SOLNP+: A Derivative-Free Solver for Nonlinear Constrained Programming

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SICIAM ZO Optimization Workshop

May 24, 2023

Derivative-Free General Nonlinear Programming

$$\begin{aligned} &\min\nolimits_{s\in\mathbb{R}^d} f(s) \\ s.t. \quad & h_1(s) \ = \ 0, \\ & l_h \leqslant h_2(s) \leqslant u_h, \\ & l_s \leqslant s \leqslant u_s. \end{aligned} \quad \xrightarrow{\text{Adding Slack}} \quad \begin{aligned} &\min\nolimits_{x\in\mathbb{R}^d} \ f(x) \\ s.t. \ \ & g(x) = 0, \\ & l_x \leqslant x \leqslant u_x. \end{aligned}$$

- All functions are smooth functions.
- The solver only has access to zero-order information.
- Function evaluation may be expensive.
- There may be some noises in function evaluation.
- Many applications in real practice.

Applications of Derivative-Free Algorithm

- Aircraft design: Giunta, Anthony A., et al. *Multidisciplinary optimisation of a supersonic transport using design of experiments theory and response surface modelling*, 1997.
- Parameter estimation in time series: Bennedsen, Mikkel, Eric Hillebrand, and Jingying Zhou Lykke, *Global temperature projections from a statistical energy balance model using multiple sources of historical data*, 2022.
- Selecting the tuning parameters of deep neural network: Snoek, Jasper, Hugo Larochelle, and Ryan P. Adams*, Practical bayesian optimization of machine learning algorithms*, 2012.
- Prompt Optimization…

Popular Methods

- Model-Based Trust-Region methods: minimization of model functions in adaptively chosen trust region.
  - Example: Powell’s Derivative-Free Optimization (PDFO) solvers.
- Model-Based Descend method: use model functions to find a descent direction and search along the direction.
  - Example: Implicit filtering, SOLNP+.
- Direct search method: compare the current points with some near points to reduce function value.
  - Example: Nonlinear Optimization with Mesh Adaptive Directional Search (NOMAD), Nelder-Mead Simplex method.
- Generic, Simulated Annealing,⋯

SOLNP+: History

- First proposed by Ye in 1989.
- Originally implemented (SOLNP) in Matlab, 1989.
- R implementation (Rsolnp) by Alexios Ghalanos and Stefan Theussl, 2011.
- New and C implementation (SOLNP+) with improvements, 2022.

SOLNP+: Overview

- Use finite difference to approximate the gradient.
- Approximate the constraints by linear function.
- Use Augmented Lagrangian Method (ALM) to solve the nonlinear constrained problem.
- Use Sequential Quadratic Programming (SQP) and BFGS update to solve ALM subproblems.

SOLNP+ : Approximate Gradient and Constraints

- Use finite difference to calculate the approximated gradient.

$$[\nabla_\delta f(x)]_i = \frac{f(x+\delta e_i) - f(x)}{\delta}, \ e_i = [0, \ \cdots, 1, \ \cdots 0].$$

- Approximate the nonlinear constraints by linear function:

$$g(x) = 0 \quad \Longrightarrow \quad g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k) = 0.$$

SOLNP+ Outer Iteration: ALM Framework

- Modified Augmented Lagrangian function

$$\begin{aligned} L_k(x,y) = f(x) - y^T \left[g(x) - (g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k))\right] \\ + \frac{\rho_k}{2} \left\|g(x) - (g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k))\right\|_2^2 . \end{aligned}$$

- Primal Update (Robinson, 1972):

$$\begin{aligned} \min \ & L_k(x, y_k) \\ \text{s.t. } & g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k) = 0, \\ & l_x \leq x \leq u_x, \end{aligned}$$

where y_k is the approximated Lagrange multiplier with respect to the linear constraints.

Solve ALM Subproblem: Find Feasible Solution

- The linearized problem may not be feasible.
- Find (approximated) feasible solution x_k^0 by solving the following LP.

$$
\begin{aligned}
&\min \tau \\
&\text{s.t. } g(x_k)(1-\tau) + \nabla_{\delta_k} g(x_k)^T (x - x_k) = 0, \\
&\qquad l_x \leq x \leq u_x, \\
&\qquad \tau \geq 0
\end{aligned}
$$

- When τ is small, we find a near feasible start point.
- Start from x_k^0 , move along the direction that is in the null space of $\nabla_{\delta_k} g(x_k)^T$.

SOLNP+ Inner Iteration: SQP and BFGS Update

- SOLNP+ generates the following sequential quadratic programming (SQP) to solve the ALM subproblem.

$$\begin{aligned} \min \ & \frac{1}{2}(x - x_k^i)^T H_k^i (x - x_k^i) + \nabla_{\delta_k} L_k(x_k^i, y_k)^T (x - x_k^i) \\ \text{s.t. } & g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k) = b_k, \\ & l_x \leq x \leq u_x. \end{aligned}$$

where $b_k = g(x_k) + \nabla_{\delta_k} g\left(x^k\right)^T \left(x_k^0 - x_k\right)$ and BFGS update:

$$H_k^{i+1} = H_k^i + \frac{tt^T}{t^T s} - \frac{(H_k^i s)(H_k^i s)^T}{s^T H_k^i s}, \qquad H_1^0 = I.$$

where $t = \nabla_{\delta_k} L_k(x_k^{i+1}, y_k) - \nabla_{\delta_k} L_k(x_k^i, y_k)$ and $s = x_k^{i+1} - x_k^i.$

Solve SQP: QP Subproblem

- Let $\hat{x}_k^i$ be the solution of the following QP.

$$\begin{aligned} \min\ & \frac{1}{2}(x - x_k^i)^T H_k^i (x - x_k^i) + \nabla_{\delta_k} L_k(x_k^i, y_k)^T (x - x_k^i) \\ \text{s.t.}\ & g(x_k) + \nabla_{\delta_k} g(x_k)^T (x - x_k) = b_k, \\ & l_x \leq x \leq u_x. \end{aligned}$$

- SOLNP+ applies IPM to solve it and performs line search between $\hat{x}_k^i$ and x_k^i to reduce $L_k(x, y_k)$
- Use Lagrange multiplier of linear constraints as an approximation to the real multiplier.

