SYMMETRIC CONFIDENCE REGIONS AND CONFIDENCE INTERVALS FOR NORMAL MAP FORMULATIONS OF STOCHASTIC VARIATIONAL INEQUALITIES

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Abstract. Stochastic variational inequalities (SVI) model a large class of equilibrium problems subject to data uncertainty, and are closely related to stochastic optimization problems. The SVI solution is usually estimated by a solution to a sample average approximation (SAA) problem. This paper considers the normal map formulation of an SVI, and proposes a method to build asymptotically exact confidence regions and confidence intervals for the solution of the normal map formulation, based on the asymptotic distribution of SAA solutions. The confidence regions are single ellipsoids with high probability. We also discuss the computation of simultaneous and individual confidence intervals.

 $\textbf{Key words.} \ \ \text{confidence region, confidence interval, stochastic variational inequality, sample average approximation, stochastic optimization, normal map}$

1. Introduction. This paper considers a stochastic variational inequality (SVI), in which the function that defines the variational inequality is an expectation function. Let (Ω, \mathcal{F}, P) be a probability space, and ξ be a random vector that is defined on Ω and supported on a closed subset Ξ of \mathbb{R}^d . Let O be an open subset of \mathbb{R}^q , and F be a measurable function from $O \times \Xi$ to \mathbb{R}^q , such that for each $x \in O$ the expectation $f_0(x) = E[F(x, \xi)]$ is well defined. Let S be a polyhedral convex set in \mathbb{R}^q . The SVI problem is to find a point $x \in S \cap O$ such that

$$0 \in f_0(x) + N_S(x), \tag{1.1}$$

where $N_S(x) \subset \mathbb{R}^q$ denotes the normal cone to S at x:

$$N_S(x) = \{ v \in \mathbb{R}^q \mid \langle v, s - x \rangle \le 0 \text{ for each } s \in S \}.$$

We use $\langle \cdot, \cdot \rangle$ to denote the scalar product of two vectors of the same dimension. Here and elsewhere, the symbol \subset stands for set inclusion and allows the two sets compared to coincide.

The function f_0 defined above is a function from O to \mathbb{R}^q . We are interested in situations in which f_0 does not have a closed form expression and is approximated by a sample average function. Let ξ^1, \dots, ξ^n be independent and identically distributed (i.i.d.) random variables with distribution same as that of ξ . Define the sample average function $f_n: O \times \Omega \to \mathbb{R}^q$ by

$$f_n(x,\omega) = n^{-1} \sum_{i=1}^n F(x,\xi^i(\omega)).$$
 (1.2)

The sample average approximation (SAA) problem is to find a point $x \in S \cap O$ such that

$$0 \in f_n(x,\omega) + N_S(x). \tag{1.3}$$

In the rest of this paper, we will write $f_n(x,\omega)$ as $f_n(x)$ when clear from the context. We will consider the normal map formulations (to be defined below) of both (1.1) and (1.3). The major objective is to

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develop a method to build confidence regions and confidence intervals for the solution of the normal map formulation of (1.1). We will explain how to obtain confidence regions and intervals for the solution of (1.1) in Section 6. For brevity, we refer to a solution to (1.1) or its normal map formulation as a true solution, and a solution to (1.3) or its normal map formulation as an SAA solution.

Under certain regularity conditions, the SAA solutions almost surely converge to a true solution as the sample size n goes to infinity; see Gürkan, Özge and Robinson [9], King and Rockafellar [11], and Shapiro, Dentcheva and Ruszczyński [35, Section 5.2.1]. [11, Theorem 2.7] and [35, Section 5.2.2] provided the asymptotic distribution of SAA solutions. Xu [41] showed that the SAA solutions converge to the set of true solutions in probability at an exponential rate under some assumptions on the moment generating functions of certain random variables; see [36] for related results on the exponential convergence rate. For work on stability of stochastic optimization problems, see [3, 4, 30, 34] and numerous references therein.

As discussed in Pflug [21], there are two basic approaches to constructing confidence regions for the true solution of a stochastic optimization problem. The first approach is based on the asymptotic distribution of SAA solutions, and the second is based on properties about boundedness in probability with known tail behavior. The latter approach was used in [21] to construct universal confidence sets for the true solution, among other results. Vogel [40] continued that approach and developed a general method for universal confidence sets, taking account for random feasible sets and nonunique optimal solutions.

The method in this paper belongs to the first approach in the above classification. Our goal is to construct asymptotically exact confidence regions that are convenient to compute along with confidence intervals, under assumptions that guarantee the SVI and its SAA approximations to have locally unique solutions. Our work is closely related to Demir [2]. In that dissertation, Demir considered the normal map formulation of the SVI and obtained in [2, Equation (36)] an expression for confidence regions of the true solution. That expression depended on quantities not directly computable. [2, Theorem 3.16] modified it, resulting in a formula for the set called S^n in [2]. That formula looks similar to (4.2) of the present paper, but it uses $d(f_0)_S(z_n)(z_n - z)$ (in our notation) instead of $d(f_n)_S(z_n)(z - z_n)$ in (4.2). We show in this paper that the set (4.2) is an asymptotically exact confidence region of the true solution, by proving that the probability for it to contain the true solution converges to the prescribed level of confidence. The development in [2] did not justify its method with an asymptotic exactness result, aside from using some restrictive assumptions.

The starting point of the asymptotic analysis in this paper is Theorem 3.1, which is proved in [16] and related to results in [2, 11, 35]. Equations (3.4) and (3.5) in that theorem describe the asymptotic distribution of the solution (denoted by z_n) to the normal map formulation of the SAA problem (1.3) in terms of a piecewise linear function L_K and a normal random vector Y_0 . Because L_K depends on the true solution z_0 and is unknown before z_0 is found, we need to replace it by a suitable estimator in order to establish a confidence region for z_0 . For the general situations considered in this paper, the dependence of L_K on the location of z_0 is discontinuous, due to the nonsmooth structure of S. Such discontinuity is a major issue to be addressed for establishing computable confidence regions, and this paper handles this issue using a different approach from those in [15, 16].

In [15, 16], L_K is replaced by estimators designed to converge to L_K in probability. The consistency of those estimators relies on the exponential convergence rate of z_n to z_0 . When L_K is piecewise linear with multiple pieces, its estimators constructed in [15, 16] have multiple pieces with high probability, producing asymmetric confidence regions that are factions of ellipsoids pieced together. In the present paper, we use a property of general piecewise affine functions (Theorem 2.2) to show that for large n

the two vectors $-d(f_n)_S(z_n)(z_0-z_n)$ and $L_K(z_n-z_0)$ are close to each other even though $d(f_n)_S(z_n)$ may be a very different function from L_K . Accordingly, we can use $-d(f_n)_S(z_n)(z_0-z_n)$ to replace $L_K(z_n-z_0)$ in (3.5) without losing the limiting property (Theorem 3.3). This leads to a computable confidence region for z_0 given in (4.2) or (4.6) without the need of constructing a consistent estimator for L_K . The main advantage with the new method comes from Proposition 3.5, which implies that the confidence region built from this method is with high probability a single ellipsoid (or can be approximated by a degenerate ellipsoid in the singular case). This brings much efficiency for describing confidence regions or computing simultaneous confidence intervals. Another advantage of the new method is that it does not rely on the exponential convergence rate of z_n . Lastly, we mention that with this method the confidence region obtained from a particular z_n may be very different from that obtained from another z_n , since $d(f_n)_S(z_n)$ can be very different for different z_n . This does not conflict with the asymptotic exactness of the confidence region.

Given the results on confidence regions and simultaneous confidence intervals, a natural question is whether individual confidence intervals for components of z_0 can be computed in a parallel manner, by using $d(f_n)_S(z_n)$ to replace L_K in (3.4). Since $d(f_n)_S(z_n)$ is an invertible linear function with high probability, the individual confidence interval given by this approach can be expressed by a closed-form formula (5.17). Theorem 5.1 shows that the probability for that interval to contain the *j*th component of z_0 converges to a quantity related to the random variable $\Gamma = (L_K)^{-1}(Y_0)$, and that quantity equals the desired confidence level $1 - \alpha$ when the condition in (5.5) holds. Based on that convergence result and given the simple format of (5.17), one can use (5.17) as an approximative confidence interval for $(z_0)_j$ to compare with confidence intervals obtained from other methods (such as methods developed in [13] to compute asymptotically exact individual confidence intervals using estimators in [15, 16]), which generally require more computation when L_K has more than two pieces.

Examples of stochastic variational inequalities of the form (1.1) include stochastic Nash equilibrium problems in which players' cost functions are expected values of certain random variables, such as the energy market problem studied in [9, 10]. Stochastic variational inequalities also arise as first-order conditions of optimization problems whose objective functions are expectations. If the exact values of some coefficients of the objective function are unknown, and are estimated using sample data average, then the solution obtained for such a problem is essentially an SAA solution. The method of this paper can be applied to such problems to provide a quantitative measure on the effect of sample variations on solutions obtained for those problems. We have applied this method to a type of statistical learning problems [17].

Below we briefly introduce the normal map formulation of variational inequalities. The normal map induced by the function $f_0: O \to \mathbb{R}^q$ and the polyhedron $S \subset \mathbb{R}^q$ is defined to be a function $(f_0)_S: \Pi_S^{-1}(O) \to \mathbb{R}^q$, with

$$(f_0)_S(z) = f_0(\Pi_S(z)) + (z - \Pi_S(z)) \text{ for each } z \in \Pi_S^{-1}(O),$$
(1.4)

where $\Pi_S(z)$ denotes the Euclidean projection of z on S, and $\Pi_S^{-1}(O)$ is the set of points $z \in \mathbb{R}^q$ such that $\Pi_S(z) \in O$. If a point $x \in S \cap O$ satisfies (1.1), then the point $z = x - f_0(x)$ satisfies $\Pi_S(z) = x$ and

$$(f_0)_S(z) = 0. (1.5)$$

Conversely, if z satisfies (1.5), then $x = \Pi_S(z)$ satisfies $x - f_0(x) = z$ and solves (1.1). Thus, equation (1.5) is an equivalent formulation for (1.1), and is referred to as the normal map formulation of (1.1).

In general, for any function g from (a subset of) \mathbb{R}^q to \mathbb{R}^q and any closed and convex set C in \mathbb{R}^q , one can define the normal map induced by g and C, denoted by g_C , in the same way as (1.4) with g in place of f and C in place of S. For example, the normal map induced by the sample average function f_n and the set S is a function $(f_n)_S: O \to \mathbb{R}^q$ defined as

$$(f_n)_S(z) = f_n(\Pi_S(z)) + (z - \Pi_S(z))$$
 for each $z \in \Pi_S^{-1}(O)$.

The following is the normal map formulation for the SAA problem (1.3):

$$(f_n)_S(z) = 0. (1.6)$$

Equation (1.6) is related to (1.3) in the same way as (1.5) is to (1.1).

The above definition for the normal map is from Robinson [26, 27]. The normal map concept is closely related to the Minty parametrization [18], in the sense that the variable z can be considered as the parameter in the Minty parametrization of the graph of N_S : the mapping $z \to (\Pi_S(z), z - \Pi_S(z))$ is one-to-one from \mathbb{R}^q onto the graph of N_S , and the equation (1.5) is a reformulation of (1.1) in terms of z using that parametrization.

Because S is a polyhedral convex set by assumption, the Euclidean projector Π_S is a piecewise affine function (see Section 2 below for the precise definition of piecewise affine functions). It coincides with an affine function on each of a family of finitely many q-dimensional polyhedral convex sets. This family is called the normal manifold of S, and each set in this family is called an q-cell, where the symbol q refers to the dimension of those sets. The union of all the q-cells is \mathbb{R}^q . Any two distinct q-cells are either disjoint, or meet at a common proper face of them. (A face of a convex set P in \mathbb{R}^q is defined to be a convex subset F of P such that if x_1 and x_2 belong to P and $\lambda x_1 + (1 - \lambda)x_2 \in F$ for some $\lambda \in (0,1)$, then x_1 and x_2 actually belong to F, see, e.g., [28]. F is a proper face of P, if it is a nonempty face of P and is not P itself.) For detailed discussions on the normal manifold and properties of piecewise affine functions, see [22, 23, 26, 32].

