Algorithms for Deterministically Constrained Stochastic Optimization

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involving joint work with

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presented at

International Conference on Continuous Optimization (ICCOPT)

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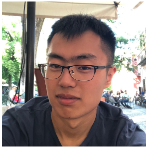
Collaborators and references

- A. S. Berahas, F. E. Curtis, D. P. Robinson, and B. Zhou, "Sequential Quadratic Optimization for Nonlinear Equality Constrained Stochastic Optimization," *SIAM Journal on Optimization*, 31(2):1352–1379, 2021.
- A. S. Berahas, F. E. Curtis, M. J. O'Neill, and D. P. Robinson, "A Stochastic Sequential Quadratic Optimization Algorithm for Nonlinear Equality Constrained Optimization with Rank-Deficient Jacobians," https://arxiv.org/abs/2106.13015.
- F. E. Curtis, D. P. Robinson, and B. Zhou, "Inexact Sequential Quadratic Optimization for Minimizing a Stochastic Objective Subject to Deterministic Nonlinear Equality Constraints," https://arxiv.org/abs/2107.03512.
- F. E. Curtis, M. J. O'Neill, and D. P. Robinson, "Worst-Case Complexity of an SQP Method for Nonlinear Equality Constrained Stochastic Optimization," https://arxiv.org/abs/2112.14799.

Talks at ICCOPT

Wednesday, 10:25am-11:45am, Rauch 241

- Baoyu Zhou, "SQP Methods for Inequality Constrained Stochastic Optimization"
- Raghu Bollapragada, "Adaptive Sampling Stochastic Sequential Quadratic Programming"
- Jiahao Shi, "Accelerating Sequential Quadratic Programming for Equality Constrained Stochastic Optimization using Predictive Variance Reduction"

Outline

Outline

Constrained optimization (deterministic)

Consider

$$\boxed{\begin{aligned} \min_{x\in\mathbb{R}^n}\ & f(x) \\ \text{s.t. } & c_{\mathcal{E}}(x) = 0 \\ & c_{\mathcal{I}}(x) \leq 0 \end{aligned}}$$

where $f : \mathbb{R}^n \to \mathbb{R}$, $c_{\mathcal{E}} : \mathbb{R}^n \to \mathbb{R}^{m_{\mathcal{E}}}$, and $c_{\mathcal{I}} : \mathbb{R}^n \to \mathbb{R}^{m_{\mathcal{I}}}$ are smooth

- Physics-constrained, resource-constrained, etc.
- Long history of algorithms (penalty, SQP, interior-point, etc.)
- Comprehensive theory (even with lack of constraint qualifications)
- Effective software (Ipopt, Knitro, LOQO, etc.)

Constrained optimization (stochastic constraints)

Consider

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \ & f(x) \\ \text{s.t. } & c_{\mathcal{E}}(x) = 0 \\ & c_{\mathcal{I}}(x, \omega) \lesssim 0 \end{aligned}$$

where $f : \mathbb{R}^n \to \mathbb{R}$, $c_{\mathcal{E}} : \mathbb{R}^n \to \mathbb{R}^{m_{\mathcal{E}}}$, and $c_{\mathcal{I}} : \mathbb{R}^n \times \Omega \to \mathbb{R}^{m_{\mathcal{I}}}$

- Various modeling paradigms:
- . . . stochastic optimization
- . . . (distributionally) robust optimization
- . . . chance-constrained optimization

Constrained optimization (stochastic objective)

Consider

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \ & f(x) \equiv \mathbb{E}[F(x,\omega)] \\ \text{s.t.} \ & c_{\mathcal{E}}(x) = 0 \\ & c_{\mathcal{I}}(x) \leq 0 \end{aligned}$$

where $f : \mathbb{R}^n \times \mathbb{R}$, $F : \mathbb{R}^n \times \Omega \to \mathbb{R}$, $c_{\mathcal{E}} : \mathbb{R}^n \to \mathbb{R}^{m_{\mathcal{E}}}$, and $c_{\mathcal{I}} : \mathbb{R}^n \to \mathbb{R}^{m_{\mathcal{I}}}$

- ω has probability space $(\Omega, \mathcal{F}, P)$
- $\mathbb{E}[\cdot]$ with respect to P
- Classical applications under uncertainty, constrained DNN training, etc.
- Besides cases involving a deterministic equivalent...
- ... very few algorithms so far (mostly penalty methods)

What kind of algorithm do we want?

