Appendix 00000000

# Stochastic-Gradient-based Algorithms for Solving Nonconvex Constrained Optimization Problems

Frank E. Curtis, Lehigh University

presented at

Numerical Analysis Seminar

University of Maryland, College Park

October 15, 2024



Stochastic Algorithms for Nonconvex Constrained Optimization

## Outline

Motivation

Stochastic Algorithms for Nonconvex Optimization

Extensions and Experimental Results

#### Conclusion

#### Appendix

Stochastic Algorithms for Nonconvex Constrained Optimization

## Outline

#### Motivation

Stochastic Algorithms for Nonconvex Optimization

Extensions and Experimental Results

#### Conclusion

Appendix

 $\substack{ \operatorname{Appendix} \\ \operatorname{00000000} }$ 

# Learning: Prediction function

#### **Aim**: Determine a prediction function p from a family $\mathcal{P}$ such that

#### $p(a_j)$

yields an accurate prediction corresponding to any given input feature vector  $a_j$ .

Appendix 00000000

## Learning: Prediction function, parameterized

Let us say that the family is parameterized by some vector x such that

#### $p(a_j, x)$

yields an accurate prediction corresponding to any given input feature vector  $a_j$ .

# Learning: Supervised

In supervised learning, we have known input-output pairs  $\{(a_j, b_j)\}_{i=1}^{n_o}$ . Then,

$$\min_{x \in \mathbb{R}^n} \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(p(a_j, x), b_j)$$

becomes our empirical-loss training problem to determine the optimal x.

 $\substack{\text{Appendix}\\00000000}$ 

# Learning: Supervised and regularized

If we aim to impose some structure on the solution x, then we may consider

$$\min_{x \in \mathbb{R}^n} \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(p(a_j, x), b_j) + r(x)$$

where r is a *regularization* function.

 $\substack{ \operatorname{Appendix} \\ 00000000 }$ 

## Learning: Supervised and regularized

If we aim to impose some structure on the solution x, then we may consider

$$\min_{x \in \mathbb{R}^n} \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(p(a_j, x), b_j) + r(x)$$

where r is a *regularization* function. Is this good for *informed* learning?

#### Learning: Supervised and informed through model design

One approach is to embed information in the prediction function itself, so

$$\min_{x \in \mathbb{R}^n} \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(\mathbf{p}(a_j, x), b_j)$$

ensures that information is enforced with every forward pass. (Is this enough and/or efficient?)

### Learning: Supervised and informed with *soft* constraints

Added to the loss (e.g., mean-squared error), we might consider

$$\min_{x \in \mathbb{R}^n} \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(p(a_j, x), b_j) + \frac{1}{n_c} \sum_{j=1}^{n_c} \phi(p(\tilde{a}_j, x), \dots, \tilde{b}_j)$$

where  $\{(\tilde{a}_j, \tilde{b}_j)\}_{j=1}^{n_c}$  are known input-output pairs and  $\phi$  encodes information.

Appendix

## Learning: Supervised and informed with *hard* constraints

Alternatively, how about *hard* constraints during training, as in

$$\begin{split} & \min_{x \in \mathbb{R}^n} \;\; \frac{1}{n_o} \sum_{j=1}^{n_o} \ell(p(a_j, x), b_j) \\ & \text{s.t.} \;\; \varphi(p(\tilde{a}_j, x), \dots, \tilde{b}_j) = 0 \;\; (\text{or} \leq 0) \;\; \text{for all} \;\; i \in \{1, \dots, n_c\} \end{split}$$

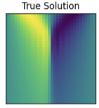
such that we restrict attention to functions that are informed implicitly?

Motivation	Stochastic Algorithms for Nonconvex Optimiz	ation
000000	000000000000	

### Motivation and challenges: Stochastic algorithms for constrained optimization

Motivated by informed learning when model design + regularization is insufficient

- physics-informed machine learning
- ▶ fair (supervised) machine learning
- ▶ ... but algorithms are general-purpose, e.g., also for simulation optimization



Epoch 10001



## Motivation and challenges: Stochastic algorithms for constrained optimization

Motivated by informed learning when model design + regularization is insufficient

- physics-informed machine learning
- ▶ fair (supervised) machine learning
- $\blacktriangleright$  ... but algorithms are general-purpose, e.g., also for simulation optimization

Same challenges and questions as for unconstrained:

- convergence/complexity guarantees (adaptive algorithms)
- computational complexity
- stability guarantees
- generalization properties