To illustrate the normal manifold concept, consider the example when $S = \mathbb{R}_+^q$, the nonnegative orthant in \mathbb{R}^q . For this example, the projector Π_S coincides with an affine function when restricted to each fixed orthant of \mathbb{R}^q , and that affine function is different for a different orthant: for example we have $\Pi_S(z) = z$ for points $z \in \mathbb{R}_+^q$, $\Pi_S(z) = 0$ for $z \in \mathbb{R}_-^q$, and $\Pi_S(z) = (z_1, 0, \dots, 0)$ for $z \in \mathbb{R}_+ \times \mathbb{R}_-^{q-1}$, so Π_S coincides with the identity function, the zero function, or the projector onto the z_1 axis, when restricted on \mathbb{R}_+^q , \mathbb{R}_-^q or $\mathbb{R}_+ \times \mathbb{R}_-^{q-1}$ respectively. Accordingly, the normal manifold of \mathbb{R}_+^q is the family of all orthants in \mathbb{R}^q .

Below we introduce some terminology and notation. A subset K of \mathbb{R}^q is called a cone if $\mu x \in K$ whenever $x \in K$ and μ is a positive real number. For a set $C \subset \mathbb{R}^q$, int C denotes its interior, and cone C is the smallest cone that contains it. (This definition for cone C is equivalent to the one given in [32, Section 2.1.1] for polyhedral convex sets C. In this paper we will only apply the definition to such sets.) We use $\|\cdot\|$ to denote the norm of an element in a normed space; unless explicitly stated otherwise, it can be any norm, as long as the same norm is used in all related contexts. We use $\mathcal{N}(0,\Sigma)$ to denote a Normal random vector with covariance matrix Σ . Weak convergence of k-dimensional random variables Y_n to Y will be denoted as $Y_n \Rightarrow Y$, which means that $Ef(Y_n)$ converges to Ef(Y) for all bounded continuous functional f on \mathbb{R}^k . Following [24], a locally Lipschitz function $g: \mathbb{R}^q \to \mathbb{R}^m$ is said to be B-differentiable at a point $x_0 \in \mathbb{R}^q$ if there is a positively homogeneous function $G: \mathbb{R}^q \to \mathbb{R}^m$, such that

$$g(x_0 + v) = g(x_0) + G(v) + o(v). (1.7)$$

(Recall that a function G is positively homogeneous, if $G(\lambda v) = \lambda G(v)$ for each nonnegative real number λ and each $v \in \mathbb{R}^q$.) Such a function G is called the B-derivative of g at x_0 and is denoted as $dg(x_0)$. Note that $dg(x_0)(h)$ is exactly the directional derivative of g at x_0 along the direction h. Indeed, as pointed out in [33], for a locally Lipschitz function in finite-dimensional spaces, B-differentiability (called the directional differentiability in the sense of Fréchet in [33]) of the function is equivalent to directional differentiability of the function for all directions. If g is differentiable at x_0 , then the B-derivative $dg(x_0)$ coincides with the standard Fréchet derivative.

The rest of this paper is organized as follows. Section 2 is a discussion on general piecewise affine functions. Section 3 establishes the main asymptotic distribution results. Section 4 provides methods to build confidence regions and simultaneous confidence intervals. Section 5 discusses computation of individual confidence intervals. Section 6 concludes the paper with numerical examples.

2. Piecewise affine functions. This section discusses general piecewise affine functions, and proves some properties to be used in subsequent development. The notation in this section is independent of the notation in the rest of this paper.

By definition, a continuous function f from \mathbb{R}^q to \mathbb{R}^m is called *piecewise affine* if there exists a finite family of affine functions $f_j: \mathbb{R}^q \to \mathbb{R}^m, j=1,\cdots,k$, such that the inclusion $f(x) \in \{f_1(x),\cdots,f_k(x)\}$ holds for each $x \in \mathbb{R}^q$ [32]. The affine functions $f_j, j=1,\cdots,k$ are called selection functions of f. If all f_j 's are linear functions then f is called *piecewise linear*.

A closely related concept is the *polyhedral subdivision* [5, 32]. A polyhedral subdivision of \mathbb{R}^q is a finite collection of polyhedral convex sets in \mathbb{R}^q , $\mathfrak{P} = \{P_1, \dots, P_l\}$, that satisfies the following conditions:

- 1. Each P_i is a polyhedral convex set of dimension q.
- 2. The union of all P_i is \mathbb{R}^q .
- 3. The intersection of each two P_i and P_j , $1 \le i \ne j \le l$, is either empty or a common proper face of both P_i and P_j .

If each $P_i \in \mathfrak{P}$ is a polyhedral convex cone, then \mathfrak{P} is a conical subdivision. It was shown in [32, Proposition 2.2.3] that for any piecewise affine function f there corresponds a polyhedral subdivision \mathfrak{P} of \mathbb{R}^q such that f coincides with an affine function on each $P \in \mathfrak{P}$. If f is piecewise linear, then the corresponding \mathfrak{P} is a conical subdivision. For example, if $S = \mathbb{R}^q_+$, then the Euclidean projector Π_S is piecewise linear, and the family of all orthants in \mathbb{R}^q is the corresponding conical subdivision. In general, for any polyhedral convex set S the Euclidean projector Π_S is piecewise affine, with the normal manifold of S being the corresponding polyhedral subdivision.

In the rest of this section, let $f: \mathbb{R}^q \to \mathbb{R}^m$ be a piecewise affine function with the corresponding subdivision \mathfrak{P} . Clearly, if f is represented by different selection functions on $P_1 \in \mathfrak{P}$ and $P_2 \in \mathfrak{P}$, and $x \in P_1 \cap P_2$, then f is nondifferentiable at x. However, it is well known that f is B-differentiable at any point in \mathbb{R}^q ; below we explain a formula for the B-derivative of f at a point $x \in \mathbb{R}^q$. For the derivation of this formula see [5] and [32, Proposition 2.2.6]. Let

$$\mathfrak{P}(x) = \{ P \in \mathfrak{P} \mid x \in P \}$$

be the subfamily of \mathfrak{P} that consists of elements in \mathfrak{P} containing x. We use $|\mathfrak{P}(x)|$ to denote the union of all $P \in \mathfrak{P}(x)$, called the *underlying* set of $\mathfrak{P}(x)$ in algebraic topology [19]. We caution the reader that $|\mathfrak{P}(x)|$ here does not mean the cardinality of $\mathfrak{P}(x)$. It is obvious that x belongs to the interior of $|\mathfrak{P}(x)|$. For each $x \in \mathbb{R}^q$, define the following family of polyhedral convex cones:

$$\mathfrak{P}'(x) = \{ \operatorname{cone}(P - x) \mid P \in \mathfrak{P}(x) \}.$$

The family $\mathfrak{P}'(x)$ is a conical subdivision of \mathbb{R}^q . The B-derivative df(x) of f at x is a piecewise linear function from \mathbb{R}^q to \mathbb{R}^m , whose corresponding subdivision is exactly $\mathfrak{P}'(x)$. If f coincides with the affine function Ax + b on the polyhedral convex set $P \in \mathfrak{P}(x)$, then

$$df(x)(h) = Ah \text{ for each } h \in \text{cone}(P - x).$$
 (2.1)

A consequence of (2.1) is that the selection functions of df(x) are exactly the linear parts of selection functions of f on elements of $\mathfrak{P}(x)$. In particular, if x is contained in the interior of some $P \in \mathfrak{P}$, then df(x) is a linear map.

While for a fixed point $x \in \mathbb{R}^q$ the B-derivative df(x) is a continuous function on \mathbb{R}^q , the dependence of df(x) on x is discontinuous, because df(x) changes abruptly to a very different function as x moves from the interior of some $P \in \mathfrak{P}$ to its boundary. For example consider Π_S with $S = \mathbb{R}^q_+$ again. As a piecewise linear function, Π_S is B-differentiable at any point $z \in \mathbb{R}^q$. At any z in the interior of \mathbb{R}^q_+ , the B-derivative $d\Pi_S(z)$ is the identity map. At any z with $z_1 = 0$ and $z_i > 0$ for $i = 2, \dots, q$, $d\Pi_S(z)$ is a piecewise linear map with two pieces:

For each
$$h \in \mathbb{R}^q$$
, $d\Pi_S(z)(h) = \begin{cases} h, & \text{if } h_1 \ge 0, \\ (0, h_2, \cdots, h_q), & \text{if } h_1 \le 0. \end{cases}$

As will become clear, the discontinuity of df(x) with respect to x is a major issue to be addressed to develop methods for confidence regions in this paper and in [15, 16]. In this paper, we handle this issue by utilizing a "symmetry" property between the B-derivatives df(x) and df(y) for two points x and y that belong to a common set in \mathfrak{P} , shown in Theorem 2.2 below. Theorem 2.2 will be used to establish our main result in Theorem 3.3. The proof of Theorem 2.2 uses the following lemma, which gives two equivalent statements for the condition $y \in |\mathfrak{P}(x)|$.

LEMMA 2.1. Let x and y be two points in \mathbb{R}^q . The following are equivalent.

- (1) $y \in |\mathfrak{P}(x)|$.
- (2) $x \in |\mathfrak{P}(y)|$.
- (3) There exists $P \in \mathfrak{P}$ such that both x and y belong to P.

Proof. Suppose $y \in |\mathfrak{P}(x)|$. Then there exists $P \in \mathfrak{P}(x)$ such that $y \in P$. The fact that $P \in \mathfrak{P}(x)$ implies $x \in P$. This proves the direction $(1) \Rightarrow (3)$.

Now suppose (3) holds. Then $P \in \mathfrak{P}(x)$. Since $y \in P$, we have $y \in |\mathfrak{P}(x)|$. This proves (3) \Rightarrow (1). It follows that (3) and (1) are equivalent. Similarly we can prove (3) and (2) are equivalent. The equivalence between (1) and (2) follows. \square

THEOREM 2.2. Let $x \in \mathbb{R}^q$, and let $y \in |\mathfrak{P}(x)|$. Then

$$df(x)(y-x) = -df(y)(x-y).$$

Proof. By Lemma 2.1, there exists $P \in \mathfrak{P}$ that contains both x and y. Let A be the matrix for the linear part of the selection function of f on P. The fact that $y \in P$ implies $y - x \in \text{cone}(P - x)$, so by (2.1) we have df(x)(y - x) = A(y - x). The fact $x \in P$ implies $x - y \in \text{cone}(P - y)$. Again by (2.1) we have df(y)(x - y) = A(x - y). \square

Proposition 2.3 below shows that $\mathfrak{P}(x)$ is a superset of $\mathfrak{P}(y)$ for all y sufficiently close to x. Recall from comments below (2.1) that the selection functions of df(x) are exactly the linear parts of selection functions of f on elements of $\mathfrak{P}(x)$. Therefore, a consequence of Proposition 2.3 is that the family of

selection functions of df(x) contains the family of selection functions of df(y), for all y sufficiently close to x.

PROPOSITION 2.3. Let $x \in \mathbb{R}^q$. There exists a neighborhood X of x, such that each $y \in X$ satisfies $\mathfrak{P}(y) \subset \mathfrak{P}(x)$.