Computation Aspects for SOLNP+

- Heuristics to update the penalty parameter ρ_k .
- Restart when the algorithm cannot make any progress.
- Line search to improve quality of solution.
- Adaptively choose δ_k to increase robustness.
- Feasibility problems
- **Large-scale unconstrained problems**

SOLNP+: Dealing with Feasibility

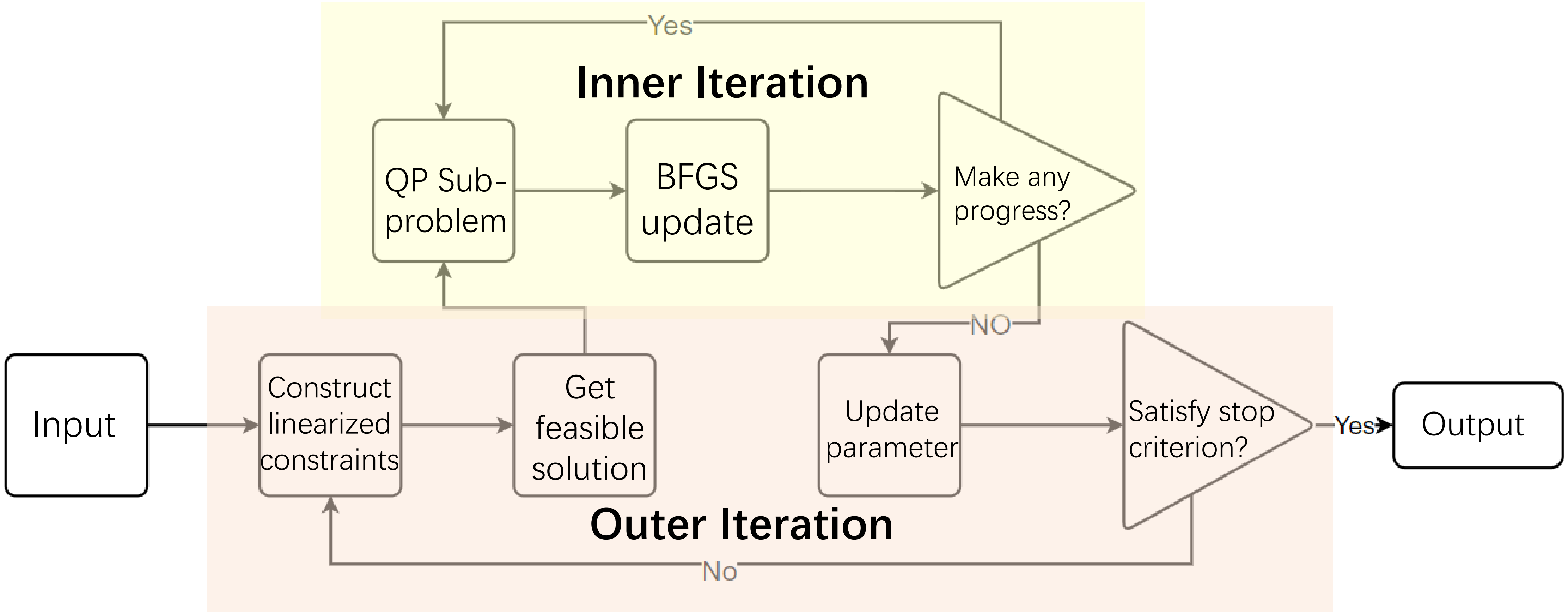
- Sometimes feasibility is hard to satisfy
- When poor feasibility is detected, SOLNP+ will switch to another formulation for satisfying feasibility

$$
\begin{aligned}
\min\ & f(x) \\
\text{s.t. } & g(x) = 0 \\
& l_s \le h(x) \le u_s \\
& l_x \le x \le u_x
\end{aligned}
\quad \xrightarrow{\text{Use } \ell_1 \text{ penalty}} \quad
\begin{aligned}
\min\ & f(x) + \mu_k e^\top u + \mu_k e^\top v \\
\text{s.t. } & g(x) + u - v = 0 \\
& h(x) - s = 0 \\
& l_s \le s \le u_s,\quad u, v \ge 0 \\
& l_x \le x \le u_x
\end{aligned}
$$

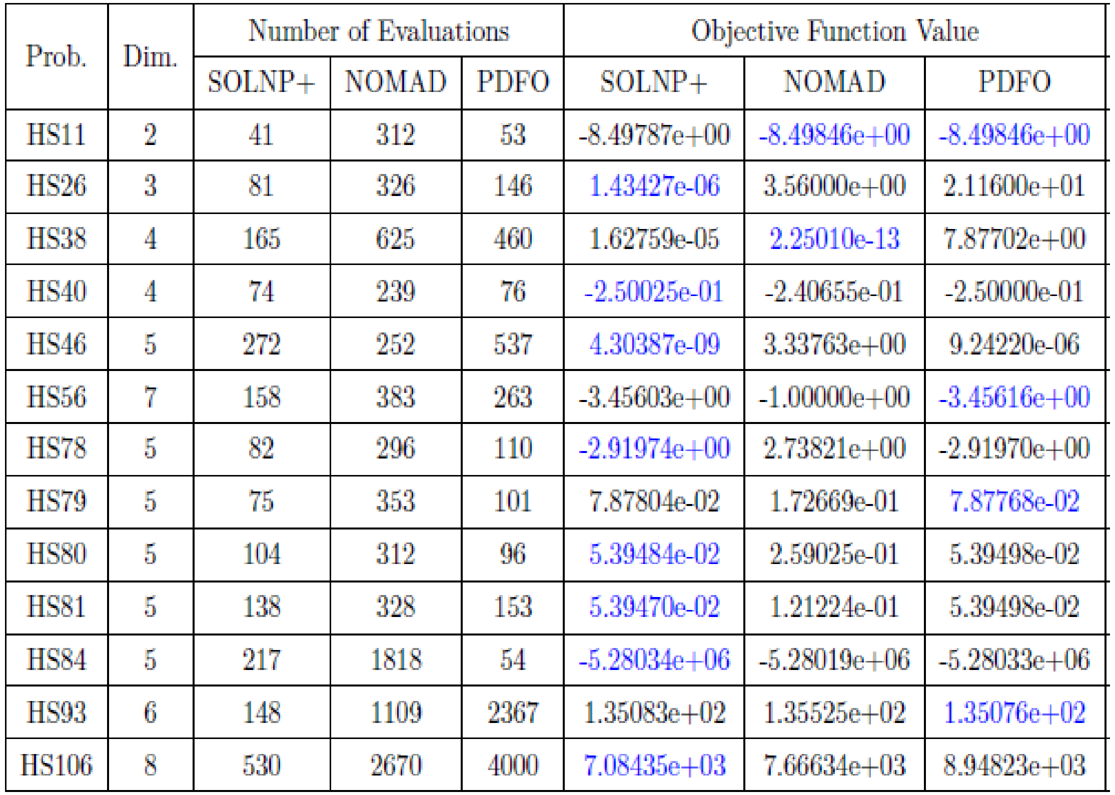
where μ_k is adjusted according to feasibility change.

