of $\mathbb{Z}^m$.

A. *Testing the Hypothesis of Specified Values for the Integers*

The first hypothesis to be investigated is written as follows:

$$\mathcal{H}_0: \ \boldsymbol{z} = \boldsymbol{z}_0, \ \text{ versus } \mathcal{H}_1: \ \boldsymbol{z} \neq \boldsymbol{z}_0 \tag{55}$$

where $\mathcal{H}_0$ and $\mathcal{H}_1$ are the null and alternative hypotheses, respectively, and $\boldsymbol{z}_0$ is a given integer vector. Unlike real-valued linear models, since $\boldsymbol{z}$ in (1) is discrete, it does make sense to test (55). From the point of view of maximum likelihood, if the null hypothesis $\mathcal{H}_0$ is true, then it must be most helpful to produce the measurements $\boldsymbol{y}$. Because the distribution of $\boldsymbol{y}$ has been specified and σ^2 assumed known, the distribution of $\hat{\boldsymbol{z}}$ has been completely determined under the null hypothesis $\mathcal{H}_0$. If the integer estimate $\hat{\boldsymbol{z}}$ is exactly equal to $\boldsymbol{z}_0$, we can compute the probability for $\mathcal{H}_0$ being true as follows:

$$P(\hat{\boldsymbol{z}} \,|\, \boldsymbol{z} = \boldsymbol{z}_0) = \int_{V_0} N(\boldsymbol{0}, \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2) d\boldsymbol{x}. \tag{56}$$

The error of first kind or significance level is then computed by $(1 - P(\hat{\boldsymbol{z}} \,|\, \boldsymbol{z} = \boldsymbol{z}_0))$. Unlike tests on the mean in real-valued linear models, we cannot first specify a number for the significance level to test (55). On the other hand, the complexity of the Voronoi cell V_0 would make the precise computation of (56) very difficult and impractical. Thus, we would rather compute the lower and upper bounds for $P(\hat{\boldsymbol{z}} \,|\, \boldsymbol{z} = \boldsymbol{z}_0)$ by using the results of Sections III and IV. The corresponding tests of (55) may be said to be *conservative* and *optimistic*, respectively.

A test of significance is almost always in favor of null hypotheses. An established theory or law (null hypothesis) will not be abandoned, unless data provide strong evidence against it. This behavior of statistical testing in favor of the null hypothesis has been well enunciated in terms of prior probability or simplicity postulate by Jeffreys [25]. However, when GPS applications are concerned, the null hypothesis $\mathcal{H}_0$ of (55) should be rejected, so far as the evidence of data casts doubt on it. The reason is obvious: if GPS integer ambiguities are incorrectly fixed, no precise positioning can be obtained. Thus, the conservative test with the lower probability bound should be recommended in practice.

Up to the present, we have assumed that the observations $\boldsymbol{y}$ contain no biases. Practically, residual biases may remain in $\boldsymbol{y}$, which will then deviate $\hat{\boldsymbol{z}}_f$ systematically from the true GPS ambiguity unknowns. If $\hat{\boldsymbol{z}}_f$ happens to be inside the Voronoi cell of $\boldsymbol{z}_0$, and if $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}\sigma^2$ is sufficiently small, then the lower bound of $P(\hat{\boldsymbol{z}} \,|\, \boldsymbol{z} = \boldsymbol{z}_0)$ may approach unity. In this case, we would almost certainly accept the null hypothesis $\mathcal{H}_0$. However, if we conduct the chi-square test of

$$\mathcal{H}_{10}: \ E(\hat{\boldsymbol{z}}_f) = \boldsymbol{z}_0 \tag{57}$$

under a certain small significance level as if (1) were a real-valued linear model, then (57) is expected to be rejected almost certainly. In other words, if the null hypothesis (57) cannot be accepted, this should mean that there exist residual biases in the observations $\boldsymbol{y}$. The data have cast doubt on the null hypothesis $\mathcal{H}_0$ of (55). As a result of this extra test, one has to make sure that the residual biases are almost impossible to force $\hat{\boldsymbol{z}}_f$ out of the Voronoi cell of $\boldsymbol{z}_0$, before $\mathcal{H}_0$ can be accepted. In practice, one has to collect more GPS data, either to support the acceptance of $\mathcal{H}_0$ or to reject it, although $P(\hat{\boldsymbol{z}} \,|\, \boldsymbol{z} = \boldsymbol{z}_0)$ was almost equal to unity.