Proof. Recall that x belongs to the interior of $|\mathfrak{P}(x)|$. Let X be a neighborhood of x in the interior of $|\mathfrak{P}(x)|$, and let $y \in X$. Since y belongs to the interior of $|\mathfrak{P}(x)|$, there exist finitely many polyhedrons P_1, \dots, P_k in $\mathfrak{P}(x)$, such that $y \in P_i$ for each $i = 1, \dots, k$ and y belongs to the interior of $\bigcup_{i=1}^k P_i$. Now, let $P \in \mathfrak{P}(y)$; we shall prove that $P = P_i$ for some $i = 1, \dots, k$, by showing that it is impossible for a set $P \in \mathfrak{P}$ that is different from any of those P_i 's to meet $\bigcup_{i=1}^k P_i$. Suppose for the purpose of contradiction that P is different from any P_i , $i = 1, \dots, k$. Then, for each i the intersection $P \cap P_i$ is a proper face of P. Consequently, the intersection between P and $\bigcup_{i=1}^k P_i$ is the union of finitely many polyhedrons of dimensions less than q. On the other hand, since P is of dimension q and $\bigcup_{i=1}^k P_i$ contains q in its interior, the intersection between P and $\bigcup_{i=1}^k P_i$ contains a full-dimensional convex set. This leads to a contradiction. We have thereby proved that $P = P_i$ for some $i = 1, \dots, k$. It follows that $\mathfrak{P}(y) \subset \mathfrak{P}(x)$.

3. Limiting properties. This section provides some limiting properties of solutions to (1.6). Those properties will be used to develop methods on confidence region and simultaneous confidence intervals.

We make two sets of assumptions. Assumption 1 below is to obtain nice properties of f_0 and f_n about integrability and convergence. Following that, Assumption 2 is to guarantee the existence, local uniqueness and stability of the true solution. The notation $T_S(x)$ that appears in Assumption 2 denotes the tangent cone to S at a point $x \in S$. Since S is a polyhedral convex set, the following definition applies:

$$T_S(x) = \{ v \in \mathbb{R}^q \mid \text{ there exists } t > 0 \text{ such that } x + tv \in S \}.$$
 (3.1)

Assumption 1. (a) $E||F(x,\xi)||^2 < \infty$ for all $x \in O$.

- (b) The map $x \mapsto F(x, \xi(\omega))$ is continuously differentiable on O for a.e. $\omega \in \Omega$, and $E||d_xF(x,\xi)||^2 < \infty$ for all $x \in O$.
- (c) There exists a square integrable random variable C such that

$$||F(x,\xi(\omega)) - F(x',\xi(\omega))|| + ||d_xF(x,\xi(\omega)) - d_xF(x',\xi(\omega))|| \le C(\omega)||x - x'||,$$

for all $x, x' \in O$ and a.e. $\omega \in \Omega$.

The notation $d_x F(x, \xi(\omega))$ here stands for the partial derivative of F w.r.t. x, a $q \times q$ matrix. The norms used in Assumption 1 can be any norms in the \mathbb{R}^q or $\mathbb{R}^{q \times q}$ space, since all norms in a finite-dimensional space are equivalent to each other. A consequence of Assumption 1 is the continuous differentiability of f_0 on O. Moreover, for any nonempty compact subset X of O, let $C^1(X, \mathbb{R}^q)$ be the Banach space of continuously differentiable mappings $f: X \to \mathbb{R}^q$, equipped with the norm

$$||f||_{1,X} = \sup_{x \in X} ||f(x)|| + \sup_{x \in X} ||df(x)||.$$
(3.2)

Under Assumption 1, the sample average function f_n converges to f_0 almost surely as an element of $C^1(X, \mathbb{R}^q)$, see, e.g., [35, Theorems 7.44, 7.48 and 7.52] and [16, Theorem 3].

Assumption 2. Suppose that x_0 solves the variational inequality (1.1). Let $z_0 = x_0 - f_0(x_0)$, $L = df_0(x_0)$, $K = T_S(x_0) \cap \{z_0 - x_0\}^{\perp}$, and assume that the normal map L_K induced by L and K, defined as $L_K(h) = L(\Pi_K(h)) + h - \Pi_K(h)$ for each $h \in \mathbb{R}^q$, is a homeomorphism from \mathbb{R}^q to \mathbb{R}^q .

We assume in the above assumption that (1.1) has a solution x_0 . To guarantee the existence of such a solution, one would need to put additional conditions on f_0 and S. For example, if f_0 is strongly monotone on S then (1.1) must have a (globally unique) solution. Detailed discussions and more general solution existence conditions for variational inequalities can be found in [6, Chapter 2], [29, Chapter 12] and references therein. The set K defined in Assumption 2 is called the critical cone to S associated with z_0 . The homeomorphism condition on L_K guarantees that x_0 is a locally unique solution of (1.1), and that (1.1) continues to have a locally unique solution around x_0 under small perturbation of f_0 , see [16, Lemma 1] and the original result in [27]. Being the normal map induced by a linear map and a polyhedral convex cone, L_K is a piecewise linear function. It was shown in [26] that L_K is a homeomorphism if and only if it is coherently oriented (a piecewise linear function is coherently oriented if the determinants of matrices representing its selection functions all have the same nonzero sign), see also [23, 31] for shortened proofs. A special case in which the coherent orientation condition holds is when the restriction of L on the linear span of K is positive definite. In particular, if f_0 is strongly monotone on O, then the entire matrix L is positive definite and L_K is a global homeomorphism.

The normal map L_K is related to the normal map $(f_0)_S$ in (1.4) in the following way. Because f_0 is differentiable at x_0 and Π_S is B-differentiable, the normal map $(f_0)_S$ is B-differentiable at z_0 by the chain rule of B-differentiability, with

$$d(f_0)_S(z_0)(h) = df_0(x_0)(d\Pi_S(z_0)(h)) + h - d\Pi_S(z_0)(h).$$
(3.3)

It was shown in [27] that L_K is exactly $d(f_0)_S(z_0)$, the B-derivative of $(f_0)_S$ at z_0 .

The following theorem is adapted from [16, Theorem 7]. Here and hereafter, we use Σ_0 to denote the covariance matrix of $F(x_0,\xi)$. Equation (3.4) in the theorem looks similar to the equation in [11, Theorem 2.7] and [35, Equation (5.74)]. Those two references are about the asymptotic distribution of x_n , a solution to (1.3), while (3.4) here describes the asymptotic distribution of z_n , a solution to (1.6).

THEOREM 3.1. Suppose that Assumptions 1 and 2 hold. Let Y_0 be a normal random vector in \mathbb{R}^q with zero mean and covariance matrix Σ_0 . Then there exist neighborhoods X_0 of x_0 in O and Z of z_0 in \mathbb{R}^q such that the following hold. For almost every $\omega \in \Omega$, there exists an integer N_ω , such that for each $n \geq N_\omega$, the equation (1.6) has a unique solution z_n in Z, and the variational inequality (1.3) has a unique solution in X_0 given by $x_n = \Pi_S(z_n)$. Moreover, $\lim_{n\to\infty} z_n = z_0$ and $\lim_{n\to\infty} x_n = x_0$ almost surely,

$$\sqrt{n}(z_n - z_0) \Rightarrow (L_K)^{-1}(Y_0),$$
 (3.4)

and

$$\sqrt{n}L_K(z_n - z_0) \Rightarrow Y_0. \tag{3.5}$$

From (3.5), the random variable $n[L_K(z_n-z_0)]^T \Sigma_0^{-1}[L_K(z_n-z_0)]$ weakly converges to a χ^2 random variable with q degrees of freedom (assuming Σ_0 is nonsingular). This leads to an expression for confidence regions of z_0 . However, that expression includes the normal map L_K in it, which is unknown unless z_0 is known because both L and K depend on z_0 or z_0 . Therefore, to obtain a computable confidence region, one needs to substitute L_K by a function that depends only on z_n and z_n , without losing the limiting property.

Recall that L_K is exactly $d(f_0)_S(z_0)$, the B-derivative of the normal map $(f_0)_S$ at z_0 . A natural estimator of L_K is therefore $d(f_n)_S(z_n)$. However, from the discontinuity of B-derivatives of piecewise

affine functions discussed above Lemma 2.1 and given that Π_S is a piecewise affine function, the Bderivative $d\Pi_S(z_n)$ is not guaranteed to converge to $d\Pi_S(z_0)$ even though z_n converges to z_0 almost surely. From (3.3) it is clear that $d(f_n)_S(z_n)$ is not guaranteed to converge to L_K . To provide an alternative estimator of L_K , the papers [15] and [16] designed some functions to converge to L_K , by utilizing the exponential convergence rate of z_n to z_0 in probability obtained under additional assumptions.

The approach taken here is different from methods in [15, 16]. Instead of designing functions that converge to L_K , we directly use $d(f_n)_S(z_n)$ to replace L_K in (3.5), knowing that $d(f_n)_S(z_n)$ is not guaranteed to converge to L_K and may be very different with different z_n . The method is based on Theorem 3.3, which says that for large n the vector $d(f_n)_S(z_n)(z_0-z_n)$ is close to $-L_K(z_n-z_0)$ with high probability, and that using $d(f_n)_S(z_n)$ to replace L_K in (3.5) along with some sign changes keeps the weak convergence result to hold. As mentioned earlier, the proof of Theorem 3.3 relies on a "symmetry" property between the B-derivatives at two different points given in Theorem 2.2. From Theorems 3.3 we derive Theorems 4.1 and 4.2, to show that the set (4.2), or (4.6) for the singular case, is an asymptotically exact confidence region for z_0 : that is, the set contains z_0 with probability converging to the prescribed level of confidence.

Comparing to methods in [15, 16], the main advantage with the new method is given by Proposition 3.5, which states that $d(f_n)_S(z_n)$ is with high probability an invertible linear function. This implies that the set (4.2) is with high probability a single ellipsoid, when Σ_0 is nonsingular. When Σ_0 is singular one could use $R_{n,0}$ in (4.12) to approximate $R_{n,\epsilon}$ in (4.6), and $R_{n,0}$ is with high probability a degenerate ellipsoid. In contrast, when L_K is piecewise linear with multiple pieces, the estimators designed in [15, 16] have multiple pieces with high probability, providing confidence regions that are factions of ellipsoids pieced together. Clearly, it is much easier to describe a single ellipsoid, or to find the minimal enclosing box of a single ellipsoid to obtain simultaneous confidence intervals. Additionally, the new method does not rely on the assumptions for the exponential convergence rate of z_n , another advantage comparing to [15, 16].

Before proceeding to the proofs, recall that the Euclidean projector Π_S coincides with an affine function on each q-cell in the normal manifold of S. We use \mathfrak{P} to denote the normal manifold of S, which is the polyhedral subdivision of \mathbb{R}^q corresponding to Π_S . As in Section 2 we use $\mathfrak{P}(z_0)$ to denote the family of q-cells containing z_0 . Lemma 3.2 below will be used in the proof of Theorem 3.3.

LEMMA 3.2. Suppose that Assumptions 1 and 2 hold. Then for almost every $\omega \in \Omega$ there exists an integer N_{ω} such that the following equality holds for each $n \geq N_{\omega}$:

$$d\Pi_S(z_0)(z_n - z_0) + d\Pi_S(z_n)(z_0 - z_n) = 0.$$
(3.6)

Proof. Recall that z_0 belongs to the interior of $|\mathfrak{P}(z_0)|$. Since z_n converges to z_0 w.p. 1, for almost every $\omega \in \Omega$ there exists an integer N_{ω} such that z_n belongs to $|\mathfrak{P}(z_0)|$ for each $n \geq N_{\omega}$. It follows from Theorem 2.2 that each such z_n satisfies (3.6). \square

Theorem 3.3 below is the main result of this paper.

