Improved Hessian estimation for adaptive random directions stochastic approximation

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Overview

Simulation Optimization

Random directions stochastic approximation (RDSA) + improved Hessian estimation

Numerical Results

Simulation Optimization

Energy Demand management

- Consumer demand, energy generation are uncertain.
- Objective is to minimize the difference.

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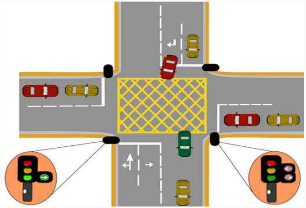
Traffic signal control

- Optimal order to switch traffic lights.
- Objective is to minimize waiting time.



Basic optimization problem

To find θ^* that minimizes the objective function $\mathrm{f}(\theta)$:

$$\boxed{\theta^* = \arg\min_{\theta \in \Theta} \mathrm{f}(\theta),} \tag{1}$$

- f: $\mathbb{R}^{\mathrm{N}} \to \mathbb{R}$ is called the objective function.
- θ is tunable N-dimensional parameter
- $\Theta \subseteq \mathbb{R}^{\mathrm{N}}$ is the feasible region in which θ takes values.

Based on objective function

Deterministic optimization problem

- Complete information about objective function f.
- First and higher order derivatives.
- Set Θ.

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Stochastic optimization problem

- We have little knowledge on the structure of f.
- f cannot be obtained directly.
- $f(\theta) \equiv E_\xi[h(\theta, \xi)]$, where ξ comprises the randomness in the system.

Complex to find θ^* only on the basis of noisy samples.

Stochastic optimization via simulation

Stochastic optimization deals with highly nonlinear and high dimensional systems. The challenges with these problems are:

- Too complex to solve analytically.
- Many simplifying assumptions are required.

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A good alternative of modelling and analysis is "Simulation"

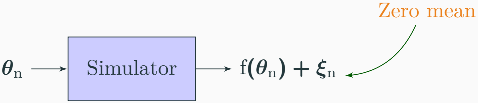

Figure 1: Simulation optimization

Stochastic approximation + Gradient descent

Stochastic analog of gradient descent

$$\theta_{n+1} = \Gamma_\Theta \left[\theta_n - a_n \widehat{\nabla} f(\theta_n)\right], \tag{2}$$

- $\widehat{\nabla} f(\theta_n)$ is an noisy estimate of the gradient $\nabla f(\theta_n)$.
- $\{a_n\}$ are pre-determined step-sizes satisfying:
  $$\sum_{n=1}^{\infty} a_n = \infty, \quad \sum_{n=1}^{\infty} a_n^2 < \infty$$
- Γ_Θ denotes the projection of a point onto Θ.

1-slide summary

Related second-order methods

(Spall 2000)[1]	Second-order SPSA (2SPSA)	4 simulations/iteration
(Spall 2009)[2]	2SPSA + feedback	4 simulations/iteration
(Prashanth L.A. et al 2016)[3]	Second-order RDSA (2RDSA)	3 simulations/iteration

Our work

We propose feedback and weighting mechanisms for improving Hessian estimate for 2RDSA algorithm.

[1] J. C. Spall (2000), "Adaptive stochastic approximation by the simultaneous perturbation method," IEEE TAC.

[2] J. C. Spall (2009), "Feedback and weighting mechanisms for improving Jacobian estimates in the adaptive simultaneous perturbation algorithm," IEEE TAC.

[3] Prashanth L. A. et al. (2016) "Adaptive system optimization using random directions stochastic approximation," IEEE TAC.

Random directions stochastic approximation (RDSA) + improved Hessian estimation

Our algorithm

- Matrix projection
- Gradient estimate

$$\theta_{n+1} = \theta_n - a_n \Upsilon(\overline{\overline{H}}_n)^{-1} \widehat{\nabla} f(\theta_n), \tag{3}$$