True Solution







Appendix 00000000

### Motivation and challenges: Stochastic algorithms for constrained optimization

Motivated by informed learning when model design + regularization is insufficient

- physics-informed machine learning
- ▶ fair (supervised) machine learning
- ▶ ... but algorithms are general-purpose, e.g., also for simulation optimization

Same challenges and questions as for unconstrained:

- convergence/complexity guarantees (adaptive algorithms)
- computational complexity
- stability guarantees
- generalization properties

New challenges for handling constraints as constraints:

- ▶ (i.e., avoid penalty methods, augmented Lagrangian, etc.)
- balancing the objective and constraints
- degeneracy and infeasibility

True Solution







Motivation	Stochastic Algorithms for Nonconvex Optimization
000000	00000000000

Extensions and Experiments 00000000000

Conclusion 0000 Appendix 00000000

# Predicting movement of a spring

Problem from https://benmoseley.blog/blog/

Appendix 00000000

### Expected-loss training problems

For the sake of generality/generalizability, the expected-loss objective function is

$$\int_{\mathcal{A}\times\mathcal{B}} \ell(p(a,x),b) \mathrm{d}\mathbb{P}(a,b) \equiv \mathbb{E}_{\omega}[F(x,\omega)] =: f(x)$$

One might consider various paradigms for imposing the constraints:

- expectation constraints
- (distributionally) robust constraints
- ▶ probabilistic (i.e., chance) constraints

In this talk, constraints values and derivatives can be computed:

 $c_{\mathcal{E}}(x) = 0$  and  $c_{\mathcal{I}}(x) \leq 0$ 

e.g., imposing a fixed set of constraints corresponding to a fixed set of sample data

## Outline

#### Motivation

#### Stochastic Algorithms for Nonconvex Optimization

**Extensions and Experimental Results** 

#### Conclusion

Appendix

## Stochastic gradient method

Consider  $\min_{x \in \mathbb{R}^n} f(x)$ , where  $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$  is Lipschitz continuous with constant L.

Algorithm SG : Stochastic gradient method

1: choose an initial point  $x_1 \in \mathbb{R}^n$  and step sizes  $\{\alpha_k\} > 0$ 2: for  $k \in \{1, 2, ...\} =: \mathbb{N}$  do 3: set  $x_{k+1} \leftarrow x_k - \alpha_k g_k$ , where  $g_k \approx \nabla f(x_k)$ 4: end for

Algorithm<sup>†</sup> behavior is defined by  $(\Omega, \mathcal{F}, \mathbb{P})$ , where

- $\Omega = \Gamma \times \Gamma \times \Gamma \times \cdots$  (sequence of draws determining stochastic gradients);
- $\blacktriangleright$   $\mathcal{F}$  is a  $\sigma$ -algebra on  $\Omega$ , the set of events (i.e., measurable subsets of  $\Omega$ ); and
- ▶  $\mathbb{P}$  :  $\mathcal{F} \to [0, 1]$  is a probability measure.

View any  $\{(x_k, g_k)\}$  as a realization of  $\{(X_k, G_k)\}$ , where for all  $k \in \mathbb{N}$ 

 $x_k = X_k(\omega)$  and  $g_k = G_k(\omega)$  given  $\omega \in \Omega$ .

<sup>†</sup>Robbins and Monro (1951); Sutton Monro = former Lehigh ISE faculty member

Stochastic Algorithms for Nonconvex Constrained Optimization

Appendix

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization $000000000000000000000000000000000000$	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000

### Convergence of SG

 $\mathbb{E}[\cdot] =$ expectation w.r.t.  $\mathbb{P}[\cdot]$ . Analyze through associated sub- $\sigma$ -algebras  $\{\mathcal{F}_k\}$ .

Assumption

For all  $k \in \mathbb{N}$ , one has that

- $\blacktriangleright \mathbb{E}[G_k | \mathcal{F}_k] = \nabla f(X_k) \text{ and }$
- $\blacktriangleright \mathbb{E}[\|G_k\|_2^2|\mathcal{F}_k] \le M + M_{\nabla f} \|\nabla f(X_k)\|_2^2$