Theorem 3.3. Suppose that Assumptions 1 and 2 hold. Then for each $\epsilon > 0$ we have

$$\lim_{n \to \infty} \text{Prob}\{\sqrt{n} \| d(f_0)_S(z_0)(z_n - z_0) + d(f_n)_S(z_n)(z_0 - z_n) \| > \epsilon\} = 0.$$
 (3.7)

Consequently,

$$-\sqrt{n}d(f_n)_S(z_n)(z_0-z_n) \Rightarrow Y_0. \tag{3.8}$$

Proof. Recall from Assumption 2 and Theorem 3.1 that $x_0 = \Pi_S(z_0)$ and $x_n = \Pi_S(z_n)$ are solutions to (1.1) and (1.3) respectively. From (3.3) we have

$$d(f_0)_S(z_0)(z_n - z_0) = df_0(x_0)(d\Pi_S(z_0)(z_n - z_0)) + z_n - z_0 - d\Pi_S(z_0)(z_n - z_0).$$
(3.9)

Similarly,

$$d(f_n)_S(z_n)(z_0 - z_n) = df_n(x_n)(d\Pi_S(z_n)(z_0 - z_n)) + z_0 - z_n - d\Pi_S(z_n)(z_0 - z_n).$$
(3.10)

It follows that $\sqrt{n} \|df_0\|_S(z_0)(z_n - z_0) + d(f_n)_S(z_n)(z_0 - z_n)\|$ is bounded from above by the sum of the following two terms.

Term (a): $\sqrt{n} \| df_0(x_0) (d\Pi_S(z_0)(z_n - z_0)) + df_n(x_n) (d\Pi_S(z_n)(z_0 - z_n)) \|$.

Term (b): $\sqrt{n} \|d\Pi_S(z_0)(z_n - z_0) + d\Pi_S(z_n)(z_0 - z_n)\|.$

By Lemma 3.2, term (b) converges to 0 almost surely, so it converges to 0 in probability. It remains to show that Term (a) converges to 0 in probability. Term (a) is bounded from above by the sum of the following two terms.

Term (c): $\sqrt{n} \| df_0(x_0) (d\Pi_S(z_0)(z_n - z_0)) - df_n(x_n) (d\Pi_S(z_0)(z_n - z_0)) \|$.

Term (d): $\sqrt{n} \| df_n(x_n) (d\Pi_S(z_0)(z_n - z_0)) + df_n(x_n) (d\Pi_S(z_n)(z_0 - z_n)) \|$.

Because $df_n(x_n)(\cdot)$ is a linear map, by Lemma 3.2 term (d) converges to 0 almost surely and therefore converges to 0 in probability. To prove the theorem it suffices to show that term (c) converges to 0 in probability.

Term (c) is bounded from above by the following

$$||df_0(x_0) - df_n(x_n)|| ||\sqrt{n}(d\Pi_S(z_0)(z_n - z_0))||$$
(3.11)

where $||df_0(x_0) - df_n(x_n)||$ is the norm of the linear operator $df_0(x_0) - df_n(x_n)$, which is bounded from above by

$$||df_0(x_0) - df_0(x_n)|| + ||df_0(x_n) - df_n(x_n)||.$$

Since x_n converges to x_0 almost surely and f_0 is continuously differentiable under Assumption 1, $\|df_0(x_0) - df_0(x_n)\|$ converges to 0 almost surely. Assumption 1 also guarantees f_n to converge to f_0 almost surely as an element of $C^1(X, \mathbb{R}^q)$ for any compact subset X of O. Let X be a compact subset of O that contains x_0 in its interior; we have $x_n \in X$ for all sufficiently large n. It follows that $\|df_0(x_n) - df_n(x_n)\|$ converges to zero almost surely. This proves that $\|df_0(x_0) - df_n(x_n)\|$ converges to zero almost surely. On the other hand, since $d\Pi_S(z_0)$ is positively homogeneous, we can rewrite $\sqrt{n}(d\Pi_S(z_0)(z_n-z_0))$ as $d\Pi_S(z_0)(\sqrt{n}(z_n-z_0))$. By (3.4), $\sqrt{n}(z_n-z_0)$ converges in distribution to a random variable, so it is (uniformly) tight; see, e.g., [39, Theorem 2.4]. It follows that $d\Pi_S(z_0)(\sqrt{n}(z_n-z_0))$ is uniformly tight, and that the quantity (3.11) converges to 0 in probability. This proves that term (c) converges to 0 in probability, and thereby proves (3.7). Equation (3.8) is a result of (3.5) and (3.7). \square

Proposition 3.5 below shows the function $d(f_n)_S(z_n)$ that appears in (3.8) is a linear invertible function with high probability. Its proof uses the following lemma.

LEMMA 3.4. Under Assumptions 1 and 2, there exist a neighborhood Z' of z_0 in \mathbb{R}^q and a neighborhood \mathbb{L} of the matrix L in $\mathbb{R}^{q \times q}$, such that for each $z' \in Z'$ and $L' \in \mathbb{L}$ the map $\Upsilon(z', L') : \mathbb{R}^q \to \mathbb{R}^q$ defined as

$$\Upsilon(z', L')(h) = L' d\Pi_S(z')(h) + h - d\Pi_S(z')(h) \text{ for each } h \in \mathbb{R}^q$$
(3.12)

is a global homeomorphism from \mathbb{R}^q to \mathbb{R}^q .

Proof. First, note that for each $z' \in \mathbb{R}^q$ the B-derivative $d\Pi_S(z')$ is exactly the Euclidean projector onto the critical cone to S associated with z' [20, 25]. Hence, the map $\Upsilon(z', L')$ is exactly the normal map induced by L' and the latter critical cone. Recall that such a normal map is a global homeomorphism if and only if it is coherently oriented (see the discussion below Assumption 2). In the rest of this proof, we find neighborhoods Z' and L to guarantee $\Upsilon(z', L')$ to be coherently oriented for $z' \in Z'$ and $L' \in L$.

Since K is the critical cone to S associated with z_0 , we have $d\Pi_S(z_0) = \Pi_K$ and $\Upsilon(z_0, L) = L_K$. Because L_K is a global homeomorphism by assumption, it is coherently oriented. The fact that K is a polyhedral convex cone implies that L_K is a piecewise linear function. Let M_1, \dots, M_k be the matrices that represent the selection functions of L_K . Since L_K is coherently oriented, the determinants of M_1, \dots, M_k have the same nonzero sign (see the definition of the coherent orientation condition below Assumption 2). By choosing $\mathbb L$ to be a sufficiently small neighborhood of L, we can guarantee that the determinants of matrices representing selection functions of $\Upsilon(z_0, L')$ to have the same nonzero sign for each $L' \in \mathbb L$. This proves that $\Upsilon(z_0, L')$ is coherently oriented for each $L' \in \mathbb L$.

By Proposition 2.3, there exists a neighborhood Z' of z_0 such that $\mathfrak{P}(z') \subset \mathfrak{P}(z_0)$ for each $z' \in Z'$. As noted in the remark above Proposition 2.3, the family of the selection functions of $d\Pi_S(z_0)$ includes that of $d\Pi_S(z')$ for each $z' \in Z'$. Thus, for each $L' \in \mathbb{L}$ and $z' \in Z'$, any selection function of $\Upsilon(z', L')$ is also a selection function of $\Upsilon(z_0, L')$, and the coherent orientation of $\Upsilon(z', L')$ follows from the coherent orientation of $\Upsilon(z_0, L')$. \square

Proposition 3.5. Under Assumptions 1 and 2,

$$\lim_{n\to\infty} \operatorname{Prob}\{d(f_n)_S(z_n) \text{ is an invertible linear map}\} = 1.$$

Proof. By the chain rule,

$$d(f_n)_S(z_n)(h) = df_n(x_n)(d\Pi_S(z_n)(h)) + h - d\Pi_S(z_n)(h)$$
 for each $h \in \mathbb{R}^q$.

The linearity of $d(f_n)_S(z_n)$ depends on the linearity of $d\Pi_S(z_n)$. The latter function is linear whenever z_n belongs to the interior of an q-cell in the normal manifold of S. Let R be the union of boundaries of all the q-cells; it follows that R is the union of finitely many polyhedral convex sets of dimensions less than q. Consider the tangent cone $T_R(z_0)$, which is defined in the same way as $T_S(x)$ in (3.1) if $z_0 \in R$ and is the empty set if $z_0 \notin R$. Let Z_0 be a neighborhood of z_0 such that $Z_0 \cap R = Z_0 \cap (z_0 + T_R(z_0))$; we have

$$\sqrt{n}(z-z_0) \in T_R(z_0)$$
 for each $z \in Z_0 \cap R$ and each integer n . (3.13)

The fact that z_n converges to z_0 almost surely implies

$$\lim_{n\to\infty}\operatorname{Prob}\{z_n\not\in Z_0\}=0.$$

On the other hand, (3.13) implies

$$\text{Prob}\{z_n \in Z_0 \cap R\} < \text{Prob}\{\sqrt{n}(z_n - z_0) \in T_R(z_0)\}.$$

It follows from (3.4) and the fact that L_K is a piecewise linear homeomorphism that

$$\lim_{n \to \infty} \text{Prob}\{\sqrt{n}(z_n - z_0) \in T_R(z_0)\} \le \text{Prob}\{(L_K)^{-1}(Y_0) \in T_R(z_0)\} = 0.$$

Because $\text{Prob}\{z_n \in R\} \leq \text{Prob}\{z_n \notin Z_0\} + \text{Prob}\{z_n \in Z_0 \cap R\}$, we have proved

$$\lim_{n \to \infty} \text{Prob}\{z_n \in R\} = 0,\tag{3.14}$$

which implies that the probability for $d(f_n)_S(z_n)$ to be a linear function converges to 1 as n goes to ∞ .

Next, choose neighborhoods Z' of z_0 and $\mathbb L$ of L as in Lemma 3.4. Since z_n converges to z_0 almost surely, z_n belongs to Z' almost surely for sufficiently large n. It was shown in the proof of Theorem 3.3 that $df_n(x_n)$ almost surely converges to $df_0(x_0)$. Consequently, $df_n(x_n)$ belongs to $\mathbb L$ almost surely for sufficiently large n. By Lemma 3.4, $d(f_n)_S(z_n)$ is a global homeomorphism almost surely for sufficiently large n, so the probability for $d(f_n)_S(z_n)$ to be an invertible function converges to 1 as n goes to ∞ . The conclusion of the proposition follows by combining the linearity and invertibility. \square

The random variable Y_0 in (3.8) has covariance matrix Σ_0 , which depends on the true solution x_0 . In computing confidence regions and intervals we will replace Σ_0 by Σ_n , the sample covariance matrix of $\{F(x_n, \xi^i)\}_{i=1}^n$. The lemma below supports such a replacement.

LEMMA 3.6. Suppose that Assumptions 1 and 2 hold. The matrix Σ_n converges to Σ_0 almost surely as $n \to \infty$.

Proof. Under the assumptions, $\frac{1}{n}\sum_{i=1}^{n}F(x,\xi^{i}(\omega))F(x,\xi^{i}(\omega))^{T}$ converges to $E[F(x,\xi)F(x,\xi)^{T}]$ almost surely uniformly on each compact subset X of O (see, e.g., [35, Theorem 7.48]). Since x_{n} converges to x_{0} almost surely, we have

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^n F(x_n, \xi^i(\omega)) F(x_n, \xi^i(\omega))^T = E[F(x_0, \xi) F(x_0, \xi)^T] \text{ almost surely.}$$

Similarly $f_n(x_n)$ converges to $f_0(x_0)$ almost surely as $n \to \infty$. This proves the lemma. \square

4. Confidence regions and simultaneous confidence intervals. This section provides formulas for confidence regions of z_0 that are computable from z_n , and provides a method to compute simultaneous confidence intervals for components of z_0 . We treat two cases separately: Theorem 4.1 considers situations in which Σ_0 (the covariance matrix of $F(x_0, \xi)$) is nonsingular, and Theorem 4.2 handles situations in which Σ_0 is singular. The confidence region is given in (4.2) or (4.6) for the two cases respectively. We use χ_l^2 to denote a χ^2 random variable with l degrees of freedom, and use $\chi_l^2(\alpha)$ to denote the number that satisfies $P(\chi_l^2 > \chi_l^2(\alpha)) = \alpha$ for $\alpha \in [0,1]$. For the rest of this section, let $\alpha \in [0,1]$ be fixed.

