Sparsity-Exploiting Sample-Average Approximation to Stochastic Programming with Applications in Designing Acoustic Tweezer

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Problem Statement

Regularized SAA to exploit sparsity

Theoretical Extensions

Application to Designing Acoustic Tweezer

Outline

1. Problem Statement
2. Regularized SAA to exploit sparsity
3. Theoretical Extensions
4. Application to Designing Acoustic Tweezer

Stochastic Programming Problem

- Consider a stochastic programming (SP) problem:

$$\min_{\mathbf{x}:\, 0 \le \mathbf{x} \le R} \{F(\mathbf{x}) := \mathbb{E}_{\mathbb{P}} f(\mathbf{x}, W)\}$$

- f deterministic. For every feasible $\mathbf{x}$, the function $f(\mathbf{x}, \cdot)$ is measurable and $F(\mathbf{x})$ is finite
- We assume box constraints for simplification of analysis
- Commonly solved via sample average approximation (SAA), a.k.a. Monte Carlo (Sampling) Method

Section 1

Problem Statement

RSAA for High-Dimensional SP and Applications

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Sample Average Approximation

- To solve:

$$\mathbf{x}^{\min} \in \underset{\mathbf{x}:\, 0 \le \mathbf{x} \le R}{\arg\min} \{F(\mathbf{x}) := \mathbb{E}_{\mathbb{P}} f(\mathbf{x}, W)\}$$

- Solve instead an approximation problem

$$\min_{\mathbf{x}:\, 0 \le \mathbf{x} \le R} \left\{ F_n(\mathbf{x}) := n^{-1} \sum_{j=1}^{n} f(\mathbf{x}, W_j) \right\}$$

  - $\{W_1, W_2, ..., W_j, ..., W_n\}$ is a sequence of samples of W
  - Simple to implement
  - Often tractably computable

SAA is a popular way of solving SP

Efficacy of SAA

- Assumptions: i.i.d., subgaussian and Lipschitz-like conditions.
- Number of samples n required to achieve ϵ accuracy with probability $1-\alpha$ in solving an p-dimensional problem:

$$\mathbb{P}[F(\mathbf{x}^{SAA}) - F(\mathbf{x}^{\min}) \leq \epsilon] \geq 1-\alpha$$

if n is large enough to satisfy[1,2,3]

$$n \gtrsim \frac{p}{\epsilon^2} \ln \frac{1}{\epsilon} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$$

Sample size n grows polynomially when number of dimensions p increases

[1] Shapiro (2003) Stochastic Programming, Handbook in OR & MS
[2] Shapiro et al. (2009) Lectures on Stochastic Programming Modeling and Theory
[3] Shapiro & Xu (2008) Optimization

High-Dimensional SP

- Question 1: What if $p \gg n$ and acquiring new samples is prohibitively costly?
- Question 2: What if most dimensions are ineffective, e.g., $\mathbf{x}^{\min} = [80; 131; 100; 0; 0; ....; 0; 0]$?
- For example:
  - Consider a problem with $p = 100,000$, where SAA requires $n \geq 100,000 \sim 10,000,000$
  - If it is known which dimensions (10 of them) are nonzero, the original problem can be reduced to $p = 10$, and then $n \geq 10 \sim 1,000$

Conventional SAA is not effective in solving high-dimensional SP

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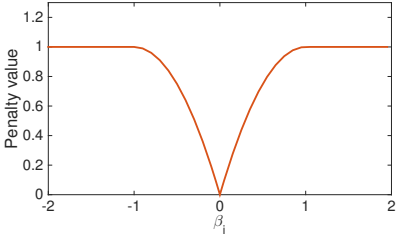
Regularized Sample Average Approximation (RSAA)

- The RSAA formulation

$$\min_{\mathbf{x}:\, 0 \le \mathbf{x} \le R} \left\{ F_{n,\lambda}(\mathbf{x}) := F_n(\mathbf{x}) + \sum_{i=1}^{p} P_\lambda(x_i) \right\}$$

- $P_\lambda : \Re_+ \to \Re_+$: minimax concave penalty (MCP):[4]



$$P_\lambda(\tau) := \int_0^\tau \frac{(a\lambda - t)_+}{a}\, dt$$
$$= \begin{cases} \lambda\tau - \frac{\tau^2}{2a} & \text{if } 0 \le \tau \le a\lambda; \\ \frac{1}{2}a\lambda^2 & \text{if } \tau > a\lambda. \end{cases}$$