Need to establish what we want/expect from an algorithm.

Note: We are interested in the fully stochastic regime.[†]

We assume:

- Feasible methods are not tractable
- ... so no projection methods, Frank-Wolfe, etc.
- "Two-phase" methods are not effective
- ... so should not search for feasibility, then optimize.
- Only enforce convergence in expectation.

Finally, want to use techniques that can generalize to diverse settings.

[†] Alternatively, see Na, Anitescu, Kolar (2021, 2022)

This talk

Consider *equality constrained* stochastic optimization:

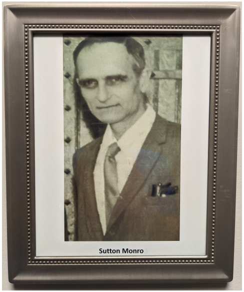
$$\min_{x\in\mathbb{R}^n} f(x) \equiv \mathbb{E}[F(x,\omega)]$$
$$\text{s.t. } c_{\mathcal{E}}(x) = 0$$

- *Adaptive* SQP method for deterministic setting
- *Stochastic* SQP method for stochastic setting
- Convergence in expection (comparable to SG for unconstrained setting)
- Worst-case complexity on par with stochastic subgradient method
- Numerical experiments are very promising
- Various open questions!

Outline

Stochastic gradient method (SG)

Invented by Herbert Robbins and Sutton Monro (1951)



Sutton Monro, former Lehigh faculty member

Stochastic gradient (*not* descent)

Consider the stochastic optimization problem

$$\min_{x \in \mathbb{R}^n} \; f(x) \equiv \mathbb{E}[F(x,\omega)]$$

where $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz continuous with constant L

Algorithm SG : Stochastic Gradient

1: choose an initial point $x_0 \in \mathbb{R}^n$ and step sizes $\{\alpha_k\} > 0$
2: **for** $k \in \{0, 1, 2, \dots\}$ **do**
3: set $x_{k+1} \leftarrow x_k - \alpha_k g_k$, where $\mathbb{E}_k[g_k] = \nabla f(x_k)$ and $\mathbb{E}_k[\|g_k - \nabla f(x_k)\|_2^2] \leq M$
4: **end for**

Not a descent method! . . . but *eventual descent in expectation*:

$$\begin{aligned} f(x_{k+1}) - f(x_k) &\leq \nabla f(x_k)^T (x_{k+1} - x_k) + \tfrac{1}{2} L \|x_{k+1} - x_k\|_2^2 \\ &= -\alpha_k \nabla f(x_k)^T g_k + \tfrac{1}{2} \alpha_k^2 L \|g_k\|_2^2 \end{aligned}$$

$$\implies \mathbb{E}_k[f(x_{k+1})] - f(x_k) \leq -\alpha_k \|\nabla f(x_k)\|_2^2 + \tfrac{1}{2} \alpha_k^2 L \mathbb{E}_k[\|g_k\|_2^2].$$

Markovian: x_{k+1} depends only on x_k and random choice at iteration k.

SG theory

Theorem SG

Since $\mathbb{E}_k[g_k] = \nabla f(x_k)$ *and* $\mathbb{E}_k[\|g_k - \nabla f(x_k)\|_2^2] \leq M$ *for all* $k \in \mathbb{N}$*:*

$$\alpha_k = \frac{1}{L} \qquad \Longrightarrow \mathbb{E}\left[\frac{1}{k}\sum_{j=1}^{k} \|\nabla f(x_j)\|_2^2\right] \leq \mathcal{O}(M)$$

$$\alpha_k = \Theta\left(\frac{1}{k}\right) \qquad \Longrightarrow \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^{k} \alpha_j\right)}\sum_{j=1}^{k} \alpha_j \|\nabla f(x_j)\|_2^2\right] \to 0$$

$$\Longrightarrow \liminf_{k\to\infty} \mathbb{E}[\|\nabla f(x_k)\|_2^2] = 0$$

Sequential quadratic optimization (SQP)