THEOREM 4.1. Suppose that Assumptions 1 and 2 hold, and that Σ_0 is nonsingular. For almost every $\omega \in \Omega$, there exists an integer N_{ω} such that Σ_n is nonsingular for $n \geq N_{\omega}$. Moreover,

$$-\sqrt{n}\sum_{n}^{-1/2}[d(f_n)_S(z_n)(z_0-z_n)] \Rightarrow \mathcal{N}(0,I_q), \tag{4.1}$$

and the probability for z_0 to belong to the set

$$\left\{ z \in \mathbb{R}^q \left| n \left[d(f_n)_S(z_n)(z - z_n) \right]^T \Sigma_n^{-1} \left[d(f_n)_S(z_n)(z - z_n) \right] \le \chi_q^2(\alpha) \right\}$$

$$(4.2)$$

converges to $1 - \alpha$ as $n \to \infty$.

Proof. Since Σ_n converges to Σ_0 almost surely (Lemma 3.6), it is nonsingular for sufficiently large n almost surely. Equation (4.1) follows from (3.8). From (4.1) the random variable

$$n[d(f_n)_S(z_n)(z_0-z_n)]^T \Sigma_n^{-1}[d(f_n)_S(z_n)(z_0-z_n)]$$

weakly converges to a χ_q^2 random variable, so the set (4.2) contains z_0 with probability converging to $1 - \alpha$. \square

THEOREM 4.2. Suppose that Assumptions 1 and 2 hold, and that Σ_0 is singular. Let $\rho > 0$ be the minimum of all positive eigenvalues of Σ_0 , and let l be the number of positive eigenvalues of Σ_0 counted with regard to their algebraic multiplicities. Let ρ_0 satisfy $0 < \rho_0 < \rho$. Decompose Σ_n as

$$\Sigma_n = U_n^T \Delta_n U_n \tag{4.3}$$

where U_n is an orthogonal $q \times q$ matrix, and Δ_n is a diagonal matrix with monotonically decreasing elements. Let D_n be the upper-left submatrix of Δ_n whose diagonal elements are at least ρ_0 . Let l_n be the number of rows in D_n , $(U_n)_1$ be the submatrix of U_n that consists of its first l_n rows, and $(U_n)_2$ be the submatrix that consists of the remaining rows of U_n . Then for almost every ω the equality $l_n = l$ holds for sufficiently large n. Moreover,

$$n[d(f_n)_S(z_n)(z_0 - z_n)]^T (U_n)_1^T D_n^{-1}(U_n)_1 [d(f_n)_S(z_n)(z_0 - z_n)] \Rightarrow \chi_l^2$$
(4.4)

and

$$n[d(f_n)_S(z_n)(z_0 - z_n)]^T (U_n)_2^T (U_n)_2 [d(f_n)_S(z_n)(z_0 - z_n)] \Rightarrow 0.$$
(4.5)

For each $\epsilon > 0$, the set

$$R_{n,\epsilon} = \left\{ z \in \mathbb{R}^q \middle| \begin{array}{l} n \left[d(f_n)_S(z_n)(z - z_n) \right]^T (U_n)_1^T D_n^{-1}(U_n)_1 \left[d(f_n)_S(z_n)(z - z_n) \right] \le \chi_{l_n}^2(\alpha) \\ \|\sqrt{n}(U_n)_2 [d(f_n)_S(z_n)(z - z_n)] \|_{\infty} \le \epsilon \end{array} \right\}$$
(4.6)

contains z_0 with probability converging to $1-\alpha$.

Proof. Let ρ and l be as defined in this theorem, and conduct an eigen-decomposition of Σ_0 as

$$\Sigma_0 = U_0^T \begin{bmatrix} D_0 & 0 \\ 0 & 0 \end{bmatrix} U_0 = \begin{bmatrix} (U_0)_1^T & (U_0)_2^T \end{bmatrix} \begin{bmatrix} D_0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} (U_0)_1 \\ (U_0)_2 \end{bmatrix}$$
(4.7)

where U_0 is orthogonal, D_0 is diagonal with monotonically decreasing positive diagonal elements, and $(U_0)_1$ and $(U_0)_2$ contains the first l and the last q-l rows of U_0 respectively. From (3.8) we have

$$-\sqrt{n} \begin{bmatrix} D_0^{-1/2} & 0\\ 0 & I_{q-l} \end{bmatrix} U_0[d(f_n)_S(z_n)(z_0 - z_n)] \Rightarrow \mathcal{N}(0, I_l) \times 0.$$
 (4.8)

From Lemma 3.6, for a.e. $\omega \in \Omega$ there exists an integer N_{ω}^1 , such that each $n \geq N_{\omega}^1$ satisfies

$$(\Delta_n)_{ii} > \rho_0$$
 for each $i = 1, \dots, l$ and $(\Delta_n)_{ii} < \rho_0$ for each $i = l + 1, \dots, q$. (4.9)

It follows that that $l_n = l$ for $n \geq N_{\omega}^1$ and that D_n converges to D_0 almost surely. For $n \geq N_{\omega}^1$, define

$$\hat{\Sigma}_n = U_n^T \begin{bmatrix} D_n & 0 \\ 0 & 0 \end{bmatrix} U_n \text{ and } \hat{\Sigma}_n^+ = U_n^T \begin{bmatrix} D_n^{-1} & 0 \\ 0 & 0 \end{bmatrix} U_n = (U_n)_1^T D_n^{-1} (U_n)_1.$$

Because of (4.9), $\hat{\Sigma}_n$ is the unique best approximation of Σ_n in Frobenius norm among all matrices of rank $\leq l$; see, e.g., [1, 7, 38]. Since the unique best approximation of a matrix depends continuously on that matrix (by an application of [29, Theorem 1.17]), and the best approximation of Σ_0 is itself, $\hat{\Sigma}_n$ almost surely converges to Σ_0 . As the pseudo-inverse of $\hat{\Sigma}_n$, $\hat{\Sigma}_n^+$ almost surely converges to the pseudo-inverse of Σ_0 (by an application of [37, Corollary 3.5]). This and (4.8) imply (4.4).

Finally, an application of [14, Theorem 3.1] implies that the angle between the row spaces of $(U_0)_2$ and $(U_n)_2$ almost surely converges to zero as $n \to \infty$. In view of [14, Equation (2.4)] and [8, Theorem 2.6.1], the matrix $(U_n)_2^T(U_n)_2$ converges to $(U_0)_2^T(U_0)_2$ almost surely. This and (4.8) imply (4.5).

Note that the choice of the matrix U_n in the decomposition of Σ_n is non-unique, when Σ_n has repeated eigenvalues. However, when (4.9) holds the matrices $(U_n)_1^T D_n^{-1}(U_n)_1$ and $(U_n)_2^T (U_n)_2$ that appear in (4.4) and (4.5) are uniquely determined by Σ_n , and depend continuously on Σ_n .

Since $l_n = l$ almost surely for sufficiently large n, from (4.4) we have

$$\lim_{n \to \infty} \text{Prob}\left\{n\left[d(f_n)_S(z_n)(z_0 - z_n)\right]^T (U_n)_1^T D_n^{-1}(U_n)_1 \left[d(f_n)_S(z_n)(z_0 - z_n)\right] \le \chi_{l_n}^2(\alpha)\right\} = 1 - \alpha. \quad (4.10)$$

By (4.5) we have

$$\lim_{n \to \infty} \text{Prob}\left\{ n[d(f_n)_S(z_n)(z_0 - z_n)]^T (U_n)_2^T (U_n)_2 [d(f_n)_S(z_n)(z_0 - z_n)] \le \epsilon \right\} = 1$$

for each $\epsilon > 0$. Since all norms are equivalent in a finite-dimensional space, we can rewrite the above equality as

$$\lim_{n \to \infty} \text{Prob}\left\{ \sqrt{n} \| (U_n)_2 [d(f_n)_S(z_n)(z_0 - z_n)] \|_{\infty} \le \epsilon \right\} = 1, \tag{4.11}$$

where $\|\cdot\|_{\infty}$ denotes the ∞ -norm. In writing (4.11), we assume that U_n is a measurable function of Σ_n so that the set in consideration is a measurable set in Ω . Equations (4.10) and (4.11) imply that the set $R_{n,\epsilon}$ contains z_0 with probability converging to $1-\alpha$. \square

Since for each $\epsilon > 0$ the set $R_{n,\epsilon}$ is an asymptotically exact $(1 - \alpha)100\%$ confidence region for z_0 , it is natural to ask whether the same is true about the set

$$R_{n,0} = \left\{ z \in \mathbb{R}^q \middle| \begin{array}{l} n \left[d(f_n)_S(z_n)(z - z_n) \right]^T (U_n)_1^T D_n^{-1}(U_n)_1 \left[d(f_n)_S(z_n)(z - z_n) \right] \le \chi_{l_n}^2(\alpha) \\ \sqrt{n}(U_n)_2 \left[d(f_n)_S(z_n)(z - z_n) \right] = 0 \end{array} \right\}. \quad (4.12)$$

We cannot prove that $R_{n,0}$ contains z_0 with probability converging to $1-\alpha$, because the quantity

$$\lim_{n\to\infty} \operatorname{Prob}\left\{\sqrt{n}(U_n)_2[d(f_n)_S(z_n)(z_0-z_n)]=0\right\}$$

may not equal 1. However, Proposition 4.3 below shows for a fixed n that the set-valued map $R_{n,\epsilon}$ is Lipschitz continuous on an interval $[0,\bar{\epsilon}]$ for some positive real number $\bar{\epsilon}$. Accordingly, any open set that contains $R_{n,0}$ must include $R_{n,\epsilon}$ for a sufficiently small ϵ . Since $R_{n,0}$ has a simpler geometric structure comparing to $R_{n,\epsilon}$, one may choose to use $R_{n,0}$ to approximate $R_{n,\epsilon}$ for computational efficiency.

PROPOSITION 4.3. Let $d(f_n)_S(z_n)$ be a fixed invertible linear function, U_n a fixed orthogonal matrix, and D_n a fixed $l_n \times l_n$ diagonal matrix with positive diagonal elements. There exist real numbers $\bar{\epsilon} > 0$ and $\sigma > 0$ such that

$$R_{n,\epsilon'} \subset R_{n,\epsilon} + \sigma |\epsilon - \epsilon'| \mathbb{B}$$

whenever $0 \le \epsilon \le \bar{\epsilon}$ and $0 \le \epsilon' \le \bar{\epsilon}$, where \mathbb{B} denotes the closed unit ball in \mathbb{R}^q .

Proof. After the coordinate transformation $U_n d(f_n)_S(z_n)$, one can view $R_{n,\epsilon}$ as a cartesian product of a fixed ellipsoid in \mathbb{R}^{l_n} and a polyhedron in \mathbb{R}^{q-l_n} , with ϵ being the right hand side of the linear constraints defining the polyhedron. The Lipschitz continuity can be seen in the transformed space. \square

It is shown in Proposition 3.5 that $d(f_n)_S(z_n)$ is an invertible linear function with high probability. When this holds, the set in (4.2) and $R_{n,0}$ in (4.12) are ellipsoids in \mathbb{R}^q , and therefore can be described using their centers, principal directions, and semi-axes. It is often desirable to provide simultaneous confidence intervals for components of z_0 , as intervals are more convenient to describe, visualize, and interpret. We can compute these intervals by finding the minimum enclosing box of a confidence region, i.e., by computing the maximal and minimal values of z_i for each $i = 1, \dots, q$ over the confidence region.