By Lipschitz continuity of  $\nabla f$  and construction of the algorithm, one finds

$$f(X_{k+1}) - f(X_k) \leq \nabla f(X_k)^T (X_{k+1} - X_k) + \frac{1}{2}L \|X_{k+1} - X_k\|_2^2$$
  
$$= -\alpha_k \nabla f(X_k)^T G_k + \frac{1}{2}\alpha_k^2 L \|G_k\|_2^2$$
  
$$\implies \mathbb{E}[f(X_{k+1})|\mathcal{F}_k] - f(X_k) \leq -\alpha_k \|\nabla f(X_k)\|_2^2 + \frac{1}{2}\alpha_k^2 L \mathbb{E}[\|G_k\|_2^2|\mathcal{F}_k]$$
  
$$\leq -\alpha_k \|\nabla f(X_k)\|_2^2 + \frac{1}{2}\alpha_k^2 L (M + M_{\nabla f} \|\nabla f(X_k)\|_2^2)$$

by the assumption and since  $f(X_k)$  and  $\nabla f(X_k)$  are  $\mathcal{F}_k$ -measurable.

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000

#### Conclusion

 $\substack{\mathrm{Appendix}\\00000000}$ 

# SG theory

Taking total expectation, one arrives at

$$\mathbb{E}[f(X_{k+1}) - f(X_k)] \le -\alpha_k (1 - \frac{1}{2}\alpha_k L M_{\nabla f}) \mathbb{E}[\|\nabla f(X_k)\|_2^2] + \frac{1}{2}\alpha_k^2 L M$$

### Theorem

$$\begin{aligned} \alpha_k &= \frac{1}{LM_{\nabla f}} &\implies \mathbb{E}\left[\frac{1}{k}\sum_{j=1}^k \|\nabla f(X_j)\|_2^2\right] \le M_k \xrightarrow{k \to \infty} \mathcal{O}\left(\frac{M}{M_{\nabla f}}\right) \\ \alpha_k &= \Theta\left(\frac{1}{k}\right) &\implies \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^k \alpha_j\right)}\sum_{j=1}^k \alpha_j \|\nabla f(X_j)\|_2^2\right] \to 0 \\ &\implies \liminf_{k \to \infty} \mathbb{E}[\|\nabla f(X_k)\|_2^2] = 0 \\ (further steps) &\implies \nabla f(X_k) \to 0 \text{ almost surely.} \end{aligned}$$

Appendix 00000000

### Constrained optimization

 $\operatorname{Consider}$ 

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

Option: Regularization / soft constraints (penalization), as in

 $\min_{x \in \mathbb{R}^n} \tau f(x) + \|c(x)\|_q^p (+y^T c(x)),$ 

then employ a (stochastic) algorithm for unconstrained optimization.

Appendix 00000000

### Constrained optimization

Consider

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

Option: Regularization / soft constraints (penalization), as in

 $\min_{x \in \mathbb{R}^n} \tau f(x) + \|c(x)\|_q^p (+y^T c(x)),$ 

then employ a (stochastic) algorithm for unconstrained optimization.

On the positive side, "exact" penalty function theory is well established:

▶ *can* solve the constrained problem, in theory.

Unfortunately, however, such an approach is not ideal:

- ▶ appropriate balance  $(\tau \text{ and/or } y)$  not known in advance
- ▶ p = 1 (nonsmooth), p = 2 (need  $\tau \searrow 0$ , ill-conditioning)

# Sequential quadratic optimization (SQP)

 $\operatorname{Consider}$ 

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

Option: With  $J \equiv \nabla c^T$  and H positive definite over Null(J), two viewpoints:

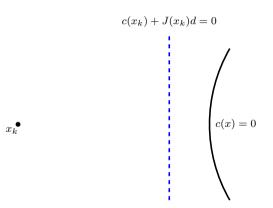
$$\begin{bmatrix} \nabla f(x) + J(x)^T y \\ c(x) \end{bmatrix} = 0 \quad \text{or} \quad$$

$$\min_{d \in \mathbb{R}^n} f(x) + \nabla f(x)^T d + \frac{1}{2} d^T H d$$
  
s.t.  $c(x) + J(x)d = 0$ 

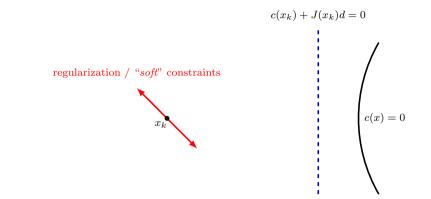
both leading to the same "Newton-SQP system":

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

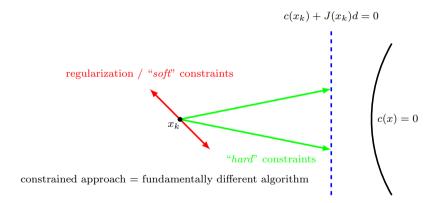
Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000



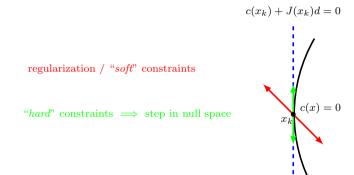
Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000



Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000
1				/



Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	



i.