B. *Testing a Composite Hypothesis on the Integers*

The second hypothesis to be discussed is formulated as follows:

$$\mathcal{H}_{20}: \ \boldsymbol{z} \in \mathcal{Z}, \ \text{ versus } \mathcal{H}_{21}: \ \boldsymbol{z} \notin \mathcal{Z} \tag{58}$$

where $\mathcal{Z}$ is a subset of given integer points, namely, $\mathcal{Z} \subseteq \mathbb{Z}^m$. $\mathcal{H}_{20}$ and $\mathcal{H}_{21}$ are the null and alternative hypotheses, respectively. If the generalized likelihood ratio statistic is applied to test hypotheses of type (58), the integer point in $\mathcal{Z}$ that maximizes the likelihood is chosen to construct the test statistic. In the case of GPS applications, the most conservative practice should be preferred, since fixing the ambiguities to an incorrect integer point means that precise positioning is impossible. Thus, the optimistic likelihood practice of tests should not be suitable in GPS applications. One might suggest that a least favorable point in $\mathcal{Z}$ is chosen to construct a test statistic. This proposal cannot be accepted either, because, in the case of testing $\boldsymbol{Hz} = \boldsymbol{c}$ with an infinitely countable number of Voronoi cells, the null hypothesis $\mathcal{H}_{20}$ will almost always be rejected.

Except for the difficulty mentioned above, if we follow the practice of testing $\mathcal{H}_0$ to test $\mathcal{H}_{20}$, we may encounter a logical difficulty from the frequentist point of view, since the true GPS ambiguity vector is unique, though unknown. Two methods may be used to circumvent this logical difficulty: i) testing (58) from the Bayesian point of view; or ii) testing (58) by treating $\mathcal{H}_{20}$ as a problem of integer interval estimation. To apply the first method, we have to assume or assign a prior probability to each integer point in $\mathcal{Z}$. The Bayesian approach enables to completely get rid of the logical difficulty elegantly, since we can naturally assign prior information on each integer point in $\mathcal{Z}$. However, the difficulty in practical application of this strategy is how to generate such prior information reasonably. A second difficulty inherent in mixed integer linear models is how to generate prior Voronoi cells for the integer points. If the prior Voronoi cell is different from that determined from the data, what is the posterior Voronoi cell while keeping the posterior estimate as integers? These questions have to be properly addressed and solved before Bayesian test for mixed integer linear models can be practically applicable. We will not follow this line, but further research should certainly be conducted in the future.

We will use the second approach to test $\mathcal{H}_{20}$. First, we compute the probability that the Voronoi cells of $\mathcal{Z}$ may contain $\boldsymbol{z}$, which is denoted by $P(\boldsymbol{z} \in \mathcal{Z})$ and is given as follows:

$$P(\boldsymbol{z} \in \mathcal{Z}) = \sum_{\boldsymbol{z}_i \in \mathcal{Z}} \int_{V_0 + \boldsymbol{z}_i} N(\boldsymbol{z}_i - \hat{\boldsymbol{z}}, \boldsymbol{Q}_{\hat{\boldsymbol{z}}_f} \sigma^2) d\boldsymbol{x}. \tag{59}$$

If $P(\boldsymbol{z} \in \mathcal{Z})$ is sufficiently close to one, and if $\hat{\boldsymbol{z}} \in \mathcal{Z}$, we believe that $\mathcal{Z}$ contains the true GPS ambiguity vector, and $\mathcal{H}_{20}$ is accepted with the probability $P(\boldsymbol{z} \in \mathcal{Z})$. Accordingly, the error of the first kind is computed by $(1 - P(\boldsymbol{z} \in \mathcal{Z}))$. As in (56), it is more feasible to compute the lower bound for $P(\boldsymbol{z} \in \mathcal{Z})$ and then use it to decide whether or not to accept $\mathcal{H}_{20}$ conservatively for GPS applications.