Since Σ_0 is unknown in practice, it is often difficult to directly check if Σ_0 is nonsingular or not. Instead, we conduct an eigen-decomposition of the sample covariance matrix Σ_n as in (4.3), and partition matrices U_n and Δ_n based on positive or zero eigenvalues. If all eigenvalues are strictly positive (larger than a prescribed tolerance), then we use (4.2) as the confidence region. Otherwise, we use $R_{n,\epsilon}$ in (4.6) for some positive ϵ or $R_{n,0}$ as the confidence region. In the latter case, the confidence region is still bounded because $d(f_n)_S(z_n)$ is invertible, and is flat in the directions represented by rows of $(U_n)_2[d(f_n)_S(z_n)]$. In particular, the set $R_{n,0}$ is a degenerate ellipsoid. One can still find the minimal enclosing box of the confidence region to obtain the simultaneous confidence intervals. Numerical tests with singular covariance matrices are conducted in [12]. Lastly, we mention that the only requirement on Σ_n for Theorems 4.1 and 4.2 to hold is its almost sure convergence to Σ_0 . Hence, any estimator of Σ_0 that converges to it almost surely can be used as Σ_n , not necessarily the sample covariance matrix.

5. Individual confidence intervals. This section discusses computation of individual confidence intervals for z_0 . An individual confidence interval for the jth component of z_0 is an interval in \mathbb{R} that contains $(z_0)_j$ with a prescribed level of confidence. It is generally narrower than the simultaneous confidence interval for the same level. The difference between widths of the two intervals are substantial in problems with moderate or large dimensions. In such problems, the minimum enclosing box of a confidence region can be much larger than the region itself, resulting in simultaneous confidence intervals too wide to be useful. The sizes of individual confidence intervals are less affected by the dimension of the problem. There are also problems where only confidence intervals of selected components in the true solution are of interest.

Computation of individual confidence intervals requires knowledge on the distribution of each individual component of z_n . As shown in (3.4), $\sqrt{n}(z_n - z_0)$ weakly converges to the distribution of a random variable $\Gamma = (L_K)^{-1}(Y_0)$. Given results in the preceding two sections, it is natural to ask whether we can substitute $L_K = d(f_0)_S(z_0)$ with $d(f_n)_S(z_n)$ in computing individual confidence intervals for z_0 . Such a direct substitution results in a confidence interval in (5.17), where r_{nj} is defined in (5.3). The equation (5.4) expresses the limiting probability for such an interval to contain $(z_0)_j$ in terms of Γ . That limiting probability equals the desired confidence level $1 - \alpha$ when the condition in (5.5) holds.

Let $\mathfrak{P}(z_0) = \{P_1, \dots, P_k\}$ be the set of q-cells in the normal manifold of S that contains z_0 . For each $i = 1, \dots, k$, let $K_i = \operatorname{cone}(P_i - z_0)$, A_i be the matrix representing $d\Pi_S(z)$ for points z in the interior of P_i , and $T_i = d(f_0)_S(z_0)(K_i)$ be the image of K_i under the function $d(f_0)_S(z_0)$. From (3.3) we can see that $d(f_0)_S(z_0)$ coincides with $dL_S(z_0)$, where L_S is the normal map induced by the linear operator L and the set S. On the cone K_i , the map $d(f_0)_S(z_0)$ is represented by the matrix

$$M_i = LA_i + I - A_i.$$

Under Assumption 2 the map $d(f_0)_S(z_0)$ is a global homeomorphism, so all the matrices M_i , $i=1,\dots,k$ are nonsingular.

As above let $\Gamma = (L_K)^{-1}(Y_0)$, and for each $i = 1, \dots, k$ define a random variable $\Gamma^i = M_i^{-1}(Y_0)$. The fact that Y_0 is a multivariant normal random variable implies that each Γ^i is a multivariant normal random variable with covariance matrix $M_i^{-1}\Sigma_0M_i^{-T}$. Accordingly, each component of Γ^i is a normal random variable. If we define a number

$$r_j^i = \sqrt{(M_i^{-1} \Sigma_0 M_i^{-T})_{jj}}$$

for each $i=1,\cdots,k$ and $j=1,\cdots,q$, then for each real number $\alpha\in(0,1)$ we have

$$\operatorname{Prob}\left(|\Gamma_j^i| \le \sqrt{\chi_1^2(\alpha)} r_j^i\right) = 1 - \alpha. \tag{5.1}$$

Let us discuss a relation between Γ and Γ^i . Since $d(f_0)_S(z_0)$ is represented by the matrix M_i on the cone K_i , we have

$$d(f_0)_S(z_0)^{-1}(y) = M_i^{-1}(y)$$
 if $y \in T_i$.

For each measurable set $W \subset K_i$ we have

$$\operatorname{Prob}(\Gamma \in W) = \operatorname{Prob}(Y_0 \in M_i(W)) = \operatorname{Prob}(\Gamma^i \in W). \tag{5.2}$$

THEOREM 5.1. Suppose that Assumptions 1 and 2 hold, and suppose that Σ_0 has a positive determinant. Let $P_i, K_i, T_i, A_i, M_i, \Gamma^i, \Gamma, r^i_j$ be defined as above. For each integer n and each $j = 1, \dots, q$, define a number

$$r_{nj} = \begin{cases} \sqrt{(d(f_n)_S(z_n)^{-1}\Sigma_n d(f_n)_S(z_n)^{-T})_{jj}} & \text{if } d(f_n)_S(z_n) \text{ is an invertible linear map,} \\ 0 & \text{otherwise.} \end{cases}$$
(5.3)

Then for each real number $\alpha \in (0,1)$ and for each $j = 1, \dots, q$,

$$\lim_{n \to \infty} \operatorname{Prob}\left(\frac{\sqrt{n}|(z_n - z_0)_j|}{r_{nj}} \le \sqrt{\chi_1^2(\alpha)}\right) \\ = \sum_{i=1}^k \operatorname{Prob}\left(\left|\frac{\Gamma_j^i}{r_j^i}\right| \le \sqrt{\chi_1^2(\alpha)} \text{ and } \Gamma^i \in K_i\right) = \sum_{i=1}^k \operatorname{Prob}\left(\left|\frac{\Gamma_j}{r_j^i}\right| \le \sqrt{\chi_1^2(\alpha)} \text{ and } \Gamma \in K_i\right).$$

$$(5.4)$$

Moreover, suppose for a given $j = 1, \dots, q$ that the following equality

$$\operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)} \ and \ \Gamma^{i} \in K_{i}\right) = \operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)}\right) \operatorname{Prob}(\Gamma^{i} \in K_{i})$$

$$(5.5)$$

holds for each $i = 1, \dots, k$. Then for each real number $\alpha \in (0, 1)$,

$$\lim_{n \to \infty} \operatorname{Prob} \left\{ |(z_n - z_0)_j| \le \frac{\sqrt{\chi_1^2(\alpha)} r_{nj}}{\sqrt{n}} \right\} = 1 - \alpha.$$
 (5.6)

Proof. Let $\alpha \in (0,1)$ be fixed. Recall from Lemma 3.6 that Σ_n converges to Σ_0 almost surely, and from the proof of Theorem 3.3 that $df_n(x_n)$ converges to $L = df_0(x_0)$ almost surely. Let Z' be a neighborhood of z_0 in the interior of $|\mathfrak{P}(z_0)|$ with $Z' \cap P_i = Z' \cap (z_0 + K_i)$ for each $i = 1, \dots, k$. We have

$$\lim_{n \to \infty} \operatorname{Prob}(z_n \in Z') = 1. \tag{5.7}$$

Writing Z' as the following union,

$$Z' = \bigcup_{i=1}^{k} (Z' \cap (z_0 + \operatorname{int} K_i)) \cup (Z' \cap (z_0 + \mathbb{R}^q / \bigcup_{i=1}^k \operatorname{int} K_i)),$$

and noting from (3.14) in the proof of Proposition 3.5 that

$$\lim_{n \to \infty} \operatorname{Prob}(z_n \in Z' \cap (z_0 + \mathbb{R}^q / \cup_{i=1}^k \operatorname{int} K_i)) = 0,$$

we find

$$\lim_{n \to \infty} \sum_{i=1}^{k} \operatorname{Prob}(z_n \in Z' \cap (z_0 + \operatorname{int} K_i)) = 1.$$
(5.8)

It is not hard to see $Z' \cap (z_0 + \operatorname{int} K_i) = Z' \cap \operatorname{int} P_i$ for each $i = 1, \dots, k$. When $z_n \in Z' \cap \operatorname{int} P_i$, $d(f_n)_S(z_n)$ is a linear map given by

$$d(f_n)_S(z_n) = df_n(x_n)A_i + I - A_i.$$

For each integer $n, j = 1, \dots, q$ and $i = 1, \dots, k$, define a quantity

$$\hat{r}_{nj}^i = r_{nj} 1_{z_n \in Z' \cap \text{int } P_i} + r_j^i 1_{z_n \notin Z' \cap \text{int } P_i}. \tag{5.9}$$

By Proposition 3.5, and from the fact that $df_n(x_n)$ and Σ_n converge to $df_0(x_0)$ and Σ_0 almost surely respectively, \hat{r}_{nj}^i converges to r_j^i in probability as $n \to \infty$.

Now, let us first consider the situations in which $k \geq 2$. These are the situations in which z_0 lies on the boundary of some q-cell. For each $i = 1, \dots, k$ and $j = 1, \dots, q$, choose an q-dimensional vector \bar{h}^{ij} such that \bar{h}^{ij} does not belong to K_i and its jth component \bar{h}^{ij}_j satisfies $|\bar{h}^{ij}_j| > r^i_j \sqrt{\chi^2_1(\alpha)}$. Define a random variable $h^{ij}_n \in \mathbb{R}^q$ by

$$h_n^{ij} = \sqrt{n}(z_n - z_0) 1_{z_n \in Z' \cap \text{int } P_i} + \bar{h}^{ij} 1_{z_n \notin Z' \cap \text{int } P_i}, \tag{5.10}$$

and define another q-dimensional random variable $\hat{\Gamma}^{ij}$ by

$$\hat{\Gamma}^{ij} = \Gamma^i 1_{\Gamma^i \in \text{int } K_i} + \bar{h}^{ij} 1_{\Gamma^i \notin \text{int } K_i}. \tag{5.11}$$

Let W be a measurable subset of int K_i with $\text{Prob}(\Gamma \in \partial W) = 0$, where ∂W stands for the boundary of W. The above definition of h_n^{ij} and the fact that \bar{h}^{ij} does not belong to K_i imply

$$\operatorname{Prob}(h_n^{ij} \in W) = \operatorname{Prob}(\sqrt{n}(z_n - z_0) \in W \text{ and } z_n \in Z' \cap \operatorname{int} P_i).$$

Recalling that $Z' \cap \operatorname{int} P_i = Z' \cap (z_0 + \operatorname{int} K_i)$ for each $i = 1, \dots, k$, we find

$$\operatorname{Prob}(\sqrt{n}(z_n-z_0)\in W \text{ and } z_n\in Z'\cap\operatorname{int} P_i)=\operatorname{Prob}(\sqrt{n}(z_n-z_0)\in W \text{ and } z_n\in Z').$$

Combining the above two equalities with (5.7), we have

$$\lim_{n \to \infty} \operatorname{Prob}(h_n^{ij} \in W) = \lim_{n \to \infty} \operatorname{Prob}(\sqrt{n}(z_n - z_0) \in W).$$

By the asymptotic distribution (3.4), the definition of Γ and equation (5.2), we have

$$\lim_{n \to \infty} \operatorname{Prob}(\sqrt{n}(z_n - z_0) \in W) = \operatorname{Prob}(\Gamma \in W) = \operatorname{Prob}(\Gamma^i \in W).$$

From the definition of $\hat{\Gamma}^{ij}$ in (5.11) and the facts $W \subset \operatorname{int} K_i$ and $\bar{h}^{ij} \notin K_i$ we have

$$\operatorname{Prob}(\Gamma^i \in W) = \operatorname{Prob}(\hat{\Gamma}^{ij} \in W).$$

Combining the above three equalities together, we find

$$\lim_{n \to \infty} \operatorname{Prob}(h_n^{ij} \in W) = \operatorname{Prob}(\hat{\Gamma}^{ij} \in W)$$

for each measurable set $W \subset \operatorname{int} K_i$ with $\operatorname{Prob}(\Gamma \in \partial W) = 0$. Because the set $\operatorname{int} K_i$ itself satisfies $\operatorname{Prob}(\Gamma \in \partial(\operatorname{int} K_i)) = 0$, the above equality holds with $\operatorname{int} K_i$ in place of W. Since h_n^{ij} and $\hat{\Gamma}^{ij}$ only take values in $\operatorname{int} K_i \cup \{\bar{h}^{ij}\}$, we have $\lim_{n \to \infty} \operatorname{Prob}(h_n^{ij} = \bar{h}^{ij}) = \operatorname{Prob}(\hat{\Gamma}^{ij} = \bar{h}^{ij})$. Also, for each $W \subset \operatorname{int} K_i$ we have $\operatorname{Prob}(\Gamma \in \partial W) = \operatorname{Prob}(\hat{\Gamma}^{ij} \in \partial W)$. It is not hard to see

$$h_n^{ij} \Rightarrow \hat{\Gamma}^{ij}$$
.