$a > 0$ and $\lambda > 0$ are penalty parameters

RSAA = SAA + MCP penalty

[4] Zhang, 2010, Ann. Stats.; Fan and Li, 2001, JASA

Section 2

Regularized SAA to exploit sparsity

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The S^3ONC Solutions

Assume $f(\cdot, W)$ twice differentiable for almost every W

First-order necessary condition (FONC): The solution $\mathbf{x}^* \in [0,\, R]^p$ satisfies that

$$\langle \nabla F_n(\mathbf{x}^*) + (P'_\lambda(x_i^*) : 1 \le i \le p), \mathbf{x} - \mathbf{x}^* \rangle \ge 0, \quad \forall \mathbf{x} \in [0,\, R]^p$$

Significant subspace second-order necessary condition (S^3 ONC): The solution $\mathbf{x}^* := (x_i^* : 1 \le i \le p) \in [0,\, R]^p$ satisfies FONC. Furthermore, for all $i \in \{i : x_i^* \in (0,\, \min\{1,\, a\lambda\})\}$, it holds that

$$\left.\frac{\partial^2 F_{n,\lambda}(\mathbf{x})}{(\partial x_i)^2}\right|_{\mathbf{x}=\mathbf{x}^*} \ge 0$$

if $\left.\frac{\partial^2 F_{n,\lambda}(\mathbf{x})}{(\partial x_i)^2}\right|_{\mathbf{x}=\mathbf{x}^*}$ exists.

S^3ONC is weaker than the second-order KKT condition

Result I: Efficacy of RSAA

Theorem 1

Assumptions:

(a) $f(\mathbf{x}, W)$ is subgaussian for any $\mathbf{x} \in [0,\, R]^p$

(b) $f(\cdot, W)$ is twice differentiable and convex for almost every W

(c) Lipschitz-like condition

(d) The true solution is sparse, i.e., $\|\mathbf{x}^{\min}\|_0 \leq s$

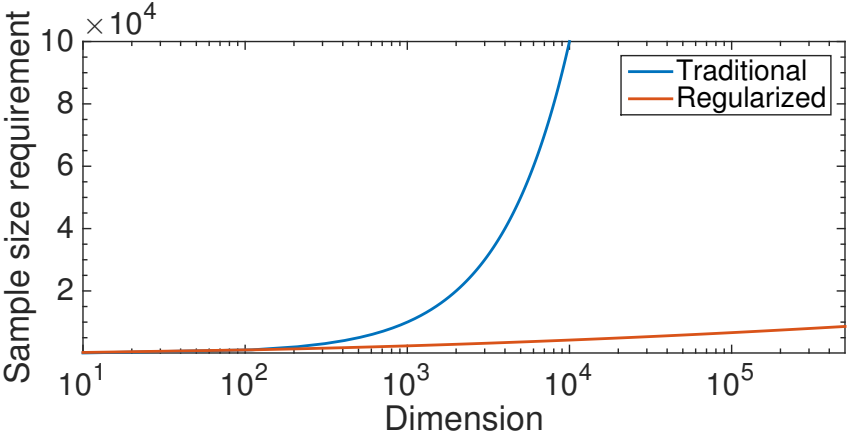
Consider an S^{3}ONC solution $\mathbf{x}^*$. If $F_{n,\lambda}(\mathbf{x}^*) \leq F_{n,\lambda}(\mathbf{0})$ almost surely, and if the sample size n satisfies

$$n \gtrsim \frac{s^{2.5}}{\epsilon^4}\left(\ln\frac{p}{\epsilon}\right)^2 + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha} \tag{1}$$

then $\mathbb{P}\left[F(\mathbf{x}^*) - F(\mathbf{x}^{true}) \leq \epsilon\right] \geq 1 - \alpha$.