Consider

$$\min_{x \in \mathbb{R}^n} \; f(x) \quad \text{s.t. } c(x) = 0$$

with $J \equiv \nabla c$ and $H \succ 0$ (for simplicity), two viewpoints:

$$\begin{bmatrix} \nabla f(x) + J(x)^T y \\ c(x) \end{bmatrix} = 0 \qquad \text{or} \qquad \min_{d \in \mathbb{R}^n} \; f(x) + \nabla f(x)^T d + \tfrac{1}{2} d^T H d \quad \text{s.t. } c(x) + J(x) d = 0$$

both leading to the same "Newton-SQP system":

$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = - \begin{bmatrix} \nabla f(x_k) \\ c_k \end{bmatrix}$$

SQP

- Algorithm guided by merit function, with adaptive parameter τ, defined by

$$\phi(x,\tau) = \tau f(x) + \|c(x)\|_1$$

a model of which is defined as

$$q(x,\tau,\nabla f(x),d) = \tau(f(x) + \nabla f(x)^T d + \tfrac{1}{2} d^T H d) + \|c(x) + J(x)d\|_1$$

- For a given $d \in \mathbb{R}^n$ satisfying $c(x) + J(x)d = 0$, the reduction in this model is

$$\Delta q(x,\tau,\nabla f(x),d) = -\tau(\nabla f(x)^T d + \tfrac{1}{2} d^T H d) + \|c(x)\|_1,$$

and it is easily shown that

$$\phi'(x,\tau,d) \leq -\Delta q(x,\tau,\nabla f(x),d)$$

SQP with backtracking line search

Algorithm SQP-B

choose $x_0 \in \mathbb{R}^n$, $\tau_{-1} \in \mathbb{R}_{>0}$, $\sigma \in (0,1)$, $\eta \in (0,1)$
for $k \in \{0,1,2,\dots\}$ **do**
    solve

$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = - \begin{bmatrix} \nabla f(x_k) \\ c_k \end{bmatrix}$$

    set τ_k to ensure $\Delta q(x_k, \tau_k, \nabla f(x_k), d_k) \gg 0$, offered by

$$\tau_k \leq \frac{(1-\sigma)\|c_k\|_1}{\nabla f(x_k)^T d_k + d_k^T H_k d_k} \quad \text{if} \quad \nabla f(x_k)^T d_k + d_k^T H_k d_k > 0$$

    backtracking line search to ensure $x_{k+1} \leftarrow x_k + \alpha_k d_k$ yields

$$\phi(x_{k+1}, \tau_k) \leq \phi(x_k, \tau_k) - \eta \alpha_k \Delta q(x_k, \tau_k, \nabla f(x_k), d_k)$$

end for

SQP with adaptive step sizes

Algorithm SQP-A

1: choose $x_0 \in \mathbb{R}^n$, $\tau_{-1} \in \mathbb{R}_{>0}$, $\sigma \in (0,1)$, $\eta \in (0,1)$
2: **for** $k \in \{0,1,2,\dots\}$ **do**
3: solve

$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = - \begin{bmatrix} \nabla f(x_k) \\ c_k \end{bmatrix}$$

4: set τ_k to ensure $\Delta q(x_k, \tau_k, \nabla f(x_k), d_k) \gg 0$, offered by

$$\tau_k \leq \frac{(1-\sigma)\|c_k\|_1}{\nabla f(x_k)^T d_k + d_k^T H_k d_k} \quad \text{if} \quad \nabla f(x_k)^T d_k + d_k^T H_k d_k > 0$$

5: set

$$\widehat{\alpha}_k \leftarrow \frac{2(1-\eta)\Delta q(x_k, \tau_k, \nabla f(x_k), d_k)}{(\tau_k L_k + \Gamma_k)\|d_k\|_2^2} \quad \text{and}$$

$$\widetilde{\alpha}_k \leftarrow \widehat{\alpha}_k - \frac{4\|c_k\|_1}{(\tau_k L_k + \Gamma_k)\|d_k\|_2^2}$$

6: set

$$\alpha_k \leftarrow \begin{cases} \widehat{\alpha}_k & \text{if } \widehat{\alpha}_k < 1 \\ 1 & \text{if } \widetilde{\alpha}_k \leq 1 \leq \widehat{\alpha}_k \\ \widetilde{\alpha}_k & \text{if } \widetilde{\alpha}_k > 1 \end{cases}$$