Since \hat{r}_{nj}^i converges in probability to the fixed number r_j^i , which is strictly positive under the assumption in this theorem about Σ_0 , we have

$$\frac{(h_n^{ij})_j}{\hat{r}_{nj}^i} \Rightarrow \frac{\hat{\Gamma}_j^{ij}}{r_j^i},$$

where $(h_n^{ij})_j$ and $\hat{\Gamma}_j^{ij}$ are the jth components of (h_n^{ij}) and $\hat{\Gamma}_j^{ij}$ respectively. It follows that

$$\lim_{n \to \infty} \operatorname{Prob}\left(\left|\frac{(h_n^{ij})_j}{\hat{r}_{nj}^i}\right| \le \sqrt{\chi_1^2(\alpha)}\right) = \operatorname{Prob}\left(\left|\frac{\hat{\Gamma}_j^{ij}}{r_j^i}\right| \le \sqrt{\chi_1^2(\alpha)}\right),\tag{5.12}$$

because the probability for $\frac{\hat{\Gamma}_{j}^{ij}}{r_{j}^{i}}$ to lie on the boundary of $[-\sqrt{\chi_{1}^{2}(\alpha)}, \sqrt{\chi_{1}^{2}(\alpha)}]$ is zero. The way $\hat{\Gamma}^{ij}$ is defined in (5.11) and the fact that $|\bar{h}_{i}^{ij}| > r_{i}^{i}\sqrt{\chi_{1}^{2}(\alpha)}$ imply

$$\operatorname{Prob}\left(\left|\frac{\hat{\Gamma}_{j}^{ij}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)}\right) = \operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)} \text{ and } \Gamma^{i} \in \operatorname{int} K_{i}\right). \tag{5.13}$$

The facts that $|\bar{h}_{j}^{ij}| > r_{j}^{i} \sqrt{\chi_{1}^{2}(\alpha)}$ and that \hat{r}_{nj}^{i} almost surely converges to r_{j}^{i} imply

$$\lim_{n\to\infty}\operatorname{Prob}\left(\big|\frac{\bar{h}_j^{ij}}{\hat{r}_{nj}^{i}}\big|\leq\sqrt{\chi_1^2(\alpha)}\right)=0.$$

We are now ready to put all pieces together to prove (5.4) for the case $k \geq 2$. By the definition of h_n^{ij} in (5.10) and the above equality, we have

$$\lim_{n \to \infty} \operatorname{Prob}\left(\left|\frac{(h_n^{ij})_j}{\hat{r}_{nj}^i}\right| \le \sqrt{\chi_1^2(\alpha)}\right)$$

$$= \lim_{n \to \infty} \operatorname{Prob}\left(\frac{\sqrt{n}|(z_n - z_0)_j|}{\hat{r}_{nj}^i} \le \sqrt{\chi_1^2(\alpha)} \text{ and } z_n \in Z' \cap \operatorname{int} P_i\right).$$
(5.14)

By the definition of \hat{r}_{nj}^i in (5.9), we can replace it by r_{nj} in the right hand side of (5.14). Combining (5.12), (5.13) and (5.14) together, we have

$$\lim_{n \to \infty} \operatorname{Prob}\left(\frac{\sqrt{n}|(z_n - z_0)_j|}{r_{nj}} \le \sqrt{\chi_1^2(\alpha)} \text{ and } z_n \in Z' \cap \operatorname{int} P_i\right)$$

$$= \operatorname{Prob}\left(\left|\frac{\Gamma_j^i}{r_j^i}\right| \le \sqrt{\chi_1^2(\alpha)} \text{ and } \Gamma^i \in \operatorname{int} K_i\right)$$

$$= \operatorname{Prob}\left(\left|\frac{\Gamma_j^i}{r_j^i}\right| \le \sqrt{\chi_1^2(\alpha)} \text{ and } \Gamma^i \in K_i\right)$$
(5.15)

where the second equality follows from the fact that the probability for Γ^i to belong to the boundary of K_i is 0. Recalling that $Z' \cap (z_0 + \text{int } K_i) = Z' \cap \text{int } P_i$, we can combine the above equality with (5.8) to prove (5.4).

Under the assumption (5.5), we have

$$\sum_{i=1}^{k} \operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)} \text{ and } \Gamma^{i} \in K_{i}\right)$$

$$= \sum_{i=1}^{k} \operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)}\right) \operatorname{Prob}\left(\Gamma^{i} \in K_{i}\right)$$

$$= \sum_{i=1}^{k} \operatorname{Prob}\left(\left|\frac{\Gamma_{j}^{i}}{r_{j}^{i}}\right| \leq \sqrt{\chi_{1}^{2}(\alpha)}\right) \operatorname{Prob}\left(\Gamma \in K_{i}\right) = 1 - \alpha,$$
(5.16)

where the third equality uses (5.2) and the fourth equality uses (5.1) and the fact that $\sum_{i=1}^{k} \text{Prob} (\Gamma \in K_i) = 1$. This proves (5.6) for the case $k \geq 2$.

The case k=1 is much simpler. In this case, z_0 lies in the interior of a single q-cell P_1 , $K_1 = \mathbb{R}^q$, $d(f_0)_S(z_0)$ is an invertible linear map, and Γ is equal to Γ^1 . Since z_n belongs to the interior of P_1 for

all sufficiently large n, the number r_{nj} converges almost surely to r_j^1 for each $j=1,\dots,q$. Equation (5.4) follows from the fact that

$$\frac{\sqrt{n}(z_n - z_0)_j}{r_{nj}} \Rightarrow \frac{\Gamma_j^1}{r_j^1},$$

and equation (5.6) follows from the equality (5.1) with i = 1. \square

Below, we discuss two situations in which the equality (5.5) holds.

The first situation is when $k \leq 2$. Obviously, when k = 1 (that is, when z_0 lies in the interior of an q-cell in the normal manifold of S), the cone K_1 is the entire space \mathbb{R}^q , and the assumption (5.5) automatically holds. It was noted by Michael Lamm that (5.5) also holds when k = 2. In the latter case, the cone K_i is a half-space for i = 1, 2. Since Γ^i is a multivariant normal random variable with mean zero, $-\Gamma^i$ and Γ^i have the same distribution. It follows that $\operatorname{Prob}\left(\left|\frac{\Gamma^i}{r^i_j}\right| \leq \sqrt{\chi_1^2(\alpha)}\right)$ and $\Gamma^i \in K_i$ are both equal to $\Gamma^i \cap \Gamma^i \cap$

The second situation is when S is a box and each Γ^i has a diagonal covariance matrix. In this case, each K_i is of the form $\{h \in \mathbb{R}^q \mid h_i \geq 0 \text{ for each } i \in I_+, h_i \leq 0 \text{ for each } i \in I_-\}$ for some disjoint subsets I_+ and I_- of $\{1, \dots, q\}$. Since each Γ^i has a diagonal covariance matrix, its components Γ^i_j are independent of each other. From such independence, and by the symmetry of a mean-0 normal random variable in \mathbb{R} with respect to the origin, it is not hard to see that (5.5) holds for every j and i.

Whenever (5.5) holds, we have (5.6), which means that the interval

$$\left[(z_n)_j - \frac{\sqrt{\chi_1^2(\alpha)} r_{nj}}{\sqrt{n}}, (z_n)_j + \frac{\sqrt{\chi_1^2(\alpha)} r_{nj}}{\sqrt{n}} \right]$$
 (5.17)

is an asymptotically exact $(1 - \alpha)$ confidence interval for $(z_0)_j$.

The numerical examples in Section 6 with $z_0 = 0$ do not belong to either of the above two cases, yet the coverage rates of individual confidence intervals obtained from this method are still reasonable. From those examples we observe that even if the difference between the two sides of (5.5) is large for some i, the difference tends to be reduced after the summation over all i's. As a result, the quantity

$$\sum_{i=1}^k \operatorname{Prob}\left(\left|\frac{\Gamma^i_j}{r^i_j}\right| \le \sqrt{\chi^2_1(\alpha)} \text{ and } \Gamma^i \in K_i\right)$$

may not be very far from $1-\alpha$. Finally, Theorem 5.1 assumes that Σ_0 is nonsingular, which implies the nonsingularity of Σ_n for large n. Even if Σ_n is singular, one can still use (5.17) to compute a confidence interval, with the caution that the coverage probability for the true solution may not be close to the prescribed level of confidence if Σ_n is very different from Σ_0 .

6. Numerical results. Before applying the proposed method to numerical examples, we summarize how to use this method in practice.

Among the assumptions, Assumption 1 is standard. For Assumption 2, instead of directly checking if the normal map L_K is a homeomorphism, we can check if one of its sufficient conditions holds (see the discussion below Assumption 2). Likewise, we can check if (5.5) holds by determining if the

problem belongs to one of the two case discussed below Theorem 5.1. In checking those assumptions, the asymptotical results in [15, 16] can be used to estimate $d(f_0)_S(z_0)$ and K.

Confidence regions of z_0 are given by the set (4.2) (if Σ_0 is nonsingular) or the set $R_{n,\epsilon}$ in (4.6) (if Σ_0 is singular), and the latter set can be approximated by $R_{n,0}$. According to Proposition 3.5, sets (4.2) and $R_{n,0}$ are ellipsoids with high probability. Computation of simultaneous confidence intervals for z_0 is done by finding the minimal bounding box of its confidence region. Individual confidence intervals of each component of z_0 can be computed using the formula (5.17), provided that (5.5) holds. The quantity r_{nj} defined in (5.3) depends on Σ_n and $d(f_n)_S(z_n)$, and the latter is a nonsingular matrix with high probability.

To convert confidence regions and intervals of z_0 into those of x_0 , the key is to use the equality $x_0 = \Pi_S(z_0)$. Suppose the set $A \subset \mathbb{R}^q$ is a $(1-\alpha)100\%$ confidence region for z_0 , then the image of A under the operator Π_S , denoted by $\Pi_S(A)$, contains x_0 with probability at least $1-\alpha$. If S is a box, then one can easily project the simultaneous confidence intervals of z_0 to obtain simultaneous confidence intervals of x_0 . The latter intervals are conservative, as the probability for the product of all those intervals to contain x_0 is at least $1-\alpha$. When S is a box, each component of x_0 is the projection of a component of z_0 onto an interval (the product of all such intervals is S), and one can project the individual confidence intervals of z_0 to obtain individual confidence intervals of x_0 . For problems in which S is not a box, the above projection method would not be easy to implement in general, and one would need to exploit special structure in those problems to obtain confidence regions and intervals of x_0 .

