Statistical Inference for Sample Average Approximation of Constrained Optimization and Variational Inequalities

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Stochastic optimization and sample average approximation

$$\min_{x \in S} E[\Phi(x, \xi)]$$

- $S \subset \mathbb{R}^n$: the feasible set, assumed to be a convex polyhedron
- $\xi(\omega)$: a random vector taking values in a set $\Xi \subset \mathbb{R}^d$
- Φ: a function from $\mathbb{R}^n \times \Xi$ to $\mathbb{R}$

Evaluating $E[\Phi(x, \xi)]$ for a given x is often impractical. A common approach is to solve the sample average approximation (SAA) problem:

$$\min_{x \in S} N^{-1} \sum_{i=1}^{N} \Phi(x, \xi^i(\omega))$$

where $\xi^1, \cdots, \xi^N$ are i.i.d. random variables with distribution same as ξ

Example: Norm-constrained minimum variance portfolio selection

The true problem[1]

$$\min_x \frac{1}{2} x^T \Sigma x \quad s.t. \quad e^T x = 1, \|x\|_1 \leq c$$

The SAA problem:

$$\min_x \frac{1}{2} x^T \Sigma_N x \quad s.t. \quad e^T x = 1, \|x\|_1 \leq c$$

- $x \in \mathbb{R}^p$: portfolio allocations among p assets
- $e \in \mathbb{R}^p$: vector of all one's
- $c \geq 1$: a constant controlling the amount of short sales allowed
- $\Sigma \in \mathbb{R}^{p \times p}$: the true covariance matrix of the random return R
- $\Sigma_N \in \mathbb{R}^{p \times p}$: the sample covariance matrix of the random return, computed from independently and identically distributed sample data $\{r_{ij}\}_{j=1}^p, i = 1, \ldots N$

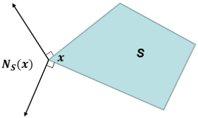
[1] It can be written as $\min_{x \in S} g(E[\Phi(x, R)])$

Stochastic variational inequalities[2] and sample average approximation

$$-E[F(x,\xi)] \in N_S(x) \qquad \text{(TRUE-VI)}$$

- $S \subset \mathbb{R}^n$: the feasible set, assumed to be a convex polyhedron
- ξ: a random vector taking values in a set $\Xi \subset \mathbb{R}^d$
- F: a function from $\mathbb{R}^n \times \Xi$ to $\mathbb{R}^n$
- $N_S(x)$: the normal cone to S at x

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



Let $\xi^1, \cdots, \xi^N$ be i.i.d. random variables with distribution same as ξ. The SAA problem is

$$-N^{-1} \sum_{i=1}^{N} F(x, \xi^i(\omega)) \in N_S(x) \qquad \text{(SAA-VI)}$$

[2]See [Chen, Wets and Zhang 2012], [Rockafellar and Wets 2016] for alternative SVI formulations

Stochastic optimization related to stochastic variational inequalities

If the objective function of the stochastic optimization problem

$$\min_{x \in S} E[\Phi(x, \xi)]$$

is differentiable at a local minimizer x_0, then x_0 satisfies the first-order necessary condition

$$-\nabla_x E[\Phi(x_0, \xi)] \in N_S(x_0).$$

The above condition becomes a stochastic variational inequality, when

$$\nabla_x E[\Phi(x_0, \xi)] = E[\nabla_x \Phi(x_0, \xi)]$$

Example: stochastic equilibria in energy markets

- 4 gas producers ($i = 1, \cdots, 4$) decide the amount of gas (x_{ij}^t) to ship to 6 markets ($j = 1, \cdots, 6$) in 4 time periods ($t = 1, \cdots, 4$)
- Each producer i tries to maximize its own profit $E[\Phi_i(x, \xi)]$

$$x_i \in \underset{x_i \in \mathbb{R}_+^{24}}{\operatorname{argmax}} E[\Phi_i(x, \xi)]$$

  - $x_i = [x_{ij}^t]_{tj}$: variables of producer i
  - $x = [x_{ij}^t]_{tij}$: the vector of all variables
  - Φ_i: the profit function of producer i. It depends on x_j for $j \neq i$, since the total amount of production affects gas price
  - $\xi = [\xi^t]_t$: the random oil price