SOLNP+ Solver

SOLNP+ is written in ANSI C and under active development.



Computational Results I: Noiseless functions



Prob.	Dim.	Number of Evaluations			Objective Function Value		
		SOLNP+	NOMAD	PDFO	SOLNP+	NOMAD	PDFO
HS11	2	41	312	53	-8.49787e+00	-8.49846e+00	-8.49846e+00
HS26	3	81	326	146	1.43427e-06	3.56000e+00	2.11600e+01
HS38	4	165	625	460	1.62759e-05	2.25010e-13	7.87702e+00
HS40	4	74	239	76	-2.50025e-01	-2.40655e-01	-2.50000e-01
HS46	5	272	252	537	4.30387e-09	3.33763e+00	9.24220e-06
HS56	7	158	383	263	-3.45603e+00	-1.00000e+00	-3.45616e+00
HS78	5	82	296	110	-2.91974e+00	2.73821e+00	-2.91970e+00
HS79	5	75	353	101	7.87804e-02	1.72669e-01	7.87768e-02
HS80	5	104	312	96	5.39484e-02	2.59025e-01	5.39498e-02
HS81	5	138	328	153	5.39470e-02	1.21224e-01	5.39498e-02
HS84	5	217	1818	54	-5.28034e+06	-5.28019e+06	-5.28033e+06
HS93	6	148	1109	2367	1.35083e+02	1.35525e+02	1.35076e+02
HS106	8	530	2670	4000	7.08435e+03	7.66634e+03	8.94823e+03

Table 1: Test results on Hock and Schittkowski Hock and Schittkowski [1980] problems. The blue color means that the solver returns an approximate optimal solution with better objective value.

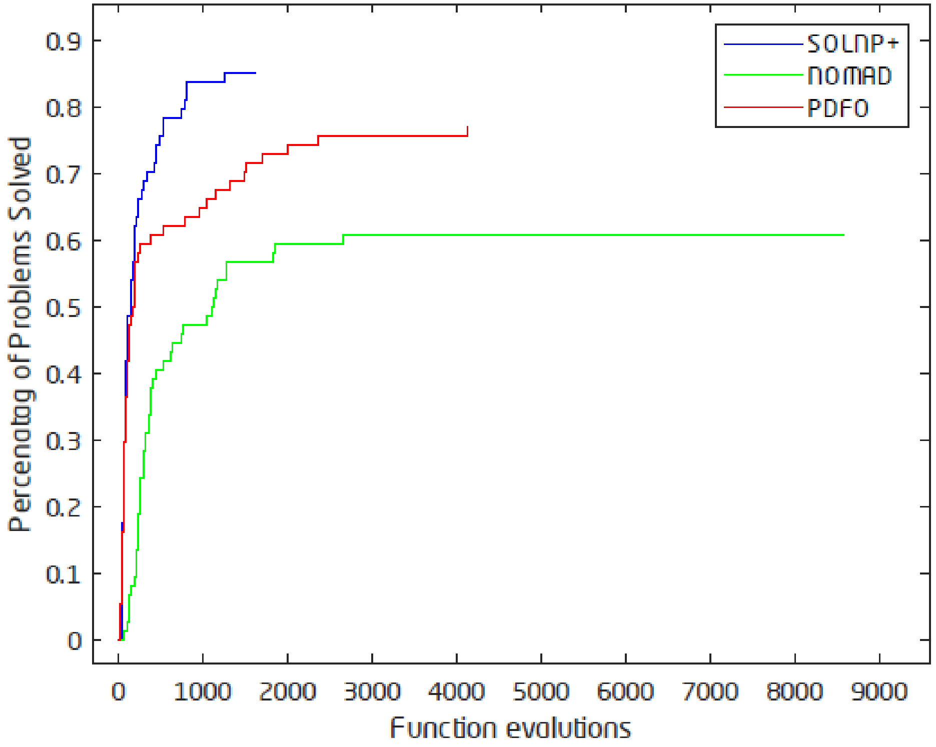


Figure 1: Test result of 74 problems in Hock and Schittkowski Hock and Schittkowski [1980] problems. Total running time of SOLNP+, NOMAD, PDFO are 1.410250e+00s, 2.251209e+03s and 5.324220e+00s.

TM Ragonneau and Z Zhang. Pdfo: Cross-platform interfaces for powells derivative-free optimization solvers (version 1.1), 2021.
Le Digabel, Sébastien. "Algorithm 909: NOMAD: Nonlinear optimization with the MADS algorithm." *ACM Transactions on Mathematical Software (TOMS)* 37.4 (2011): 1-15.and Christophe Tribes.