Appendix 00000000

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000

## Stochastic SQP

Algorithm guided by merit function with adaptive parameter  $\tau$  defined by

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

#### Algorithm : Stochastic SQP

- 1: choose  $x_1 \in \mathbb{R}^n, \, \tau_0 \in (0,\infty), \, \{\beta_k\} \in (0,1]^{\mathbb{N}}$
- 2: for  $k \in \{1, 2, ...\}$  do
- 3: compute step: solve

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

4: update merit parameter: set  $\tau_k$  to ensure

$$\phi'(x_k, \tau_k, d_k) \le -\Delta q(x_k, \tau_k, g_k, d_k) \ll 0$$

5: compute step size: set

$$\alpha_k = \Theta\left(\frac{\beta_k \tau_k}{\tau_k L_{\nabla f} + L_J}\right)$$

6: then  $x_{k+1} \leftarrow x_k + \alpha_k d_k$ 7: end for

### Convergence theory in *deterministic setting*

#### Assumption

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

#### Theorem

- $\{\alpha_k\} \ge \alpha_{\min} \text{ for some } \alpha_{\min} > 0$
- $\{\tau_k\} \ge \tau_{\min}$  for some  $\tau_{\min} > 0$
- $\Delta q(x_k, \tau_k, \nabla f(x_k), d_k) \to 0$  implies optimality error vanishes, specifically,

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

# Stochastic setting: What do we want?

What we want/expect from the algorithm?

Note: We are interested in the stochastic approximation (SA) regime.

Ultimately, there are *many* questions to answer:

- convergence guarantees
- complexity guarantees
- tradeoff analysis (Bottou and Bousquet)
- generalization
- large-scale implementations
- ▶ beyond first-order (SG) methods

Appendix 00000000

#### Fundamental lemma

Recall in the unconstrained setting that

$$\mathbb{E}[f(X_{k+1})|\mathcal{F}_{k}] - f(X_{k}) \leq -\alpha_{k} \|\nabla f(X_{k})\|_{2}^{2} + \frac{1}{2}\alpha_{k}^{2} L\mathbb{E}[\|G_{k}\|_{2}^{2}|\mathcal{F}_{k}]$$

#### Lemma

For all  $k \in \mathbb{N}$  one finds (before taking expectations)

$$\begin{array}{l} \phi(X_{k+1},\mathcal{T}_{k+1}) - \phi(X_k,\mathcal{T}_k) \\ \leq \underbrace{-\mathcal{A}_k \Delta q(X_k,\mathcal{T}_k,\nabla f(X_k),D_k^{\mathrm{true}})}_{\mathcal{O}(\beta_k), \quad "deterministic"} \\ + \underbrace{\frac{1}{2}\mathcal{A}_k \beta_k \Delta q(X_k,\mathcal{T}_k,G_k,D_k)}_{\mathcal{O}(\beta_k^2), \; stochastic/noise} + \underbrace{\mathcal{A}_k \mathcal{T}_k \nabla f(X_k)^T (D_k - D_k^{\mathrm{true}})}_{due \; to \; adaptive \; \mathcal{A}_k} \end{array}$$

## Good merit parameter behavior

#### Theorem 4

Let  $\mathcal{E} :=$  event that  $\{\mathcal{T}_k\}$  eventually remains constant at  $\mathcal{T}' \ge \tau_{\min} > 0$ . Then, conditioned on  $\mathcal{E}$ .

$$\begin{split} \beta_k &= \Theta(1) \implies \mathbb{E}\left[\frac{1}{k} \sum_{j=1}^k \Delta q(X_j, \mathcal{T}', \nabla f(X_j), D_j^{\text{true}})\right] = \mathcal{O}(M) \\ \beta_k &= \Theta\left(\frac{1}{k}\right) \implies \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^k \beta_j\right)} \sum_{j=1}^k \beta_j \Delta q(X_j, \mathcal{T}', \nabla f(X_j), D_j^{\text{true}})\right] \to 0 \end{split}$$