This Cournot-Nash equilibrium problem can be reformulated as a stochastic variational inequality:

$$0 \in -E \begin{bmatrix} \nabla_{x_1} \Phi_1(x, \xi) \\ \vdots \\ \nabla_{x_4} \Phi_4(x, \xi) \end{bmatrix} + N_{\mathbb{R}_+^{96}}(x)$$

The inference question

- In practice, we often solve the SAA problem to find the SAA solution, x_N
- How does data uncertainty affect the reliability of the SAA solution?
- One way to answer this question is by building confidence regions and intervals for the true solution, x_0, based on knowledge about x_N
- An asymptotically exact confidence region $C(x_N)$ is a set in $\mathbb{R}^n$ that depends on x_N and satisfies

$$\lim_{N\to\infty} P\left(x_0 \in C(x_N)\right) = 1 - \alpha$$

- We build confidence regions and intervals by utilizing the asymptotic distribution of SAA solutions

The normal map formulation of variational inequalities[3]

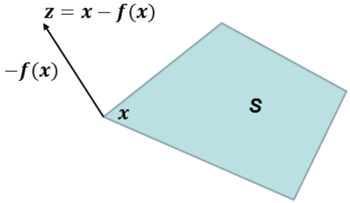
The normal map associated with a function $f : S \to \mathbb{R}^n$ and a set $S \subset \mathbb{R}^n$ is a function $f_S : \mathbb{R}^n \to \mathbb{R}^n$, defined as

$$f_S(z) = f(\Pi_S(z)) + z - \Pi_S(z) \text{ for each } z \in \mathbb{R}^n$$

where $\Pi_S(z)$ is the Euclidean projection of z on S

$$\boxed{-f(x) \in N_S(x)} \quad \underset{x=\Pi_S(z)}{\overset{z=x-f(x)}{\rightleftarrows}} \quad \boxed{f_S(z) \quad = \quad 0}$$

- Π_S is piecewise affine
- The normal manifold of S: the polyhedral subdivision of $\mathbb{R}^n$ corresponding to Π_S
- f_S is piecewise smooth if f is smooth, and is piecewise affine if f is affine



[3]Details about normal maps can be found in [Robinson 1992], [Ralph 1993], [Facchinei and Pang 2003], [Scholtes 2012] and references therein

The true problems and SAA problems

- Define the true function as $f_0(x) = E[F(x, \xi)]$ and the SAA function

$$f_N(x) = -N^{-1} \sum_{i=1}^{N} F(x, \xi^i(\omega))$$

- Write (TRUE-VI) as

$$-f_0(x) \in N_S(x)$$

and (SAA-VI) as

$$-f_N(x) \in N_S(x)$$

- Their corresponding normal map formulations are

$$(f_0)_S(z) = 0 \quad \text{(SVI-NM)} \qquad \text{and} \qquad (f_N)_S(z) = 0 \quad \text{(SAA-NM)}$$

- Let $z_0 = x_0 - f_0(x_0)$ and $z_N = x_N - f_N(x_N)$ be solutions to the normal map formulations

Convergence of SAA solutions to the true solution[4]

Under certain ▸ Assumptions

- For a.e. ω, (SAA-VI) has a locally unique solution x_N for N large enough, with $\lim_{N\to\infty} x_N = x_0$
- The corresponding solution z_N to (SAA-NM) is also locally unique, with $\lim_{N\to\infty} z_N = z_0$ almost surely
- Let Σ_0 be the covariance matrix of $F(x_0,\xi)$, and $\mathcal{N}(0,\Sigma_0)$ be a normal r.v. in $\mathbb{R}^n$ with zero mean and covariance matrix Σ_0. Then,

$$\sqrt{N} L_K(z_N - z_0) \Rightarrow \mathcal{N}(0,\Sigma_0) \qquad \text{(Conv-Dist-}z\text{)}$$

$$\sqrt{N}(x_N - x_0) \Rightarrow \Pi_K \circ (L_K)^{-1}(\mathcal{N}(0,\Sigma_0)) \qquad \text{(Conv-Dist-}x\text{)}$$

  where $L = \nabla_x E[F(x_0,\xi)]$, $K = T_S(x_0) \cap E[F(x_0,\xi)]^{\perp}$, L_K is the normal map associated with L and K, and $(L_K)^{-1}$ is its inverse
- L_K is a piecewise linear approximation of the normal map $(f_0)_S$ around z_0

[4] See related results in [Dupacova and Wets 1988], [King and Rockafellar 1993], [Gürkan, Özge and Robinson 1999], [Demir 2000], [Shapiro, Dentcheva and Ruszczyński 2009], [Gürkan and Pang 2009], [Xu 2010] etc.