RSAA has improved dependence on p v.s. the conventional SAA, $n \gtrsim \frac{p}{\epsilon^2}\ln\frac{1}{\epsilon} + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}$

Benefit of RSAA: Poly-Logarithmic Dependence in p



RSAA: Compensation of exponential growth in p by increasing n polynomially

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Result II: Efficacy of RSAA Under Additional Regularity

Theorem 2

Assumptions:

- The same set of assumptions as in Theorem 1
- F is strongly convex and continuously differentiable

Consider an S^{3}ONC solution $\mathbf{x}^*$. If $F_{n,\lambda}(\mathbf{x}^*) \leq F_{n,\lambda}(\mathbf{0})$ almost surely, and if the sample size n satisfies

$$n \gtrsim \frac{s^{1.5}}{\epsilon^3}\left(\ln\frac{p}{\epsilon}\right)^{1.5} + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}$$

then $\mathbb{P}\left[F(\mathbf{x}^*) - F(\mathbf{x}^{true}) \leq \epsilon\right] \geq 1 - \alpha$.

Better than both

- Conventional SAA: $n \gtrsim \frac{p}{\epsilon^2}\ln\frac{1}{\epsilon} + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}$
- RSAA without strong convexity: $n \gtrsim \frac{s^{2.5}}{\epsilon^4}\left(\ln\frac{p}{\epsilon}\right)^2 + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}$

Result III: Efficacy of RSAA Under Additional Regularity

Theorem 3

Assumptions:

- The same set of assumptions as in Theorem 2
- $\min\{|x_i^{\min}| : |x_i^{\min}| \neq 0, i = 1, ..., p\} \geq$ threshold

Consider an S^{3}ONC solution $\mathbf{x}^*$. If $F_{n,\lambda}(\mathbf{x}^*) \leq F_{n,\lambda}(\mathbf{0})$ almost surely, and if the sample size n satisfies

$$n \gtrsim \frac{s}{\epsilon^2} \ln \frac{p}{\epsilon} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$$

then $\mathbb{P}\left[F(\mathbf{x}^*) - F(\mathbf{x}^{true}) \leq \epsilon\right] \geq 1 - \alpha$.

Much better than conventional SAA: $n \gtrsim \frac{p}{\epsilon^2} \ln \frac{1}{\epsilon} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$. Substantially better rate in p without compromise on the rate in ϵ.

Result IV: Efficacy of RSAA Under the Least Regularities

Theorem 4

Assumptions:

- $f(\mathbf{x}, W)$ is subgaussian for any $\mathbf{x} \in [0, R]^p$
- $f(\cdot, W)$ is twice differentiable for almost every W
- The true solution is sparse, i.e., $\|\mathbf{x}^{\min}\|_0 \leq s$
- Lipschitz-like condition

Consider the global minimal solution $\mathbf{x}^*$. If

$$n \gtrsim \frac{s}{\epsilon^3}\left(\ln\frac{p}{\epsilon}\right)^{1.5} + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}$$

then $\mathbb{P}\left[F(\mathbf{x}^*) - F(\mathbf{x}^{true}) \leq \epsilon\right] \geq 1 - \alpha$.

Summary of Results

	$n \gtrsim$	Global	$f(\cdot, W)$ convex	F strongly convex & differen -tiable	$\min_{i \in \mathcal{S}} \hat{x}_i^{\min}$ $\geq$ threshold
SAA	$\frac{p}{\epsilon^2} \ln \frac{1}{\epsilon} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$	✓	×	×	×
RSAA	$\frac{s}{\epsilon^3} \left(\ln \frac{p}{\epsilon}\right)^{1.5} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$	✓	×	×	×
	$\frac{s^{2.5}}{\epsilon^4} \left(\ln \frac{p}{\epsilon}\right)^{2} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$	×	✓	×	×
	$\frac{s^{1.5}}{\epsilon^3} \left(\ln \frac{p}{\epsilon}\right)^{1.5} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$	×	✓	✓	×
	$\frac{s}{\epsilon^2} \ln \frac{p}{\epsilon} + \frac{1}{\epsilon^2} \ln \frac{1}{\alpha}$	×	✓	✓	✓

- *In general:* poly-logarithmic dependence in p at the compromise on increased dependence in ϵ
- *A special case:* poly-logarithmic dependence in p at no compromise on increased dependence in ϵ

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Algorithms that guarantees S^3ONC

- S^3ONC is a weaker condition than the second-order KKT
- Algorithms that guarantees the second-order KKT exist in literature
  - Ye (1998)[5], Bian et al. (2015)[6], and Haeser, Liu, Ye, Math Program (2018).