## Good merit parameter behavior

#### Theorem 4

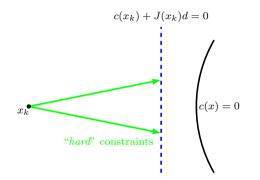
Let  $\mathcal{E} :=$  event that  $\{\mathcal{T}_k\}$  eventually remains constant at  $\mathcal{T}' \ge \tau_{\min} > 0$ . Then, conditioned on  $\mathcal{E}$ .

$$\begin{split} \beta_k &= \Theta(1) \implies \mathbb{E}\left[\frac{1}{k} \sum_{j=1}^k \left(\|\nabla f(X_j) + J(X_j)^T Y_j^{\text{true}}\|_2 + \|c(X_j)\|_2\right)\right] = \mathcal{O}(M) \\ \beta_k &= \Theta\left(\frac{1}{k}\right) \implies \mathbb{E}\left[\frac{1}{\left(\sum_{j=1}^k \beta_j\right)} \sum_{j=1}^k \beta_j \left(\|\nabla f(X_j) + J(X_j)^T Y_j^{\text{true}}\|_2 + \|c(X_j)\|_2\right)\right] \to 0 \end{split}$$

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization $000000000000000000000000000000000000$	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000

## Key observation

Key observation is that  $c(X_k)$  and  $J(X_k)$  are  $\mathcal{F}_k$ -measurable.



Therefore,  $\mathbb{E}[D_k|\mathcal{F}_k] = \text{true step if } \nabla f(X_k)$  were known.

## Numerical results: https://github.com/frankecurtis/StochasticSQP

Stochastic SQP (hard constraints) vs. stochastic subgradient (soft constraints)

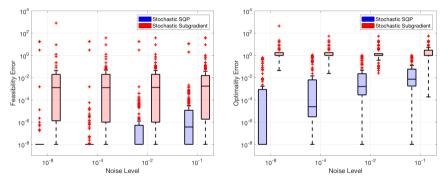


Figure: Box plots for feasibility errors (left) and optimality errors (right).

## Outline

#### Motivation

Stochastic Algorithms for Nonconvex Optimization

#### Extensions and Experimental Results

#### Conclusion

Appendix

Appendix 00000000

## Summary

Since our original work, we have considered various extensions.

- stronger convergence guarantees (almost-sure convergence)
- convergence of Lagrange multiplier estimates
- relaxed constraint qualifications
- worst-case complexity guarantees
- generally constrained problems (with inequality constraints as well)
- interior-point methods
- iterative linear system solvers and inexactness
- diagonal scaling methods for saddle-point systems

Motivation	Stochastic Algorithms for Nonconvex Optimization
000000	00000000000

### Almost-sure convergence of merit function value

Convergence of the algorithm is driven by the exact merit function

 $\phi_{\tau}(X) = \tau f(X) + \|c(X)\|$ 

Reductions in a local model of  $\phi_{\tau}$  can be tied to a stationarity measure

 $\Delta q_{\tau}(X, \nabla f(X), H, D^{\text{true}}) \sim \|\nabla f(X) + J(X)^T Y\|^2 + \|c(X)\|$ 

#### Lemma

Suppose  $\mathbb{E}[G_k|\mathcal{F}_k] = \nabla f(X_k)$  and  $\mathbb{E}[||G_k - \nabla f(X_k)|\mathcal{F}_k||^2] \leq M$ . Then, by a classical theorem of Robbins and Siegmund (1971), one finds that, almost surely,

$$\begin{split} &\lim_{k\to\infty} \{\phi_\tau(X_k)\} \text{ exists and is finite and} \\ &\lim_{k\to\infty} \Delta q_\tau(X_k, \nabla f(X_k), H_k, D_k^{\text{true}}) = 0 \end{split}$$

## Almost-sure convergence of the primal iterates

#### Theorem

Suppose there exists  $x_* \in \mathcal{X}$  with  $c(x_*) = 0$ ,  $\mu \in \mathbb{R}_{>1}$ , and  $\epsilon \in \mathbb{R}_{>0}$  such that for all