7: set $x_{k+1} \leftarrow x_k + \alpha_k d_k$ and continue or update L_k and/or Γ_k and return to step 5
8: **end for**

Convergence theory

Assumption

- *f, c, ∇f, and J bounded and Lipschitz*
- *singular values of J bounded below (i.e., the LICQ)*
- $u^T H_k u \geq \zeta \|u\|_2^2$ *for all* $u \in \text{Null}(J_k)$ *for all* $k \in \mathbb{N}$

Theorem SQP-B

- $\{\alpha_k\} \geq \alpha_{\min}$ *for some* $\alpha_{\min} > 0$
- $\{\tau_k\} \geq \tau_{\min}$ *for some* $\tau_{\min} > 0$
- $\Delta q(x_k, \tau_k, \nabla f(x_k), d_k) \to 0$ *implies*

$$\|d_k\|_2 \to 0, \quad \|c_k\|_2 \to 0, \quad \|\nabla f(x_k) + J_k^T y_k\|_2 \to 0$$

Outline

Motivation

SG and SQP

Stochastic SQP

Extensions

Conclusion

Stochastic setting

Consider the stochastic problem:

$$\min_{x \in \mathbb{R}^n} \; f(x) \equiv \mathbb{E}[F(x,\omega)] \quad \text{s.t. } c(x) = 0$$

Let us assume only the following:

Assumption

For all $k \in \mathbb{N}$, one can compute g_k with

$$\mathbb{E}_k[g_k] = \nabla f(x_k) \;\; \textit{and} \;\; \mathbb{E}_k[\|g_k - \nabla f(x_k)\|_2^2] \leq M$$

Search directions computed by:

$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = - \begin{bmatrix} g_k \\ c_k \end{bmatrix}$$

Important: Given x_k, the values (c_k, J_k, H_k) are determined

Stochastic SQP with adaptive step sizes

(For simplicity, assume Lipschitz constants L and Γ are known.)

Algorithm : Stochastic SQP

choose $x_0 \in \mathbb{R}^n$, $\tau_{-1} \in \mathbb{R}_{>0}$, $\sigma \in (0,1)$, $\{\beta_k\} \in (0,1]$

for $k \in \{0,1,2,\ldots\}$ **do**

solve

$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = -\begin{bmatrix} g_k \\ c_k \end{bmatrix}$$

set τ_k to ensure $\Delta q(x_k, \tau_k, g_k, d_k) \gg 0$, offered by

$$\tau_k \leq \frac{(1-\sigma)\|c_k\|_1}{g_k^T d_k + d_k^T H_k d_k} \quad \text{if} \quad g_k^T d_k + d_k^T H_k d_k > 0$$

set

$$\widehat{\alpha}_k \leftarrow \frac{\beta_k \Delta q(x_k, \tau_k, g_k, d_k)}{(\tau_k L + \Gamma)\|d_k\|_2^2} \quad \text{and}$$

$$\widetilde{\alpha}_k \leftarrow \widehat{\alpha}_k - \frac{4\|c_k\|_1}{(\tau_k L + \Gamma)\|d_k\|_2^2}$$

set

$$\alpha_k \leftarrow \begin{cases} \widehat{\alpha}_k & \text{if } \widehat{\alpha}_k < 1 \\ 1 & \text{if } \widetilde{\alpha}_k \leq 1 \leq \widehat{\alpha}_k \\ \widetilde{\alpha}_k & \text{if } \widetilde{\alpha}_k > 1 \end{cases}$$

set $x_{k+1} \leftarrow x_k + \alpha_k d_k$

end for

Good merit parameter behavior

Lemma

For all $k \in \mathbb{N}$, for any realization of g_k, one finds

$$\begin{aligned}&\phi(x_k + \alpha_k d_k, \tau_k) - \phi(x_k, \tau_k)\\ \leq\ &\underbrace{-\alpha_k \Delta q(x_k, \tau_k, \nabla f(x_k), d_k^{\text{true}})}_{\mathcal{O}(\beta_k),\ \text{“deterministic”}} + \underbrace{\tfrac{1}{2}\alpha_k \beta_k \Delta q(x_k, \tau_k, g_k, d_k)}_{\mathcal{O}(\beta_k^2),\ \text{stochastic/noise}} + \underbrace{\alpha_k \tau_k \nabla f(x_k)^T (d_k - d_k^{\text{true}})}_{\text{due to adaptive } \alpha_k}\end{aligned}$$