An example with q=2. Here, we apply the method to the same example used in [15, 16]. In this example, $q=2, d=6, S=\mathbb{R}^2_+, F:\mathbb{R}^2\times\mathbb{R}^6\to\mathbb{R}^2$ is defined by

$$F(x,\xi) = \begin{bmatrix} \xi_1 & \xi_2 \\ \xi_3 & \xi_4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \xi_5 \\ \xi_6 \end{bmatrix}, \tag{6.1}$$

and the random vector ξ follows the uniform distribution over the box $[0,2] \times [0,1] \times [0,2] \times [0,4] \times [-1,1] \times [-1,1]$. The true problem is

$$0 \in \begin{bmatrix} 1 & 1/2 \\ 1 & 2 \end{bmatrix} \ x + N_{\mathbb{R}^2_+}(x). \tag{6.2}$$

The solution to (6.2) is $x_0 = 0$, and the solution of the corresponding normal map formulation is $z_0 = x_0 - E[F(x_0, \xi)] = 0$. The covariance matrix of $F(x_0, \xi) = (\xi_5, \xi_6)$ is given by

$$\Sigma_0 = \begin{bmatrix} 1/3 & 0\\ 0 & 1/3 \end{bmatrix},$$

and the B-derivative $d(f_0)_{\mathbb{R}^2_+}(z_0)$ is a piecewise linear function represented by matrices

$$\begin{bmatrix} 1 & 1/2 \\ 1 & 2 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1/2 \\ 0 & 2 \end{bmatrix}$$
 and
$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

in orthants \mathbb{R}^2_+ , $\mathbb{R}_+ \times \mathbb{R}_-$, $\mathbb{R}_- \times \mathbb{R}_+$ and \mathbb{R}^2_- respectively. Accordingly, if we define random variables Γ^i as in Section 5, then the covariance matrices of them are

$$\begin{bmatrix} 0.6296 & -0.3704 \\ -0.3704 & 0.2963 \end{bmatrix}, \begin{bmatrix} 0.3333 & -0.3333 \\ -0.3333 & 0.6667 \end{bmatrix}, \begin{bmatrix} 0.3542 & -0.0417 \\ -0.0417 & 0.0833 \end{bmatrix} \text{ and } \begin{bmatrix} 0.3333 & 0 \\ 0 & 0.3333 \end{bmatrix}$$

respectively. An SAA problem with n = 10 is given by

$$0 \in \begin{bmatrix} 0.9292 & 0.5400 \\ 0.7536 & 2.1111 \end{bmatrix} x + \begin{bmatrix} -0.1319 \\ -0.2906 \end{bmatrix} + N_{\mathbb{R}^2_+}(x).$$

The SAA solution is $x_{10} = (0.0782, 0.1097)$, $z_{10} = (0.0782, 0.1097)$, and the sample covariance matrix of $F(x_{10}, \xi)$ is

$$\Sigma_{10} = \begin{bmatrix} 0.4169 & 0.0137 \\ 0.0137 & 0.1865 \end{bmatrix}.$$

The B-derivative $d\Pi_{\mathbb{R}^2_+}(z_{10})$ is exactly the identity map on \mathbb{R}^2 , and the B-derivative $d(f_{10})_{\mathbb{R}^2_+}(z_{10})$ is the linear map represented by the matrix

$$\begin{bmatrix} 0.9292 & 0.5400 \\ 0.7536 & 2.1111 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0.9292 & 0.5400 \\ 0.7536 & 2.1111 \end{bmatrix}.$$

The confidence regions in (4.2) are given by

$$\{z \in \mathbb{R}^2 \mid 10(z - z_{10})^T \begin{bmatrix} 4.8810 & 9.3398 \\ 9.3398 & 24.2564 \end{bmatrix} (z - z_{10}) \le \chi_2^2(\alpha) \}.$$

Figure 6.1(a) shows boundaries of the above confidence regions. The center of these regions is z_{10} , marked by '×' in the graph. From the innermost to the outermost, the curves correspond to boundaries of confidence regions for z_0 at levels 10%, ..., 90% respectively. The point z_0 is marked by '+' and lies just beyond the 90% confidence region. The dashed rectangle shown in the figure is the minimum enclosing box of the 90% region. Figure 6.1(b) shows confidence regions for z_0 obtained from a different SAA problem with sample size n = 30, $x_{30} = 0$ and $z_{30} = (-0.0483, -0.0114)$. Table 6.1 shows the 90% simultaneous and individual confidence intervals for z_0 obtained from the above two SAA problems.

	n = 10				n = 30			
	Est	Est Sim CI Ind CI		Est	Sim CI	Ind CI		
		[-0.52, 0.68]						
$(z_0)_2$	0.11	[-0.16, 0.38]	[-0.10, 0.32]	-0.01	[-0.23, 0.21]	[-0.18, 0.16]		

To test the coverage of confidence intervals obtained from the proposed method, we generate 200 SAA problems with n=10 and 200 SAA problems with n=30 from different random seeds, solve them using the PATH solver of GAMS, and compute simultaneous and individual confidence intervals for z_0 of levels 90%, 95% and 99% from the solution for each SAA problem. We count how many times the 2-dimensional box formed by simultaneous confidence intervals cover z_0 , and record the numbers in the row labeled by z_0 in Table 6.2. For example, the 90% simultaneous confidence intervals obtained from 171 SAA problems with n=10 cover z_0 jointly. We also count how many times each component of z_0 is contained in the corresponding individual confidence intervals, and record the numbers in the remaining rows of Table 6.2. For example, the 90% individual confidence intervals for $(z_0)_1$ obtained from 164 SAA problems with n=10 cover the true value $(z_0)_1=0$.

Fig. 6.1. Confidence regions for z_0 in the example q=2 at levels $10\%, \dots, 90\%$

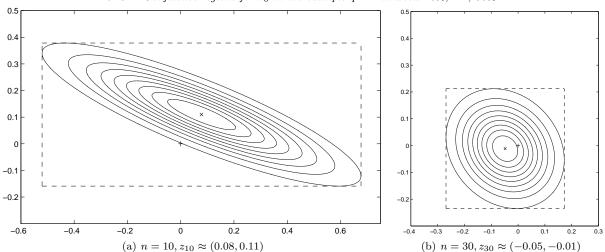


Table 6.2 True solution coverage by confidence intervals in the example q=2 from 200 SAA problems

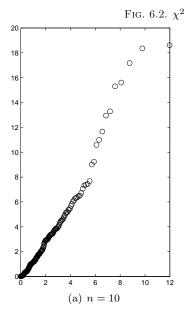
	n	= 10		n = 30			
	$\alpha = 0.1$	0.05	0.01	$\alpha = 0.1$	0.05	0.01	
$\overline{z_0}$	171	180	187	184	192	197	
$(z_0)_1$	164	185	194	172	188	198	
$(z_0)_2$	159	175	191	176	186	196	

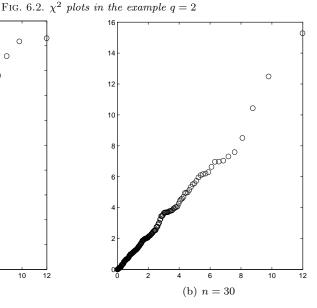
The proposed method generates confidence regions and simultaneous confidence intervals based on the asymptotic distribution in (4.1) (or (4.4) for singular cases). We evaluate how closely z_n follow the asymptotic distribution using χ^2 plots. We use the same SAA problems generated above for coverage tests. For each SAA problem with n = 10 we compute the squared distance

$$n[d(f_n)_S(z_n)(z_0-z_n)]^T \Sigma_n^{-1}[d(f_n)_S(z_n)(z_0-z_n)],$$

and order these distances from smallest to largest as $d_{(1)}^2 \leq d_{(2)}^2 \leq \cdots \leq d_{(200)}^2$. For each $j=1,\cdots,200$, let $q_{c,2}((j-1/2)/200)$ be the 100(j-1/2)/200 quantile of the χ^2 distribution with 2 degrees of freedom. We then graph the pairs $(q_{c,2}((j-1/2)/200),d_{(j)}^2)$ for $j=1,\cdots,200$ in Figure 6.2(a), in which the horizontal axis is for quantiles and the vertical axis is for squared distances. Figure 6.2(b) is obtained similarly, from the 200 SAA problems with sample size n=30. In each figure the points nearly follow a straight line through the origin with slope around 1, and the slope of the line in Figure 6.2(b) is closer to 1. This suggests that the expression on the left hand side of (4.1) approximately follows the standard normal distribution.

Examples with q = 10. We let q = 10, d = 110, $S = \mathbb{R}^{10}_+$, and $F : \mathbb{R}^{10} \times \mathbb{R}^{110} \to \mathbb{R}^{10}$ be defined as $F(x,\xi) = \Lambda(\xi)x + b(\xi)$, where $\Lambda(\xi)$ is a 10×10 matrix whose entries are the first 100 components





of ξ , and $b(\xi) \in \mathbb{R}^{10}$ consists of the last 10 components of ξ . Each diagonal entry of $\Lambda(\xi)$ is uniformly distributed on the interval [0,4], each entry above the main diagonal is uniformly distributed on [0,3], and each entry below the main diagonal is uniformly distributed on [0,2]. Thus, $E[\Lambda(\xi)] = \Lambda_0$ with $(\Lambda_0)_{ii} = 2$, $(\Lambda_0)_{ij} = 1.5$ for i < j and $(\Lambda_0)_{ij} = 1$ for i > j. We consider three different choices for the uniform distribution of $b(\xi)$, to obtain three different examples. In example 1, each component of $b(\xi)$ is uniformly distributed on [-1,1], so $E[b(\xi)]_i = 0$ for each i. In example 2, the first five components of $b(\xi)$ are uniformly distributed on [-1,0.8] and the last five components uniformly distributed on [-1,1]. In example 3, each component of $b(\xi)$ is uniformly distributed on [-1,0.8]. The true solution z_0 is given by

```
\begin{array}{l} z_0=0\in\mathbb{R}^{10} \text{ in example 1,} \\ z_0=[0.21,\ 0.43,\ 0.85,\ 1.7,\ 3.4,\ -6.6,\ -6.6,\ -6.6,\ -6.6,\ -6.6]^T\times 10^{-2} \text{ in example 2,} \\ z_0=[0.01,\ 0.01,\ 0.03,\ 0.05,\ 0.1,\ 0.21,\ 0.42,\ 0.83,\ 1.67,\ 3.34]^T\times 10^{-2} \text{ in example 3.} \end{array}
```

For each example, we generate 200 SAA problems with n=50, compute the SAA solutions, and obtain simultaneous and individual confidence intervals for z_0 of levels 90%, 95% and 99% from each SAA solution. Table 6.3 lists the averages of the 90% confidence intervals for $(z_0)_1$ and $(z_0)_{10}$ obtained from the 200 SAA problems, for each example. Table 6.4 is analogous to Table 6.2. It summarizes the joint coverage of the true solution by simultaneous confidence intervals obtained from the 200 SAA problems for each example, and the coverage of $(z_0)_1$ and $(z_0)_{10}$ by the corresponding individual confidence intervals.

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Table 6.3 Average 90% confidence intervals for $(z_0)_1$ and $(z_0)_{10}$ in examples q=10 over 200 SAA problems

	Exan	ple 1	Exan	nple 2	Example 3		
	Sim CI	Ind CI	Sim CI	Ind CI	Sim CI	Ind CI	
$(z_0)_1$	[-0.49, 0.30]	[-0.26, 0.07]	[-0.40, 0.30]	[-0.19, 0.09]	[-0.44, 0.28]	[-0.23, 0.07]	
$(z_0)_{10}$	[-0.41, 0.28]	[-0.20, 0.08]	[-0.46, 0.25]	[-0.25, 0.04]	[-0.33, 0.30]	[-0.15, 0.11]	

 ${\it Table 6.4} \\ {\it True solution coverage by confidence intervals in examples with q=10 from 200 SAA problems}$

	Exa	ample 1		Example 2			Example 3		
	$\alpha = 0.1$	0.05	0.01	$\alpha = 0.1$	0.05	0.01	$\alpha = 0.1$	0.05	0.01
z_0	198	199	200	196	198	200	197	197	198
$(z_0)_1$	156	178	194	172	186	192	164	179	195
$(z_0)_{10}$	173	183	195	176	188	197	172	184	195

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