 $x\in \mathcal{X}_{\epsilon,x_*}:=\{x\in \mathcal{X}: \|x-x_*\|_2\leq \epsilon\}$ 

one finds that

$$\phi_{\tau}(x) - \phi_{\tau}(x_{*}) \begin{cases} = 0 & \text{if } x = x_{*} \\ \in (0, \mu(\tau \| Z(x)^{T} \nabla f(x) \|_{2}^{2} + \| c(x) \|_{2})] & \text{otherwise}, \end{cases}$$

where for all  $x \in \mathcal{X}_{\epsilon,x_*}$  one defines  $Z(x) \in \mathbb{R}^{n \times (n-m)}$  as some orthonormal matrix whose columns form a basis for the null space of J(x). Then, if  $\limsup_{k \to \infty} \{ \|X_k - x_*\|_2 \} \le \epsilon$  almost surely, it follows that

$$\{\phi_{\tau}(X_k)\} \xrightarrow{a.s.} \phi_{\tau}(x_*), \quad \{X_k\} \xrightarrow{a.s.} x_*, \quad and \quad \left\{ \begin{bmatrix} \nabla f(X_k) + J(X_k)^T Y_k^{\text{true}} \\ c(X_k) \end{bmatrix} \right\} \xrightarrow{a.s.} 0.$$

## Lagrange multiplier convergence

#### Theorem

Suppose  $(x_*, y_*)$  is a stationary point. Then, for any  $k \in \mathbb{N}$ , one finds  $||X_k - x_*||_2 \leq \epsilon$  implies

$$\|Y_k - y_*\|_2 \le \kappa_y \|X_k - x_*\|_2 + r^{-1} \|\nabla f(X_k) - G_k\|_2$$
  
and  $\|Y_k^{\text{true}} - y_*\|_2 \le \kappa_y \|X_k - x_*\|_2$  for some  $(\kappa, r) \in \mathbb{R}_{>0} \times \mathbb{R}_{>0}$ .

Computed multipliers always have error. Consider averaged multipliers  $\{Y_k^{avg}\}$ :

#### Theorem

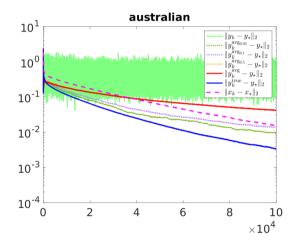
If the iterate sequence converges almost surely to  $x_*$ , i.e.,  $\{X_k\} \xrightarrow{a.s.} x_*$ , then

$$\{Y_k^{\mathrm{true}}\} \xrightarrow{a.s.} y_* \quad and \quad \{Y_k^{\mathrm{avg}}\} \xrightarrow{a.s.} y_*.$$

Motivation	Stochastic Algorithms for Nonconvex Optimization
000000	00000000000

 $\substack{\text{Appendix}\\00000000}$ 

## Constrained logistic regression: australian dataset (LIBSVM)



## Complexity of $\mathcal{O}(\epsilon^{-2})$ for deterministic algorithm

All reductions in the merit function can be cast in terms of smallest  $\tau$ .

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

#### Theorem

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

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

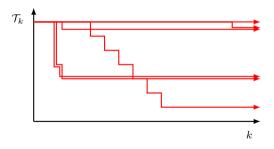
in a number of iterations no more than

$$\left(\frac{\tau_0(f_1 - f_{\inf}) + \|c_1\|_1}{\min\{\kappa_1, \kappa_2 \tau_{\min}\}}\right) \epsilon^{-2}.$$

		Stochastic Algorithms for Nonconvex Optimization
--	--	--

## Challenge in the stochastic setting

We are minimizing a function that is changing during the optimization.



▶ Details

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

#### Theorem

Suppose the algorithm is run  $k_{\max}$  iterations with  $\beta_k = \gamma/\sqrt{k_{\max}+1}$  and

▶ the merit parameter is reduced at most  $s_{\max} \in \{0, 1, ..., k_{\max}\}$  times.

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

$$\mathbb{E}[\|\nabla f(X_{k_*}) + J(X_{k_*})^T Y_{k_*}\|_2^2 + \|c(X_{k_*})\|_1] \\ \leq \frac{\tau_{-1}(f_0 - f_{\inf}) + \|c_0\|_1 + M}{\sqrt{k_{\max} + 1}} + \frac{(\tau_{-1} - \tau_{\min})(s_{\max}\log(k_{\max}) + \log(1/\delta))}{\sqrt{k_{\max} + 1}}$$

#### Theorem

If the stochastic gradient estimates are sub-Gaussian, then with probabiliy  $1-ar{\delta}$ 

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

Motivation	Stochastic Algorithms for Nonconvex Optimization
000000	000000000000

## Inequality-constrained: Fair learning

Consider an  $\epsilon$ -constraint method for fair machine learning:

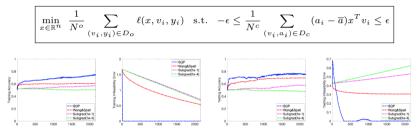


FIG. 5.5. CPU time versus training accuracy, training infeasibility error, testing accuracy, and testing infeasibility error for a representative run of SQP, Wang & Spall, subgradient  $(10^{-1})$ , and subgradient  $(10^{-4})$  with the German data set.