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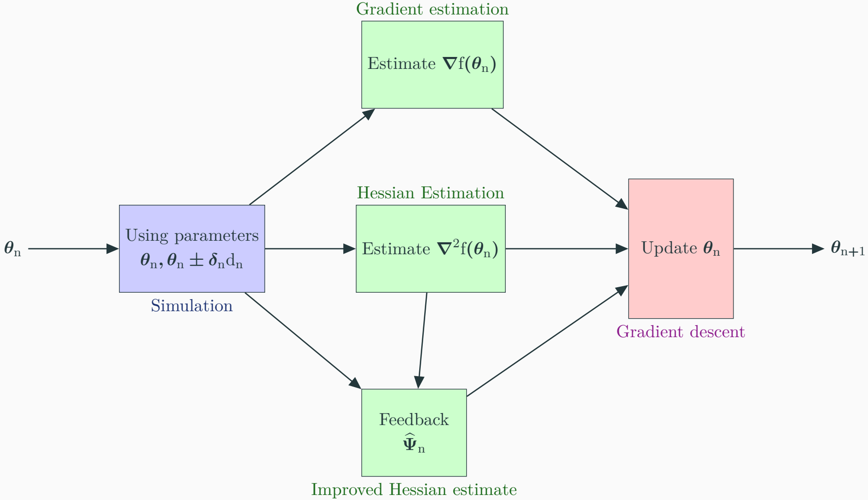
$$\theta_{n+1} = \theta_n - a_n \Upsilon(\overline{H}_n)^{-1} \widehat{\nabla} f(\theta_n), \tag{3}$$

$$\overline{H}_n = (1 - b_n)\overline{H}_{n-1} + b_n(\widehat{H}_n - \widehat{\Psi}_n), \tag{4}$$

- Optimal step-sizes
- Hessian estimate
- Feedback term

Overall flow of 2RDSA-IH



RDSA gradient estimate

Function measurements

$$y_n^+ = f(\theta_n + \delta_n d_n) + \xi_n^+, \quad y_n^- = f(\theta_n - \delta_n d_n) + \xi_n^-$$

RDSA gradient estimate

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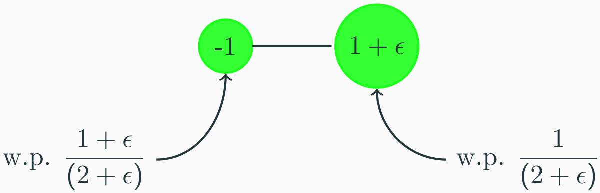
Gradient estimate

$$\widehat{\nabla} f(\theta_n) = \frac{1}{1+\epsilon} d_n \left[\frac{y_n^+ - y_n^-}{2\delta_n} \right]. \tag{5}$$

Asymmetric Bernoulli distribution for $d_n^i, i = 1, \ldots, N$:



2RDSA Hessian estimate

Function measurements

$$y_n^+ = f(\,\theta_n + \delta_n d_n\,) + \xi_n^+, \;\; y_n^- = f(\,\theta_n - \delta_n d_n\,) + \xi_n^-, \;\; y_n = f(\,\theta_n\,) + \xi_n$$

2RDSA Hessian estimate

Function measurements

$$y_n^+ = f(\theta_n + \delta_n d_n) + \xi_n^+, \;\; y_n^- = f(\theta_n - \delta_n d_n) + \xi_n^-, \;\; y_n = f(\theta_n) + \xi_n$$

Hessian estimate $\widehat{H}_n$

$$\begin{aligned}
\widehat{H}_n &= M_n \left(\frac{y_n^+ + y_n^- - 2y_n}{\delta_n^2} \right) \\
&= M_n \left[\left(\frac{f(\theta_n + \delta_n d_n) + f(\theta_n - \delta_n d_n) - 2f(\theta_n)}{\delta_n^2} \right) \right. \\
&\qquad\qquad \left. + \left(\frac{\xi_n^+ + \xi_n^- - 2\xi_n}{\delta_n^2} \right) \right] \\
&= M_n \left(\boxed{d_n^{T} \nabla^2 f(\theta_n) d_n} + O(\delta_n^2) + \boxed{\left(\frac{\xi_n^+ + \xi_n^- - 2\xi_n}{\delta_n^2} \right)} \right). \qquad (6)
\end{aligned}$$

Want to recover $\nabla^2 f(\theta_n)$ from this

Zero-mean

How to choose $\mathrm{M_n}$?