Computational Results II: Functions with Noise

- We consider the following problem,

$$
\begin{aligned}
&\min\nolimits_{x\in\mathbb{R}^d} \quad f(x)\\
&s.t.\ \ g(x)=0,\\
&\qquad\quad l_x \leqslant x \leqslant u_x.
\end{aligned}
$$

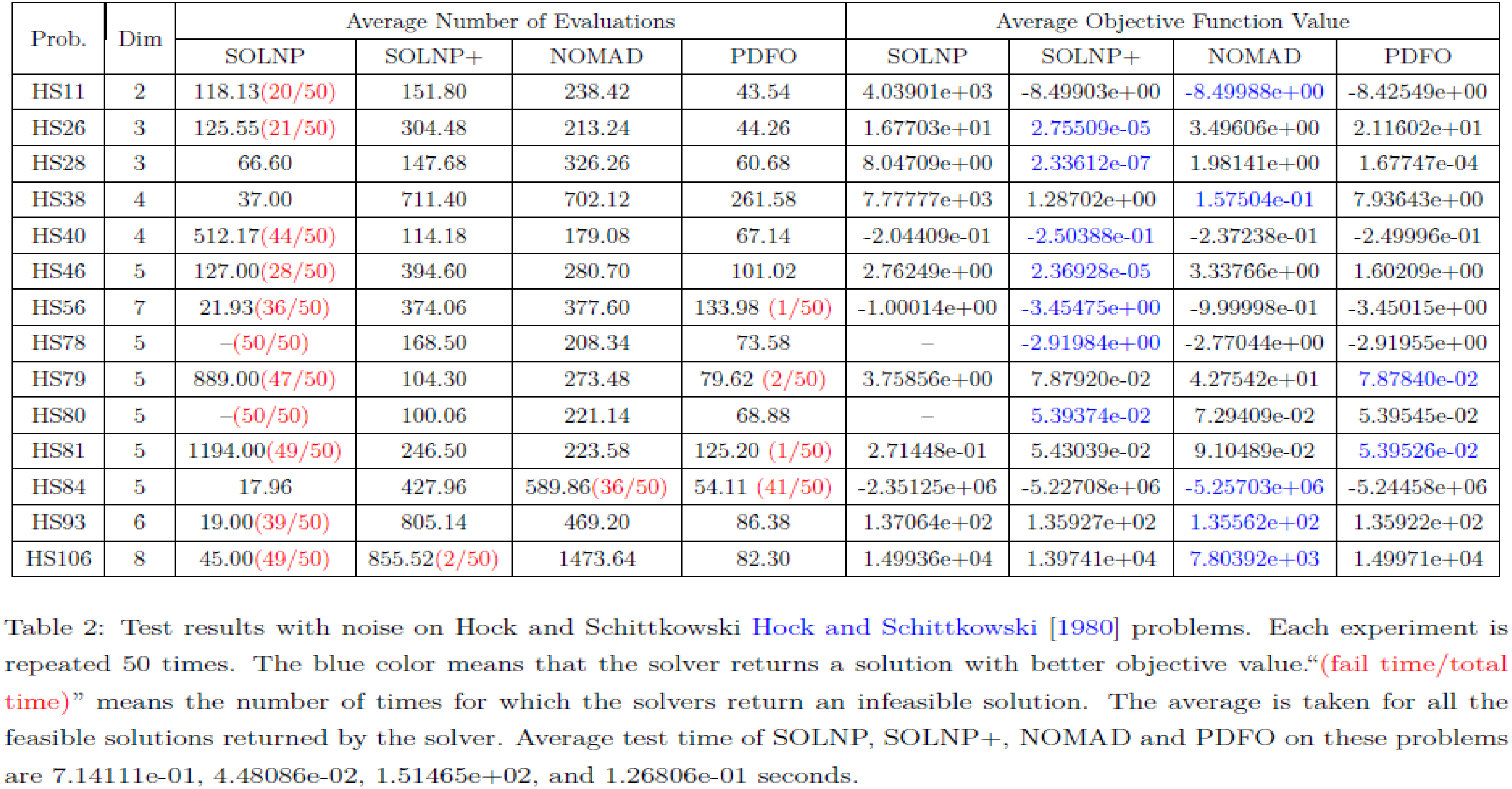
with observed value

$$
\begin{aligned}
\widehat{f}(x) &= f(x)(1+\sigma N_1(x)),\\
\widehat{g}(x) &= g(x)(1+\sigma N_2(x))
\end{aligned}
$$

where $N_i(x) \sim N(0,I)\ i.i.d.\ ,\ \sigma = 10^{-4}.$

- If the infeasibility error of the point is less than 10^{-3}, we regard it as feasible point.

Computational Results II: Noise functions



Prob.	Dim	Average Number of Evaluations				Average Objective Function Value			
		SOLNP	SOLNP+	NOMAD	PDFO	SOLNP	SOLNP+	NOMAD	PDFO
HS11	2	118.13(20/50)	151.80	238.42	43.54	4.03901e+03	-8.49903e+00	-8.49988e+00	-8.42549e+00
HS26	3	125.55(21/50)	304.48	213.24	44.26	1.67703e+01	2.75509e-05	3.49606e+00	2.11602e+01
HS28	3	66.60	147.68	326.26	60.68	8.04709e+00	2.33612e-07	1.98141e+00	1.67747e-04
HS38	4	37.00	711.40	702.12	261.58	7.77777e+03	1.28702e+00	1.57504e-01	7.93643e+00
HS40	4	512.17(44/50)	114.18	179.08	67.14	-2.04409e-01	-2.50388e-01	-2.37238e-01	-2.49996e-01
HS46	5	127.00(28/50)	394.60	280.70	101.02	2.76249e+00	2.36928e-05	3.33766e+00	1.60209e+00
HS56	7	21.93(36/50)	374.06	377.60	133.98 (1/50)	-1.00014e+00	-3.45475e+00	-9.99998e-01	-3.45015e+00
HS78	5	–(50/50)	168.50	208.34	73.58	–	-2.91984e+00	-2.77044e+00	-2.91955e+00
HS79	5	889.00(47/50)	104.30	273.48	79.62 (2/50)	3.75856e+00	7.87920e-02	4.27542e+01	7.87840e-02
HS80	5	–(50/50)	100.06	221.14	68.88	–	5.39374e-02	7.29409e-02	5.39545e-02
HS81	5	1194.00(49/50)	246.50	223.58	125.20 (1/50)	2.71448e-01	5.43039e-02	9.10489e-02	5.39526e-02
HS84	5	17.96	427.96	589.86(36/50)	54.11 (41/50)	-2.35125e+06	-5.22708e+06	-5.25703e+06	-5.24458e+06
HS93	6	19.00(39/50)	805.14	469.20	86.38	1.37064e+02	1.35927e+02	1.35562e+02	1.35922e+02
HS106	8	45.00(49/50)	855.52(2/50)	1473.64	82.30	1.49936e+04	1.39741e+04	7.80392e+03	1.49971e+04

Table 2: Test results with noise on Hock and Schittkowski Hock and Schittkowski [1980] problems. Each experiment is repeated 50 times. The blue color means that the solver returns a solution with better objective value.“(fail time/total time)” means the number of times for which the solvers return an infeasible solution. The average is taken for all the feasible solutions returned by the solver. Average test time of SOLNP, SOLNP+, NOMAD and PDFO on these problems are 7.14111e-01, 4.48086e-02, 1.51465e+02, and 1.26806e-01 seconds.