Assumptions

Assumption 1: Implies the continuous differentiability of f_0 on O, the almost sure convergence $f_N \to f_0$ as an element of $C^1(X, \mathbb{R}^n)$ for any compact set $X \subset O$, and the weak convergence of $\sqrt{N}(f_N - f_0)$

(a) $E\|F(x,\xi)\|^2 < \infty$ for all $x \in O$, where O is an open set in $\mathbb{R}^n$.
(b) The map $x \mapsto F(x, \xi(\omega))$ is cont diff on O for a.e. $\omega \in \Omega$.
(c) There exists a square integrable random variable C such that $\|F(x,\xi(\omega)) - F(x',\xi(\omega))\| + \|dF(x,\xi(\omega)) - dF(x',\xi(\omega))\| \leq C(\omega)\|x - x'\|$, for all $x', x \in O$ and a.e. $\omega \in \Omega$.

Assumption 2: Guarantees the existence, local uniqueness, and stability of the true solution under small perturbation of f_0

Suppose that $x_0 \in O$ solves (SVI). 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 is a homeomorphism from $\mathbb{R}^n$ to $\mathbb{R}^n$

Properties of the limiting distributions

$$\underbrace{(L_K)^{-1}(\mathcal{N}(0,\Sigma_0))}_{\text{limiting distribution of } \sqrt{N}(z_N - z_0)} \quad \text{and} \quad \underbrace{\Pi_K \circ (L_K)^{-1}(\mathcal{N}(0,\Sigma_0))}_{\text{limiting distribution of } \sqrt{N}(x_N - x_0)}$$

- For a given $q \in \mathbb{R}^n$, $\Pi_K \circ (L_K)^{-1}(q)$ is the solution h of a linear VI:

$$-Lh + q \in N_K(h)$$

  and when L is symmetric it is the unique solution of the QP

$$\min_{h \in K} \frac{1}{2} h^T L h - q^T h$$

- $(L_K)^{-1}(q) = h - Lh + q$
- If K is a subspace, $\Pi_K \circ (L_K)^{-1}(q)$ and $(L_K)^{-1}(q)$ are linear functions of q, and x_N and z_N are asymptotically normal
- If K is a polyhedral convex cone but not a subspace, then $\Pi_K \circ (L_K)^{-1}(q)$ and $(L_K)^{-1}(q)$ are piecewise linear functions with multiple pieces, and x_N and z_N are not asymptotically normal

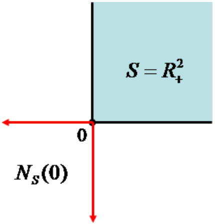
Example: a linear complementarity problem

- $F : \mathbb{R}^2 \times \mathbb{R}^6 \to \mathbb{R}^2$ given by $F(x,\xi) = \begin{bmatrix} \xi_1 & \xi_2 \\ \xi_3 & \xi_4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \xi_5 \\ \xi_6 \end{bmatrix}$
- ξ uniformly distributed on $[0,2] \times [0,1] \times [0,2] \times [0,4] \times [-1,1] \times [-1,1]$
- Then $f_0(x) = E[F(x,\xi)] = \begin{bmatrix} 1 & 1/2 \\ 1 & 2 \end{bmatrix} x$

Let $S = \mathbb{R}^2_+$. The SVI is an LCP:

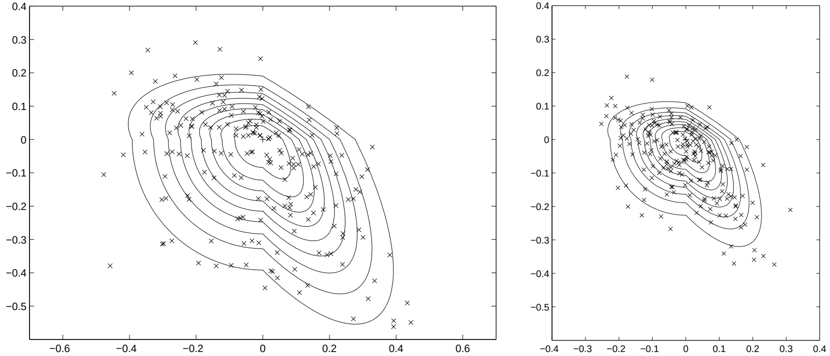
$$-f_0(x) \in N_{\mathbb{R}^2_+}(x),$$

which has a unique solution $x_0 = 0$, and $z_0 = x_0 - f_0(x_0) = 0$ is the unique solution for (SVI-NM)



Here, $L = \begin{bmatrix} 1 & 1/2 \\ 1 & 2 \end{bmatrix}$ and $K = S = \mathbb{R}^2_+$

In the example: scatter plots for z_N



- Left: solutions to 200 SAA problems with $N = 10$; Right: $N = 30$
- Curves are boundaries of sets

$$\{z \in \mathbb{R}^2 \mid N\big[L_K(z - z_0)\big]^T \Sigma_0^{-1}\big[L_K(z - z_0)\big] \leq \chi^2_N(\alpha)\}$$

which contain z_N with (approximately) probability $1 - \alpha$ for $\alpha = 0.1, \cdots, 0.9$

A computable, asymptotically exact confidence region for z_0

- From $\sqrt{N} L_K(z_N - z_0) \Rightarrow \mathcal{N}(0, \Sigma_0)$, an asymptotically exact $(1-\alpha)100\%$ confidence region for z_0[5] is

$$\left\{ z \in \mathbb{R}^n \mid N \left[L_K(z_N - z) \right]^T \Sigma_0^{-1} \left[L_K(z_N - z) \right] \le \chi_n^2(\alpha) \right\} \qquad \text{(CR0)}$$

- However, (CR0) is not computable as Σ_0 and L_K are unknown
- Interestingly, an asymptotically exact, and computable, confidence region is given by

$$\left\{ z \in \mathbb{R}^n \mid N \left[d(f_N)_S(z_N)(z - z_N) \right]^T \Sigma_N^{-1} \left[d(f_N)_S(z_N)(z - z_N) \right] \le \chi_n^2(\alpha) \right\} \qquad \text{(CR1)}$$

  - $d(f_N)_S(z_N)(z - z_N)$: the directional derivative of $(f_N)_S$ at z_N for the direction $z - z_N$
  - Σ_N: the sample covariance matrix of $F(x_N, \xi)$[6]

- With high probability, $d(f_N)_S(z_N)$ is linear and (CR1) is an ▸ ellipsoid

[5] $\chi_n^2(\alpha)$ satisfies $P(U > \chi_n^2(\alpha)) = \alpha$ for a χ^2 r.v. U with n deg of freedom
[6] Different from Σ_N in the portfolio selection example

In the example: Confidence regions for z_0 computed from z_{10}

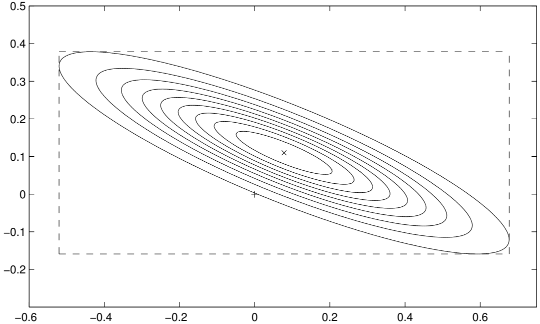
An SAA for the LCP (N=10): $$-\begin{bmatrix} 0.93 & 0.54 \\ 0.75 & 2.11 \end{bmatrix} x + \begin{bmatrix} 0.13 \\ 0.29 \end{bmatrix} \in N_{\mathbb{R}^2_+}(x)$$