Theorem

If $\{\tau_k\}$ eventually remains fixed at sufficiently small $\tau_{\min} > 0$, then for large k

$$\beta_k = \Theta(1) \implies \mathbb{E}\left[\frac{1}{k}\sum_{j=1}^{k} \Delta q(x_j, \tau_{\min}, \nabla f(x_j), d_j^{\text{true}})\right] \leq \mathcal{O}(M)$$

$$\beta_k = \Theta\left(\frac{1}{k}\right) \implies \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^{k} \beta_j\right)} \sum_{j=1}^{k} \beta_j \Delta q(x_j, \tau_{\min}, \nabla f(x_j), d_j^{\text{true}})\right] \to 0$$

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Theorem

If $\{\tau_k\}$ eventually remains fixed at sufficiently small $\tau_{\min} > 0$, then for large k

$$\beta_k = \Theta(1) \implies \mathbb{E}\left[\frac{1}{k}\sum_{j=1}^{k} (\|g_j + J_j^T y_j^{\text{true}}\|_2 + \|c_j\|_2)\right] \leq \mathcal{O}(M)$$

$$\beta_k = \Theta\left(\frac{1}{k}\right) \implies \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^{k}\beta_j\right)}\sum_{j=1}^{k} \beta_j (\|g_j + J_j^T y_j^{\text{true}}\|_2 + \|c_j\|_2)\right] \to 0$$

Numerical results

Matlab software: https://github.com/frankecurtis/StochasticSQP

CUTE problems with noise added to gradients with different noise levels

- Stochastic SQP: 10^3 iterations
- Stochastic Subgradient: 10^4 iterations and tuned over 11 values of τ

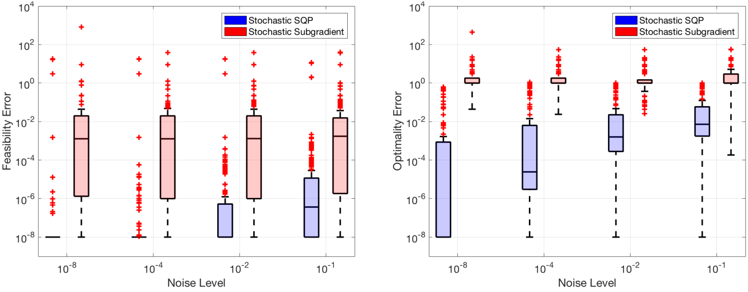


Figure: Box plots for feasibility errors (left) and optimality errors (right).

Outline

- Motivation
- SG and SQP
- Stochastic SQP
- Extensions
- Conclusion

Complexity of deterministic algorithm

All reductions in the merit function can be cast in terms of smallest τ.

Lemma 5

If $\{\tau_k\}$ eventually remains fixed at sufficiently small $\tau_{\min}$, then for any $\epsilon \in (0,1)$ there exists $(\kappa_1, \kappa_2) \in (0,\infty) \times (0,\infty)$ such that, for all k,

$$\|\nabla f(x_k) + J_k^T y_k\| > \epsilon \text{ or } \sqrt{\|c_k\|_1} > \epsilon \implies \Delta q(x_k, \tau_k, d_k) \geq \min\{\kappa_1, \kappa_2 \tau_{\min}\}\epsilon.$$

Since $\tau_{\min}$ is determined by the initial point, *it will be reached.*

Theorem 6

For any $\epsilon \in (0,1)$, there exists $(\kappa_1, \kappa_2) \in (0,\infty) \times (0,\infty)$ such that

$$\|\nabla f(x_k) + J_k^T y_k\| \leq \epsilon \text{ and } \sqrt{\|c_k\|_1} \leq \epsilon$$

in a number of iterations no more than

$$\left(\frac{\tau_{-1}(f_0 - f_{\inf}) + \|c_0\|_1}{\min\{\kappa_1, \kappa_2 \tau_{\min}\}}\right)\epsilon^{-2}.$$