Computational Results III: Feasibility Problem

Solver	Solved	Time/s	Function Evaluation
SOLNP+	53/129	601.9	213298
PDFO	55/129	3056.7	324265

Test Result on the feasibility problems with dimension less than 200 of Cutest problem set.
Solved means the solvers return a point with infeasibility less than 0.001.

Gould, Nicholas IM, Dominique Orban, and Philippe L. Toint. "CUTEst: a constrained and unconstrained testing environment with safe threads for mathematical optimization." *Computational optimization and applications* 60 (2015): 545-557.

Computational Results IV: Tumor Growth Problem

$$\begin{aligned}
&\min_{t_1,\cdots,t_n,a_1,\cdots,a_n} \quad P^* = P(t_{\text{end}}) + Q(t_{\text{end}}) + Q_P(t_{\text{end}}) \\
&s.t. \qquad 0 \le t_i \le t_{\text{end}}, \qquad i = 1, \cdots n, \\
&\qquad\qquad 0 \le a_i \le 1, \qquad i = 1, \cdots n, \\
&\qquad\qquad 0 \le \max_{t\in[0,t_{\text{end}}]} C(t) \le v_{\max}, \\
&\qquad\qquad 0 \le \int_0^{t_{\text{end}}} C(t)\mathrm{d}t \le v_{\text{cum}}.
\end{aligned}$$

At time t_i , we give drug of dosage a_i to the patient. P^* is the size of tumor at the end of the treatment. $C(t)$ is the drug concentration.

Tumor Growth Problem continued

- P^* is calculated by the ODE

$$
\begin{aligned}
\frac{\mathrm{d}C}{\mathrm{d}t} &= -\theta_1 C \\
\frac{\mathrm{d}P}{\mathrm{d}t} &= \theta_4 P(1 - \frac{P + Q + Q_P}{K}) + \theta_5 Q_P - \theta_3 P - \theta_1 \theta_2 C P \\
\frac{\mathrm{d}Q}{\mathrm{d}t} &= \theta_3 P - \theta_1 \theta_2 C Q \\
\frac{\mathrm{d}Q_P}{\mathrm{d}t} &= \theta_1 \theta_2 C Q - \theta_5 Q_P - \theta_6 Q_P,
\end{aligned}
$$

Georgios Arampatzis, Daniel Walchli, Pascal Weber, Henri Rastas, and Petros Koumoutsakos. (*μ*, *λ*)-ccma-es for constrained optimization with an application in pharmacodynamics. In *Proceedings of the Platform for Advanced Scientific Computing Conference*, pages 1–9, 2019

Tumor Growth Problem III

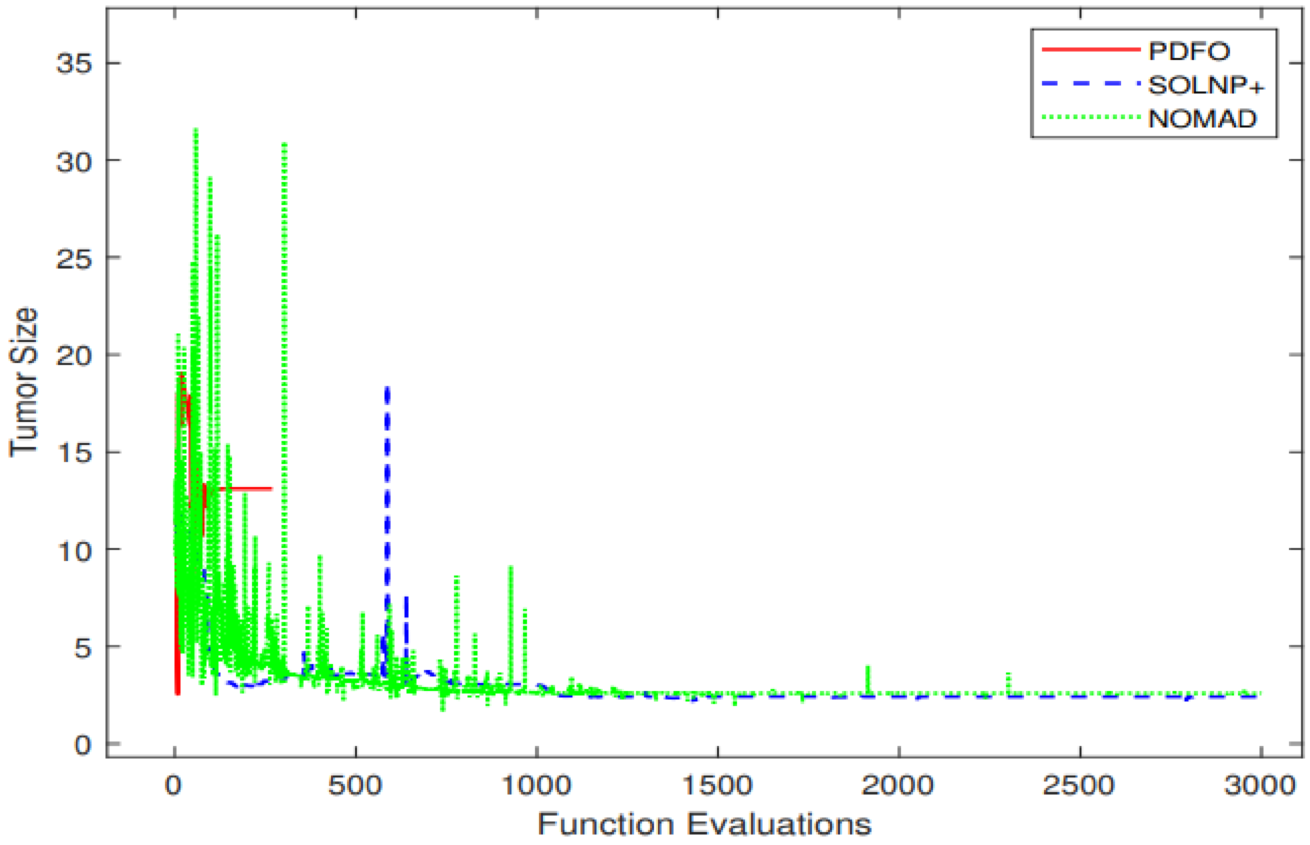


Figure 1: Convergence histories of the objective value.