A unique solution $x_{10} = (0.08, 0.11) = z_{10}$ marked as $\times$ $\quad +$: $z_0 = 0$

$$\underbrace{\begin{bmatrix} 0.42 & 0.01 \\ 0.01 & 0.19 \end{bmatrix}}_{\Sigma_{10}} \quad \underbrace{\begin{bmatrix} 0.93 & 0.54 \\ 0.75 & 2.11 \end{bmatrix}}_{d(f_{10})_{\mathbb{R}^2_+}(z_{10})} \quad \underbrace{\left\{ z \,\middle|\, 10(z - z_{10})^T \begin{bmatrix} 4.88 & 9.34 \\ 9.34 & 24.26 \end{bmatrix} (z - z_{10}) \le \chi^2_2(\alpha) \right\}}_{(1-\alpha)100\% \text{ confidence region for } z_0}$$

Shown in the figure: confidence regions for z_0 at levels $0.1, \cdots, 0.9$

90% simultaneous confidence intervals:
$(z_0)_1$: [-0.52, 0.68]
$(z_0)_2$: [-0.16, 0.38]
$(x_0)_1$: [0, 0.68]
$(x_0)_2$: [0, 0.38]



Individual confidence intervals for z_0 and x_0 (target level: 90%)

- Consider cells in the normal manifold of $\mathbb{R}^2_+$:
  $\{0\}, \{0\} \times \mathbb{R}_+, \mathbb{R}_+ \times \{0\}, \{0\} \times \mathbb{R}_-, \mathbb{R}_- \times \{0\}, \mathbb{R}^2_+, \mathbb{R}^2_-, \mathbb{R}_+ \times \mathbb{R}_-, \mathbb{R}_- \times \mathbb{R}_+,$
- C_{i_N}: the cell with the smallest dimension, among all cells that intersect the 95% region. Here it is $\{0\}$
- P_N: the 2-dim cell that contains z_N in its interior. Here it is $\mathbb{R}^2_+$
- Let $\tilde{z}_{i_N}$ be any point in ri C_{i_N}, and $K_N = \text{cone}(P_N - \tilde{z}_{i_N})$. Here it is $\mathbb{R}^2_+$
- With limiting probability $\geq 95\%$, K_N gives the cone that contains z_N in the polyhedral subdivision of $\mathbb{R}^2$ corresponding to L_K
- Let $M = (d(f_N)_S(z_N))^{-1}\Sigma_N^{1/2}$, and compute a number ℓ_N such that

$$\frac{\Pr\left(|(MZ)_j| \leq \ell_N, \ \text{ and } \ MZ \in K_N\right)}{\Pr\left(MZ \in K_N\ \right)} = 0.95, \quad \text{where } Z \sim \mathcal{N}(0, I)$$

- $\liminf_{N\to\infty} \text{Prob}\left(\sqrt{N}|(z_N - z_0)_j| \leq \ell_N\right) \geq 0.90$
- 90% individual confidence intervals for z_0 and x_0 (computation of intervals for x_0 is analogous)
  $(z_0)_1$: [-0.16, 0.32], $(z_0)_2$: [0, 0.22], $(x_0)_1$: [0, 0.32], $(x_0)_2$: [0, 0.22]

An alternative method

- Under additional assumptions, z_N converges to z_0 at an exponential rate
- At z_N we can define a function $\Phi_N(z_N) : \mathbb{R}^n \times \mathbb{R}^n$ so that

$$\lim_{N\to\infty} \text{Prob}\left[\sup_{h\in\mathbb{R}^n} \frac{\|\Phi_N(z_N)(h) - L_K(h)\|}{\|h\|} < \frac{\phi}{N^{1/3}}\right] = 1$$

- Replacing L_K by $\Phi_N(z_N)$ in the weak convergence results gives a different method for computing confidence regions and intervals

Portfolio selection example: Confidence intervals and coverage rates

- $\mathcal{A} = \{j : (x_0)_j \neq 0\}$
- 200 replications
- Avgcov: average coverage; Medcov: median coverage
- Avglen: average length