[5] Ye (1998) Math Program

[6] Bian et al. (2015) Math Program

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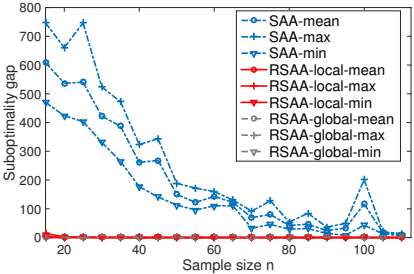
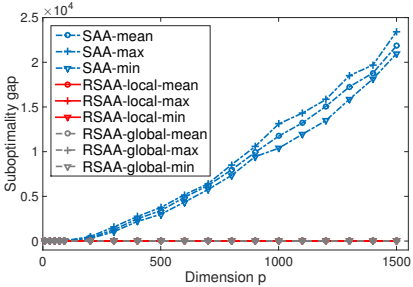
Numerical result





Summary

- RSAA: A new formulation of SAA to exploit sparsity[7]
- Aimed for high-dimensional stochastic programming
  $RSAA: \ n \geq \text{poly}(\ln p) \ \ v.s. \ \ SAA: \ n \geq \text{poly}(p)$
- RSAA admits FPTAS[8]
- Critical assumption on constraints: Box constraints

[7] Liu et al., Forthcoming in Math Program, 2018
[8] Haeser, Liu and Ye, Forthcoming in Math Program, 2018

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Section 3

Theoretical Extensions

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Theoretical Extension

- If initialized with a convex approximation, sharper bounds:

$$\tilde{O}\left(\frac{s^3}{\epsilon^3}(\ln p)^3 + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}\right)$$

  for convex case, initialized with convex program
- For linear constraints, $\{\mathbf{x} : C\mathbf{x} = \mathbf{b}, \mathbf{x} \geq 0\}$

$$\tilde{O}\left(\frac{(rk(C) - spark(C) + s)^3}{\epsilon^3}(\ln p)^3 + \frac{1}{\epsilon^2}\ln\frac{1}{\alpha}\right)$$

- For nonconvex objective function, for any S^3ONC in Γ-sublevel set:

$$\tilde{O}\left(\frac{(rk(C) - spark(C) + s)^3}{(\epsilon - \Gamma)^3}(\ln p)^3 + \frac{1}{(\epsilon - \Gamma)^2}\ln\frac{1}{\alpha} + \frac{\Gamma}{(\epsilon - \Gamma)^2}\right)$$

- Extendable to approximately sparse problems

$$\tilde{O}\left(\frac{(rk(C) - spark(C) + s)^3}{(\epsilon - \Gamma - \hat{\varepsilon})^3}(\ln p)^3 + \frac{1}{(\epsilon - \Gamma - \hat{\varepsilon})^2}\ln\frac{1}{\alpha} + \frac{\Gamma}{(\epsilon - \Gamma - \hat{\varepsilon})^2}\right)$$

Liu et al., 2018, Under review

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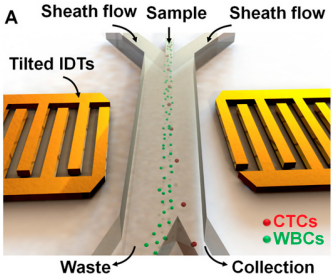
Section 4

Application to Designing Acoustic Tweezer

Acoustic Tweezer for Cell Separation

Differentiating one or multiple cell types from a heterogeneous group of cells using standing acoustic waves[9]



- bio-compatible, contact-less, and label-free (Laser, surface adherence, etc.)
- basic cell biology research
- cell-based regenerative therapies
- cell-level disease diagnostics
- 200μm v.s. 15μm
- Ultrasound frq: (19.4 MHz), Channel: 75 μm high, 1000μm wide.
- 83% accuracy

Emerging technology for cell manipulation

[9] Guo et al., PNAS, 2015; Ding et al., PNAS, 2014

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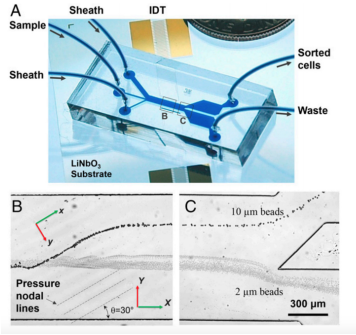
Acoustic Tweezer for Cell Separation