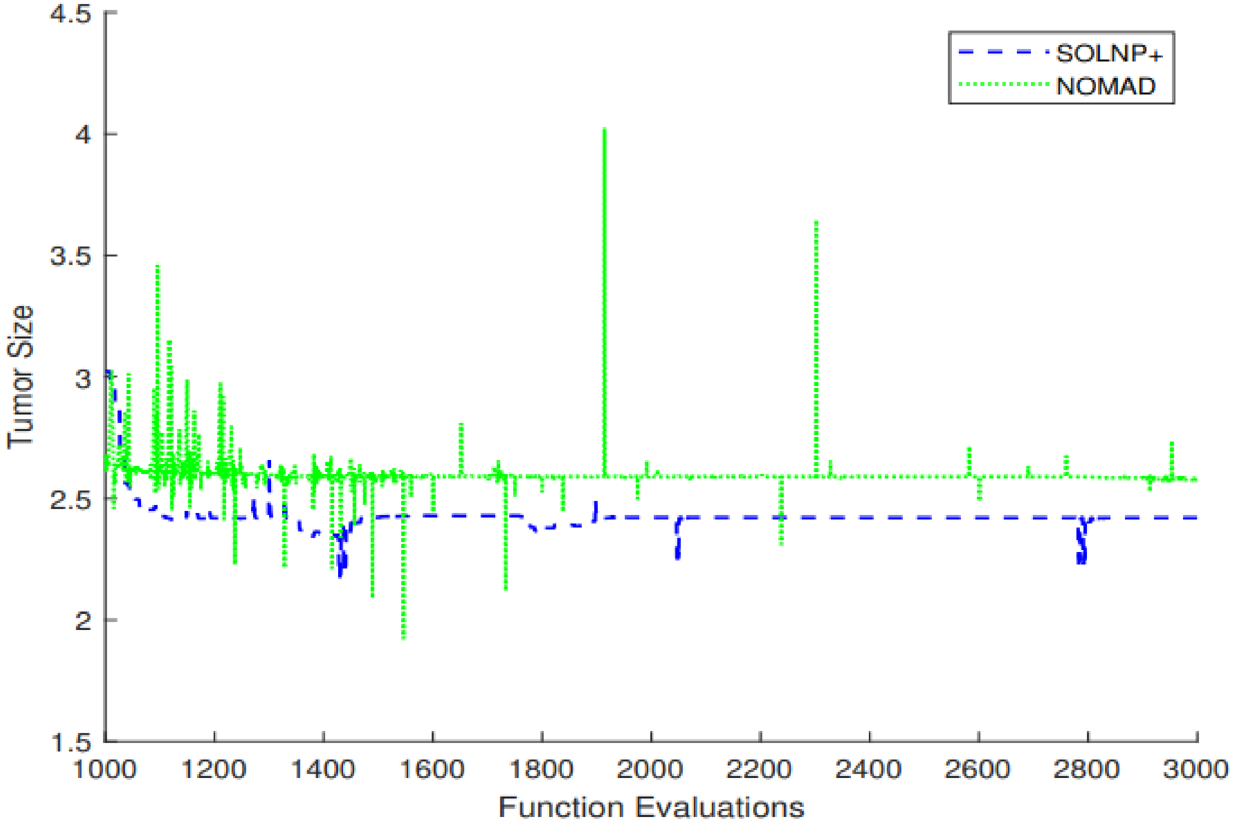


Figure 2: Convergence histories of the objective value after 1000 evaluations.

SOLNP+: Large-scale Unconstrained Problem

- Multipoint ZO gradient estimates (Duchi, 2014)

$$\hat{\nabla} f(x) := \frac{\phi(n)}{\delta} \sum_{i=1}^{b} \left[\left(f\left(x + \delta u_i\right) - f(x) \right) u_i \right]$$

When u_i is chosen as e_i, it becomes coordinate *i*.

- With gradient estimates, SOLNP+ implements ZO version of
  - SGD (Ghadimi, 2013)
  - DRSOM (Zhang, 2022) with interpolation

J.C.Duchi, M. I. Jordan, M. J. Wainwright, and A. Wibisono, “Optimal rates for zero-order convex optimization: The power of two function evaluations,”IEEE Trans.Inf Theory, vol.61,no.5,pp.2788-2806,2015.doi: 10.1109/TIT.2015.2409256.
S. Ghadimi and G. Lan, “Stochastic first-and zeroth-order methods for nonconvex stochastic programming,” *SIAM J. Optimiz.*, vol. 23, no. 4, pp. 2341–2368, 2013. doi: 10.1137/120880811
Zhang, Chuwen, et al. "DRSOM: A Dimension Reduced Second-Order Method and Preliminary Analyses." *arXiv preprint arXiv:2208.00208* (2022).