$1-\alpha = 90\%$		Our method			Normal estimation		
N and p		Avgcov $\mathcal{A}$	Medcov $\mathcal{A}$	Avglen $\mathcal{A}$	Avgcov $\mathcal{A}$	Medcov $\mathcal{A}$	Avglen $\mathcal{A}$
N=200	p=30	0.937	0.94	0.163	0.887	0.89	0.13
N=500	p=30	0.94	0.94	0.101	0.883	0.88	0.085
N=600	p=100	0.896	0.89	0.125	0.862	0.85	0.104
N=1000	p=100	0.928	0.94	0.099	0.89	0.89	0.083
$1-\alpha = 95\%$		Our method			Normal estimation		
N and p		Avgcov $\mathcal{A}$	Medcov $\mathcal{A}$	Avglen $\mathcal{A}$	Avgcov $\mathcal{A}$	Medcov $\mathcal{A}$	Avglen $\mathcal{A}$
N=200	p=30	0.965	0.965	0.210	0.94	0.94	0.183
N=500	p=30	0.97	0.96	0.129	0.945	0.91	0.112
N=600	p=100	0.97	0.96	0.083	0.945	0.89	0.073
N=1000	p=100	0.972	0.97	0.065	0.945	0.935	0.057

Energy market equilibrium example: Coverage rates ($\alpha = 0.05$)

- $\upsilon_j^{.05}$: Normal estimation
- $\tilde{h}_j^{.04}$: The presented method with $\alpha_1 = 0.01$, $\alpha_2 = 0.04$
- $\tilde{h}_j^{.025}$: The presented method with $\alpha_1 = 0.025$, $\alpha_2 = 0.025$
- 2000 replications

Percentile	$N = 200$			$N = 2,000$		
	$\upsilon_j^{.05}$	$\tilde{h}_j^{.04}$	$\tilde{h}_j^{.025}$	$\upsilon_j^{.05}$	$\tilde{h}_j^{.04}$	$\tilde{h}_j^{.025}$
MIN	88.20 %	88.70%	89.05 %	94.60 %	95.70 %	97.20 %
Q1	94.75 %	95.70 %	97.08%	94.85 %	96.00 %	97.50 %
MEDIAN	94.90 %	95.83 %	97.45%	95.30 %	96.25 %	97.95 %
Q3	95.05%	95.95 %	97.60%	95.40 %	96.5 %	98.35 %
MAX	100 %	100 %	100 %	100 %	100 %	100 %

Summary

- Development and justification of methods to build computable confidence regions and intervals for the true solutions of the expected-value formulation of stochastic variational inequalities
- Applied to stochastic Cournot-Nash production/distribution problems, sparse-penalized statistical regression and portfolio selection

This presentation is mainly based on the following papers:

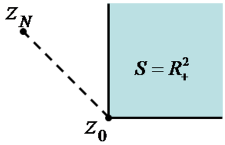
- Lamm, Lu. 2016. Generalized conditioning based approaches to compute confidence intervals for stochastic variational inequalities. Submitted
- Lamm, Lu and Budhiraja. 2016. Individual confidence intervals for solutions to expected value formulations of stochastic variational inequalities. *Mathematical Programming B*
- Lu. 2014. Symmetric confidence regions and confidence intervals for normal map formulations of stochastic variational inequalities. *SIAM Journal on Optimization*. Vol. 24, No. 3, pp. 1458-1484
- Lu and Budhiraja. Confidence regions for stochastic variational inequalities. *Mathematics of Operations Research*, 2013, Vol. 38, No. 3, pp. 545-568

Derivation of (CR1)

- A key observation: z_N in a neighborhood of z_0 satisfies

$$d\Pi_S(z_0)(z_N - z_0) + d\Pi_S(z_N)(z_0 - z_N) = 0$$

where $d\Pi_S(z_0)(z_N - z_0)$ is the directional derivative of Π_S at z_0 for the direction $z_N - z_0$



- This property holds, as long as z_0 and z_N are contained in a common n-cell

- With $\sqrt{N} L_K(z_N - z_0) \Rightarrow \mathcal{N}(0, \Sigma_0)$ and $L_K = d(f_0)_S(z_0)$, it can be shown

$$-\sqrt{N} d(f_N)_S(z_N)(z_0 - z_N) \Rightarrow \mathcal{N}(0, \Sigma_0)$$

which implies (CR1) is an asymptotically exact confidence region for z_0