Differentiating one or multiple cell types from a heterogeneous group of cells using standing acoustic waves[10]



- Tweeze a cell by combination of
  1. Acoustic radiation force
  2. Gravitational force
  3. Buoyancy force
  4. Stokes drag force
- ARF dependent on density and pressibility
- Determine energy density
- Choose interdigitated transducers angles/distances

A lot of parameter tweaking is necessary

[10] Guo et al., PNAS, 2015; Ding et al., PNAS, 2014

Acoustic radiation force

Time averaged acoustic drag force depends on density and pressibility of cell[11]

$$\mathbf{F}_{ARF} = -\frac{4}{3}\pi N \sin(2Nd) E_{ac} \psi R^3 N \mathbf{u}$$

Acoustic contract factor:

$$\psi = \frac{5\rho_p - 2\rho_f}{2\rho_p - \rho_f} - \frac{\beta_\rho}{\beta_f}$$

- ρ_p and ρ_f: densities of particle and fluid, resp.
- β_p and β_f: pressibilities of particle and fluid, resp.
- N: wave number
- R: radius of particle
- E_{ac}: acoustic energy density
- d: distance from acoustic pressure node
- $\mathbf{u}$: unit vector from pressure node to pressure antinode

[11] Ding et al., PNAS, 2014

Dynamics

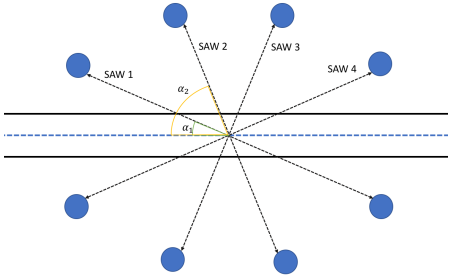
Dynamics:[12] [13]

$$
\begin{aligned}
\frac{dx}{dt} =& v_f + v_{r,x} \\
\frac{dy}{dt} =& v_{r,y} \\
\mathbf{F}_{drag} =& -6\mu\pi R\mathbf{v} \\
v_f =& \frac{\Delta P}{2\mu} b^2 \left[1 - \frac{Z^2}{b^2} + 4 \sum_{n=1}^{\infty} \frac{(-1)^n}{\beta_n^3} \cdot \frac{\cosh(\beta_n y/b)}{\cosh(\beta_n a/b)} \cos(\beta_n Z/b) \right] \\
\frac{dv_{r,x}}{dt} m =& F_{ARF,x} + F_{drag,x} \\
\frac{dv_{r,y}}{dt} m =& F_{ARF,y} + F_{drag,y}
\end{aligned}
$$

[12] Ding et al., PNAS, 2014

[13] Guo et al., PNAS, 2015

Design of acoustic tweezer



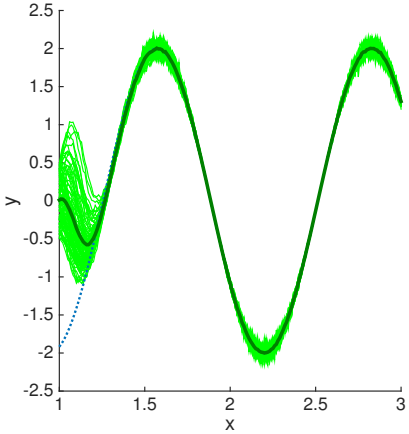
$$\min_{E_{ac,l}} \mathbb{E}\left[\sum_{p=1}^{P}\int_{t=0}^{T}[y_p(t)-y_p^{Target}(t)]^2dt\right]$$

$$s.t.\quad E_{ac,l}(t)\geq 0,\quad t\in[t_0,\,t_f],$$

Other dynamics linear in $E_{ac,l}(t)$

Pressibilities can be uncertain, initial condition can be uncertain.

Preliminary results



- 100 samples
- More than $200 \times 20 = 4000$ decision variables

Uryasev, Guo and Liu, Ongoing project, 2018

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Conclusions

- RSAA: A new formulation of SAA to exploit sparsity
- Application to acoustic tweezer design (ATD)
- More general constraints to be considered in future: Currently, RSAA assumes box/linear constraints
- More experiments for ATD: Currently, preliminary simulation results

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