ZO-DRSOM

- Dimension reduced second-order method (DRSOM) automatically adjust stepsize α_k of directions
  - gradient $g_k = \nabla f(x_k)$
  - momentum $d_k = x_k - x_{k-1}$
  - other directions added in D_k …

$$x_{k+1} = x_k + \begin{bmatrix} -g_k & d_k \end{bmatrix} \begin{bmatrix} \alpha_k^1 \\ \alpha_k^2 \end{bmatrix} = x_k + D_k \alpha_k$$

- DRSOM solves small trust region subproblem (TRS) to determine α_k

$$\begin{aligned} \min_{\alpha \in \mathbb{R}^2} \ & f(x_k) + g_k^\top D_k \alpha + \frac{1}{2} \alpha^\top D_k^\top H_k D_k \alpha \\ \text{s.t.} \ & \|D_k \alpha\|_2 \leq \Delta \end{aligned}$$

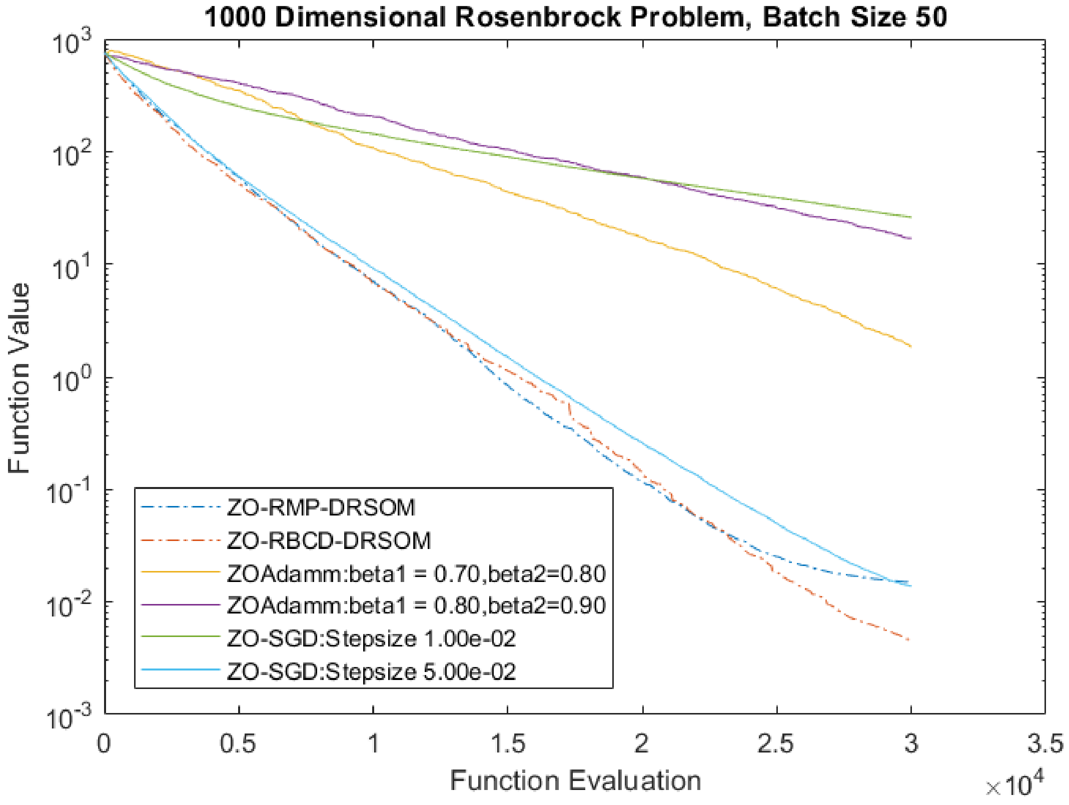
- We use two way to calculate the gradient.
  - ZO-RMP-DRSOM: Use Randomized Multi-Point Method
  - ZO-RBCD-DRSOM: Use Randomized Block Coordinate Descent
- ZO-DRSOM uses interpolation to approximate $D_k^T H_k D_k$ in TRS

Experiments in Large Problems: Rosenbrock

- Rosenbrock function is a well-known nonconvex functions in the form of

$$f(\boldsymbol{x}) = \sum_{i=1}^{n-1} 100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2$$

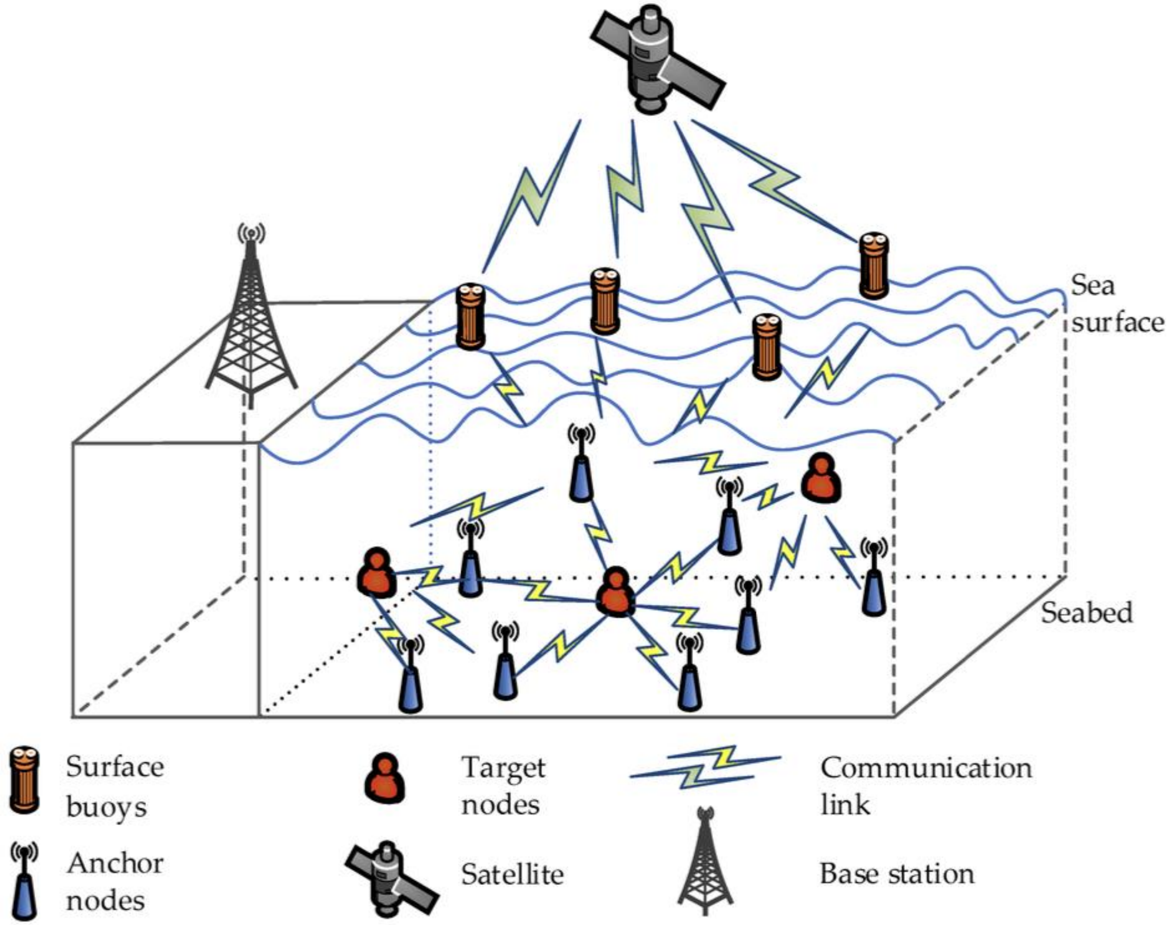
- ZO-Adamm, ZO-SGD and ZO-DRSOM are tested in a 1200 dimensional Rosenbrock problem.
- ZO-RMP-DRSOM, ZO-RBCD-DRSOM and ZO-SGD decrease most smoothly. However, inappropriate parameters lead to inappropriate performance of ZO-SGD.