Worst-case iteration complexity of $\widetilde{\mathcal{O}}(\epsilon^{-4})$

Theorem 7

Suppose the algorithm is run

- $k_{\max}$ *iterations with*
- $\beta_k = \gamma/\sqrt{k_{\max}+1}$ *and*
- *the merit parameter is reduced at most* $s_{\max} \in \{0, 1, \dots, k_{\max}\}$ *times.*

Let k_* *be sampled uniformly over* $\{1, \dots, k_{\max}\}$*. Then, with probability* $1-\delta$*,*

$$\mathbb{E}[\|g_{k_*} + J_{k_*}^T y_{k_*}^{\text{true}}\|_2^2 + \|c_{k_*}\|_1] \leq \frac{\tau_{-1}(f_0 - f_{\inf}) + \|c_0\|_1 + M}{\sqrt{k_{\max}+1}} + \frac{(\tau_{-1} - \tau_{\min})(s_{\max}\log(k_{\max}) + \log(1/\delta))}{\sqrt{k_{\max}+1}}$$

Theorem 8

If the stochastic gradient estimates are sub-Gaussian, then w.p. $1-\bar{\delta}$

$$s_{\max} = \mathcal{O}\left(\log\left(\log\left(\frac{k_{\max}}{\bar{\delta}}\right)\right)\right).$$

Recent work (under review): No LICQ

Remove constraint qualification

- infeasible and/or degenerate problems
- step decomposition method

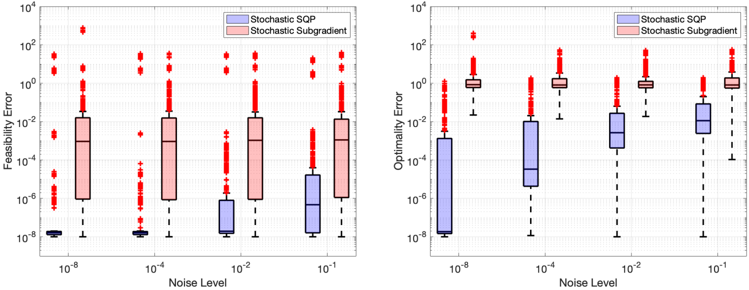


Figure: Box plots for feasibility errors (left) and optimality errors (right).

Matrix-free algorithm

Solving for the search directions can be expensive:

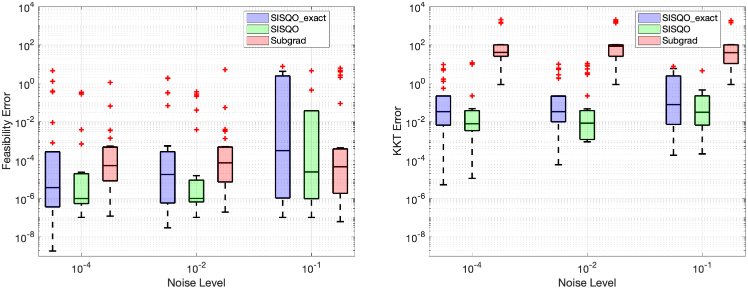
$$\begin{bmatrix} H_k & J_k^T \\ J_k & 0 \end{bmatrix} \begin{bmatrix} d_k \\ y_k \end{bmatrix} = - \begin{bmatrix} \nabla f(x_k) \\ c_k \end{bmatrix}$$

To avoid direct+exact solves,

- aim to use iterative solver(s) and
- allow inexactness in the subproblem solves.

Algorithm now involves both *stochasticity* and *inexactness*.

Results on CUTEst problems



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Summary

Consider *equality constrained* stochastic optimization:

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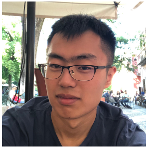
$$\text{s.t. } c_{\mathcal{E}}(x) = 0$$

- *Adaptive* SQP method for deterministic setting
- *Stochastic* SQP method for stochastic setting
- Convergence in expection (comparable to SG for unconstrained setting)
- Worst-case complexity on par with stochastic subgradient method
- Numerical experiments are very promising
- Various extensions (on-going)

Collaborators and references



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