## Projected Adam

#### Algorithm P-Adam Projection-based Adam

 $\begin{array}{l} \mathbf{Require:} \ m_{k-1} \in \mathbb{R}^d, \, v_{k-1} \in \mathbb{R}^d, \, w_k \in \mathbb{R}^d, \, g_k \in \mathbb{R}^d, \, \beta_1 \in (0,1), \, \beta_2 \in (0,1), \, \mu \in \mathbb{R}_{>0} \\ \text{Compute } \ \overline{g}_k \leftarrow (I - J(w_k)^T (J(w_k)J(w_k)^T)^{-1} J(w_k))g_k \\ \text{Set } p_k \leftarrow \beta_1 p_{k-1} + (1 - \beta_1)\overline{g}_k \\ \text{Set } q_k \leftarrow \beta_2 q_{k-1} + (1 - \beta_2)(\overline{g}_k \circ \overline{g}_k), \, \text{where } (\overline{g}_k \circ \overline{g}_k)_i = (\overline{g}_k)_i^2 \text{ for all } i \in \{1, \dots, d\} \\ \text{Set } \widehat{p}_k \leftarrow (1/(1 - \beta_1^k))p_k \\ \text{Set } \widehat{q}_k \leftarrow (1/(1 - \beta_2^k))q_k \\ \text{Compute } s_k \text{ by solving } \begin{bmatrix} \text{diag}(\sqrt{\widehat{q}_k + \mu}) & J(w_k)^T \\ J(w_k) & 0 \end{bmatrix} \begin{bmatrix} s_k \\ \lambda_k \end{bmatrix} = -\begin{bmatrix} \widehat{p}_k \\ c_k \end{bmatrix} \end{aligned}$ 

Motivation	Stochastic Algorithms	for Nonconvex	Optimization
000000	00000000000000000		

## Mass-balance

## Outline

#### Motivation

Stochastic Algorithms for Nonconvex Optimization

Extensions and Experimental Results

#### Conclusion

#### Appendix

Stochastic Algorithms for Nonconvex Constrained Optimization

## Summary

 ${\it Stochastic-gradient/Newton-based} \ algorithms \ for \ constrained \ optimization.$ 

▶ A lot of work so far, but many open questions.

Open questions:

- stochastic interior-point methods (generally constrained)?
- tradeoff analysis (Bottou and Bousquet)?
- generalization guarantees?
- beyond projected ADAM, etc.?
- Lagrange multiplier estimators?
- active-set identification?
- expectation/probabilistic constraints?

## 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," *Mathematics of Operations Research*, https://doi.org/10.1287/moor.2021.0154, 2023.
- F. E. Curtis, D. P. Robinson, and B. Zhou, "Inexact Sequential Quadratic Optimization for Minimizing a Stochastic Objective Subject to Deterministic Nonlinear Equality Constraints," to appear in INFORMS Journal on Optimization, 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," *Mathematical Programming*, https://doi.org/10.1007/s10107-023-01981-1, 2023.
- F. E. Curtis, S. Liu, and D. P. Robinson, "Fair Machine Learning through Constrained Stochastic Optimization and an e-Constraint Method," Optimization Letters, https://doi.org/10.1007/s11590-023-02024-6, 2023.
- F. E. Curtis, D. P. Robinson, and B. Zhou, "Sequential Quadratic Optimization for Stochastic Optimization with Deterministic Nonlinear Inequality and Equality Constraints," https://arxiv.org/abs/2302.14790.
- F. E. Curtis, V. Kungurtsev, D. P. Robinson, and Q. Wang, "A Stochastic-Gradient-based Interior-Point Algorithm for Solving Smooth Bound-Constrained Optimization Problems," https://arxiv.org/abs/2304.14907.