Asymmetric Bernoulli Perturbation

$$\mathrm{M_n} = \begin{bmatrix} \frac{1}{\kappa}\left((\mathrm{d_n^1})^2 - (1+\epsilon)\right) & \cdots & \frac{1}{2(1+\epsilon)^2}\mathrm{d_n^1 d_n^N} \\ \frac{1}{2(1+\epsilon)^2}\mathrm{d_n^2 d_n^1} & \cdots & \frac{1}{2(1+\epsilon)^2}\mathrm{d_n^2 d_n^N} \\ \cdots & \cdots & \cdots \\ \frac{1}{2(1+\epsilon)^2}\mathrm{d_n^N d_n^1} & \cdots & \frac{1}{\kappa}\left((\mathrm{d_n^N})^2 - (1+\epsilon)\right) \end{bmatrix}, \qquad (7)$$

where $\kappa = \tau\left(1 - \frac{(1+\epsilon)^2}{\tau}\right)$ and $\tau = \mathrm{E}(\mathrm{d_n^i})^4 = \frac{(1+\epsilon)(1+(1+\epsilon)^3)}{(2+\epsilon)}$, for any $\mathrm{i} = 1, \ldots, \mathrm{N}$.

Zero-mean feedback term

Zero-mean term

Mean of the Hessian estimate

$$\mathbb{E}\left[\widehat{H}_n \middle| \mathcal{F}_n\right] = \nabla^2 f(\theta_n) + \boxed{\mathbb{E}\left[\Psi_n(\nabla^2 f(\theta_n)) \middle| \mathcal{F}_n\right]} + O(\delta_n^2) + \mathbb{E}\left[\left(\frac{\xi_n^+ + \xi_n^- - 2\xi_n}{\delta_n^2}\right)\middle| \mathcal{F}_n\right], \quad (8)$$

[1] For any matrix P, $[P]_D$ refers to a matrix that retains only the diagonal entries of P and replaces all the remaining entries with zero.

[2] $[P]_N$ to refer to a matrix that retains only the off-diagonal entries of P, while replaces all the diagonal entries with zero.

Zero-mean feedback term

Zero-mean term

Mean of the Hessian estimate

$$\mathbb{E}\left[\widehat{\mathrm{H}}_{\mathrm{n}} \middle| \mathcal{F}_{\mathrm{n}}\right] = \nabla^2 \mathrm{f}(\theta_{\mathrm{n}}) + \boxed{\mathbb{E}\left[\Psi_{\mathrm{n}}(\nabla^2 \mathrm{f}(\theta_{\mathrm{n}})) \middle| \mathcal{F}_{\mathrm{n}}\right]} + \mathrm{O}(\delta_{\mathrm{n}}^2)$$
$$+ \mathbb{E}\left[\left(\frac{\xi_{\mathrm{n}}^+ + \xi_{\mathrm{n}}^- - 2\xi_{\mathrm{n}}}{\delta_{\mathrm{n}}^2}\right) \middle| \mathcal{F}_{\mathrm{n}}\right], \tag{8}$$

Feedback term

$$\Psi_{\mathrm{n}}(\mathrm{H}) = [\mathrm{M}_{\mathrm{n}}]_{\mathrm{D}} \left(\mathrm{d}_{\mathrm{n}}^{\mathrm{T}} [\mathrm{H}]_{\mathrm{N}} \, \mathrm{d}_{\mathrm{n}}\right) + [\mathrm{M}_{\mathrm{n}}]_{\mathrm{N}} \left(\mathrm{d}_{\mathrm{n}}^{\mathrm{T}} [\mathrm{H}]_{\mathrm{D}} \, \mathrm{d}_{\mathrm{n}}\right). \tag{9}$$

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Zero-mean feedback term

Problem

Feedback term is function of current Hessian $\nabla^2 f$.

Zero-mean feedback term

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Solution

Use $\overline{H}_{n-1}$ as a proxy for $\nabla^2 f$.

$$\widehat{\Psi}_n = \Psi_n(\boxed{\overline{H}_{n-1}}). \tag{10}$$

Rewriting the Hessian recursion

$$\overline{\mathrm{H}}_{\mathrm{n}} = \sum_{\mathrm{i}=0}^{\mathrm{n}} \tilde{\mathrm{b}}_{\mathrm{k}}(\widehat{\mathrm{H}}_{\mathrm{i}} - \widehat{\Psi}_{\mathrm{i}}). \tag{11}$$

Step-size optimization

Rewriting the Hessian recursion

$$\overline{\mathrm{H}}_{\mathrm{n}} = \sum_{\mathrm{i}=0}^{\mathrm{n}} \tilde{\mathrm{b}}_{\mathrm{k}}(\widehat{\mathrm{H}}_{\mathrm{i}} - \widehat{\Psi}_{\mathrm{i}}). \tag{11}$$