VI. Concluding Remarks

Estimation and hypothesis testing in real-valued linear models have been almost thoroughly investigated and are well documented in standard literature of statistics [29], [31], [36], [43]. In contrast, very little is known about statistical and probabilistic aspects in a mixed integer linear model, which first arose from space geodesy and has since become the standard starting model for GPS precise positioning. Although the integer LS problem (3) has been well known as the nearest or closest point problem in many areas of science/engineering and solved by using integer programming, Teunissen [50] was the first to try to rigorously address the estimation of integer unknowns in the context of GPS applications or the mixed integer linear model (1). Xu *et al.* [68] gave an alternative two-step procedure to estimate the integer unknowns of (1). Integer decorrelation techniques have been studied substantially (see, e.g., [18], [22], [23], [51], [52], [61]) but were shown by simulations to speed up the estimation procedure only if the dimension of the integer vector is not too large [65].

Compared with significant advance in numerical solutions of $\boldsymbol{\beta}$ and $\boldsymbol{z}$, very limited results have been obtained in statistical and probabilistic aspects on the estimated integers. First results on probabilistic bounds for a lattice point were given by Hassibi and Boyd [22], [23] and Viterbo and Biglieri [62]. The upper bound is derived by using the results of Shannon [45] and performs better than the corresponding upper bound of second ellipsoidal type with its region defined by (47). We should note, however, that the results of Shannon's type are valid only if the probability distributions of data are elliptically symmetric, while our upper bounds of ellipsoidal types are generally applicable. Teunissen [55], [59] also gave some lower and upper probabilistic bounds for $P(\hat{\boldsymbol{z}})$. His best possible lower bound is the same as that given by Hassibi and Boyd [22], [23], and is the largest possible of second ellipsoidal type if the shape of the ellipsoid is predetermined by using $\boldsymbol{Q}_{\hat{\boldsymbol{z}}_f}^{-1}$. We have shown that the second ellipsoidal and Shannon's types of probabilistic bounds perform poorly, although they have been most often used in the literature [23], [57]–[59], [62]. As a result, we have investigated the lower and upper probabilistic bounds of rectangular and first ellipsoidal types with maximum volume, which are much better than those used in the literature. In particular, the rectangular type of fitting results in the tightest lower and upper probabilistic bounds. They almost reproduce the probability $P(\hat{\boldsymbol{z}})$ over V_0 itself in both examples if the region covered by Shannon's type of fitting is supposed to be equivalent to two times standard deviation. Even though the first ellipsoidal type of fitting with maximum volume is better than the rectangular type in one of the examples in terms of areas of lower bounds, the rectangular type is still better in providing a tighter lower probabilistic bound.

By using interval arithmetic mathematics, we are able to eliminate an infinite number of redundant hyperplanes and thus only retain a finite number of constraints to construct the Voronoi cell V_0. We have then proposed applying the active set method to enumerate all the vertices of the Voronoi cell. As a result, V_0 has been completely constructed. Due to the complexity of V_0 for a general positive-definite matrix, we have developed methods to bound V_0 by recasting the problems of bounding as optimization models. Thus, we have derived systematically the tightest bounds of rectangular, ellipsoidal, and spherical types for the Voronoi cell V_0 from inside and outside. Accordingly, we also have obtained the lower and upper probabilistic bounds for $P(\hat{\boldsymbol{z}})$.

We have discussed the tests of two hypotheses on the integers in the mixed integer linear model (1). These tests are called conservative and optimistic, respectively, depending on whether lower or upper probabilistic bounds are used. From the point of view of practical GPS applications, conservative tests should be exercised, since fixing GPS ambiguities to an incorrect integer point is a complete failure to precise GPS positioning. On the other hand, unlike hypothesis tests in real-valued linear models, significance levels cannot be predetermined but have to be computed in statistical testing on the integers in the mixed integer linear model (1). Finally, we shall have to note that Section V is just a starting point toward hypothesis testing in mixed integer linear models, and much work remains to be done, for example, to test a more general hypothesis with real-valued and integer unknowns, and with or without prior information or random effect.

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