 $\substack{\mathrm{Appendix}\\00000000}$ 

## Thank you!

# Questions?



Stochastic Algorithms for Nonconvex Constrained Optimization

## Outline

#### Motivation

Stochastic Algorithms for Nonconvex Optimization

**Extensions and Experimental Results** 

#### Conclusion

#### Appendix

Stochastic Algorithms for Nonconvex Constrained Optimization

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization 00000000000000	Extensions and Experiments 000000000000	Conclusio 0000

onclusion 000 

## Details

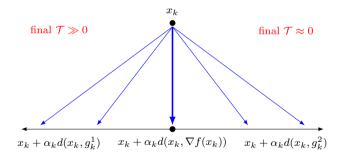


Some details on the tree construction for our complexity analysis...

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000

## Challenge in the stochastic setting

We are minimizing a function that is changing during the optimization.

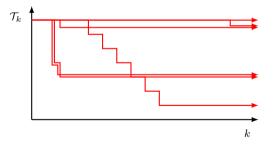


Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 00000000

#### Challenge in the stochastic setting

In the stochastic setting, minimum  $\mathcal{T}$  is not determined by the initial point.

- ▶ Even if we assume  $\mathcal{T}_k \geq \tau_{\min} > 0$  for all k in all realizations, the final  $\mathcal{T}$  is not determined.
- This means we cannot cast all reductions in terms of some fixed constant  $\tau$ .



## Our approach

In fact,  $\mathcal{T}$  reaching some minimum value is not necessary.

- ▶ Important: Diminishing probability of continued imbalance between "true" merit parameter update and "stochastic" merit parameter update.
- ▶ In iteration k, the algorithm has obtained the merit parameter value  $\mathcal{T}_{k-1}$ .
- ▶ If the true gradient is computed, then one obtains  $\mathcal{T}_k^{\text{trial,true}}$ .

#### Lemma

Suppose that the merit parameter is reduced at most  $s_{\max}$  times. For any  $\delta \in (0,1)$ , one finds that

$$\mathbb{P}\left[|\{k: \mathcal{T}_k^{trial, true} < \mathcal{T}_{k-1}\}| \le \left\lceil \frac{\ell(s_{\max}, \delta)}{p} \right\rceil\right] \ge 1 - \delta,$$

where  $p \in (0,1)$  (related to a bounded imbalance assumption we make) and

$$\ell(s_{\max}, \delta) := s_{\max} + \log(1/\delta) + \sqrt{\log(1/\delta)^2 + 2s_{\max}\log(1/\delta)} > 0.$$

## Chernoff bound

How do we get there?

Lemma (Chernoff bound, multiplicative form)

Let  $\{Y_0, \ldots, Y_k\}$  be independent Bernoulli random variables. Then, for any  $s_{\max} \in \mathbb{N}$  and  $\delta \in (0, 1)$ ,

$$\sum_{j=0}^{k} \mathbb{P}[Y_j = 1] \ge \ell(s_{\max}, \delta) \implies \mathbb{P}\left[\sum_{j=0}^{k} Y_j \le s_{\max}\right] \le \delta.$$

We construct a tree whose nodes are signatures of possible runs of the algorithm.

- A realization  $\{g_0, \ldots, g_k\}$  belongs to a node if and only if a certain number of decreases of  $\mathcal{T}$  have occurred and the probability of decrease in the current iteration is in a given closed/open interval.
- ▶ Bad leaves are those when the probability of decrease has accumulated beyond a threshold, yet the merit parameter has not been decreased sufficiently often.
- Along the way, we apply a Chernoff bound on a carefully constructed set of (independent Bernoulli) random variables to bound probabilities associated with bad leaves.

Appendix 000000000

## Node definition

- Let  $[k] := \{0, 1, \dots, k\}$  and define
  - ▶  $p_{[k]}$  = probabilities of merit parameter decreases
  - ▶  $w_{[k]}$  = counter of merit parameter decreases

Then, define nodes of the tree according to

$$G_{[k-1]} \in N(p_{[k]}, w_{[k]})$$

if and only if

$$\begin{split} G_{[k-2]} &\in N(p_{[k-1]}, w_{[k-1]}) \\ \mathbb{P}[\mathcal{T}_k < \mathcal{T}_{k-1} | \mathcal{F}_k] \in \iota(p_k) \\ \sum_{i=1}^{k-1} \mathbbm{1}[\mathcal{T}_i < \mathcal{T}_{i-1}] = w_k \end{split}$$

Motivation 000000	Stochastic Algorithms for Nonconvex Optimization	Extensions and Experiments 000000000000	Conclusion 0000	Appendix 0000000●

## Visualization