Optimization problem for weights

$$\min_{\{\tilde{\mathrm{b}}_{\mathrm{k}}\}} \sum_{\mathrm{i}=0}^{\mathrm{n}} (\tilde{\mathrm{b}}_{\mathrm{k}})^2 \delta_{\mathrm{i}}^{-4}, \text{ subject to} \tag{12}$$

$$\tilde{\mathrm{b}}_{\mathrm{i}} \geq 0 \ \forall \mathrm{i} \text{ and } \sum_{\mathrm{i}=0}^{\mathrm{n}} \tilde{\mathrm{b}}_{\mathrm{i}} = 1. \tag{13}$$

Above optimization problem solution

$$\tilde{b}_i^* = \delta_i^4 / \sum_{j=0}^{n} \delta_j^4, i = 1, \ldots, n. \quad (14)$$

[1] Step-size optimization is a relatively straightforward migration from Spall 2009.

Above optimization problem solution

$$\tilde{b}_i^* = \delta_i^4 / \sum_{j=0}^{n} \delta_j^4, i = 1, \ldots, n. \tag{14}$$

Optimal weights for original Hessian recursion

$$b_i = \delta_i^4 / \sum_{j=0}^{i} \delta_j^4. \tag{15}$$

[1]Step-size optimization is a relatively straightforward migration from Spall 2009.

Lemma

(Bias in Hessian estimate) From Prashanth L. A. et al. (2016)[1], we have a.s. that[2], for $i, j = 1, \ldots, N$,

$$\left| \mathbb{E}\left[\widehat{H}_n(i,j) \middle| \mathcal{F}_n \right] - \nabla^2_{ij} f(\theta_n) \right| = O(\delta_n^2). \tag{16}$$

Theorem

(Strong Convergence of Hessian) Under assumptions similar to those for 2SPSA and 2RDSA, we have that

$$\theta_n \to \theta^*, \overline{H}_n \to \nabla^2 f(\theta^*) \text{ a.s. as } n \to \infty.$$

[1] Prashanth L. A. et al. (2016) "Adaptive system optimization using random directions stochastic approximation," IEEE TAC.

[2] Here $\widehat{H}_n(i,j)$ and $\nabla^2_{ij} f(\cdot)$ denote the (i,j)th entry in the Hessian estimate $\widehat{H}_n$ and the true Hessian $\nabla^2 f(\cdot)$, respectively.

Numerical Results

Quadratic loss

$$f(x) = \theta^T A\theta + b^T\theta. \quad (17)$$

Fourth-order loss

$$f(x) = \theta^T A^T A\theta + 0.1 \sum_{j=1}^{N} (A\theta)_j^3 + 0.01 \sum_{j=1}^{N} (A\theta)_j^4. \quad (18)$$

Normalized MSE (NMSE)

$$\left\|\theta_{\mathrm{n}_{\mathrm{end}}} - \theta^*\right\|^2 / \left\|\theta_0 - \theta^*\right\|^2 \tag{19}$$

Normalized loss

$$\mathrm{f}(\theta_{\mathrm{n}_{\mathrm{end}}})/\mathrm{f}(\theta_0) \tag{20}$$

Table 1: Normalized loss values for fourth-order objective (18) with noise: simulation budget = 10,000 and standard error from 500 replications shown after ±

Noise parameter $\sigma = 0.1$		
	Regular	Improved Hessian estimation
2SPSA	0.132 ± 0.0267	0.104 ± 0.0355
2RDSA-Unif[1]	0.115 ± 0.0214	0.0271 ± 0.0538
2RDSA-AsymBer	0.0471 ± 0.021	0.0099 ± 0.0014

[1] 2RDSA-Unif uses Unif$[-1, 1]$ with a different $\mathrm{M_n}$.

Table 2: NMSE values for quadratic objective (17) with noise: simulation budget = 10,000 and standard error from 500 replications shown after $\pm$

Noise parameter $\sigma = 0.1$		
	Regular	Improved Hessian estimation
2SPSA	0.9491 ± 0.0131	0.5495 ± 0.0217
2RDSA-Unif	1.0073 ± 0.0140	0.1953 ± 0.0095
2RDSA-AsymBer	0.1667 ± 0.0095	0.0324 ± 0.0007

Conclusions and Future work

Conclusions

- Improved Hessian estimation scheme for the 2RDSA algorithm.
- 2RDSA-IH requires only 75% of the simulation cost per-iteration for 2SPSA, 2SPSA-IH.

Future work

To derive finite time bounds for 2RDSA-IH.

Thank you