Chen, Xiangyi, et al. "Zo-adamm: Zeroth-order adaptive momentum method for black-box optimization." *Advances in neural information processing systems* 32 (2019).

Experiments in Large Problems: SNL

- Sensor network localization (SNL) is widely used in GPS and location services.
- We known
  - Some distances between sensors
  - Some distances between sensors and anchors
  - Position of anchors
- We want to know
  - Position of sensors



Experiments in Large Problems: SNL

- SNL is the problem to recover unknown locations of sensors given some distances.
- Given anchors $a_k \in \mathbb{R}^d$, $d_{ij} \in N_x$ and $\hat{d}_{kj} \in N_a$, we need to find $x_i \in \mathbb{R}^d$ such that

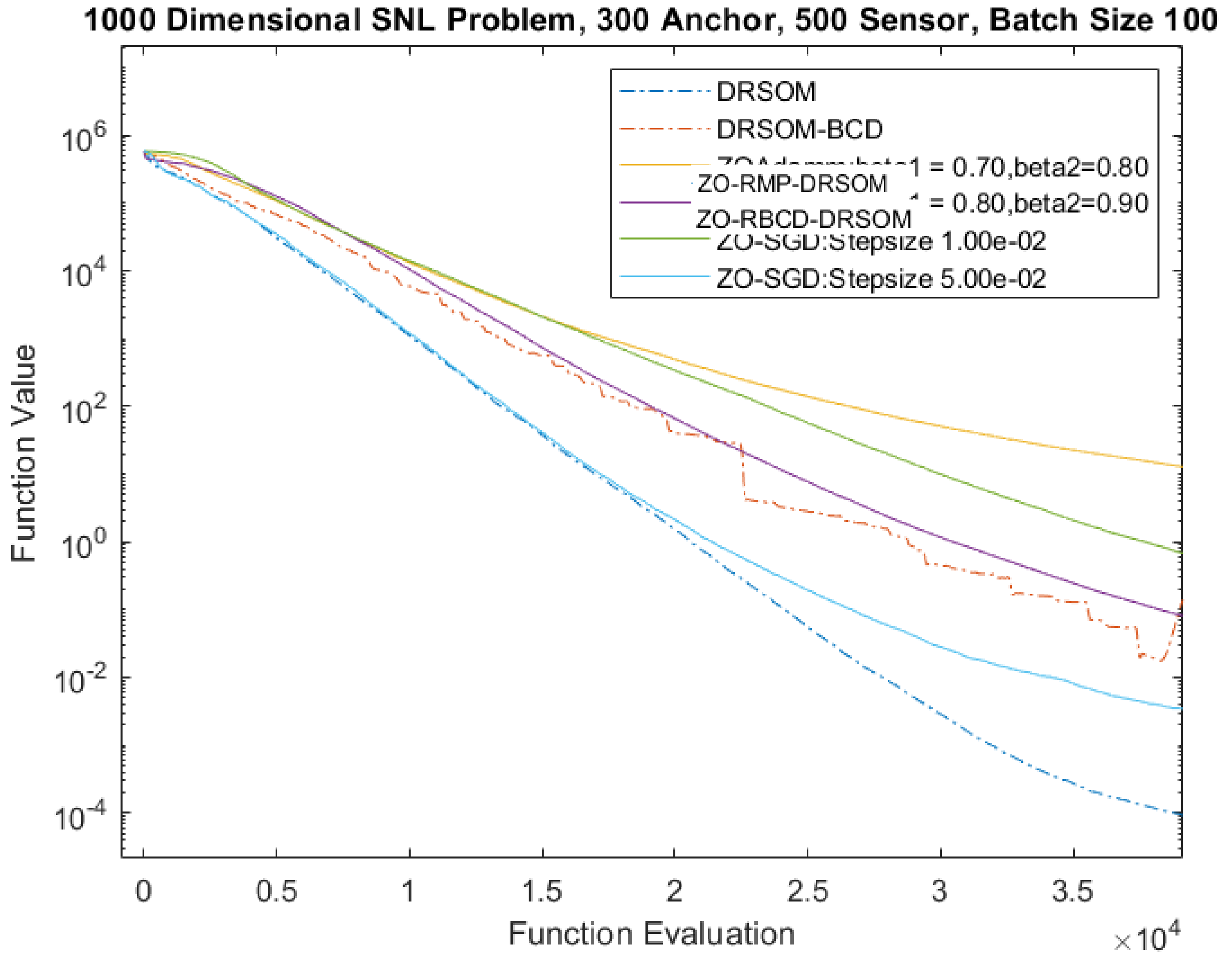
$$\begin{aligned} \|x_i - x_j\|_2^2 &= d_{ij}^2, \quad \forall (i,j) \in N_x \\ \|a_k - x_j\|_2^2 &= \hat{d}_{kj}^2, \quad \forall (k,j) \in N_a \end{aligned}$$

- Reformulate SNL as nonconvex optimization problem

$$\min_{x_i \in \mathbb{R}^d, \forall i} \ f(x) = \sum_{(i,j) \in N_x} (\|x_i - x_j\|_2^2 - d_{ij}^2)^2 + \sum_{(k,j) \in N_a} (\|a_k - x_j\|_2^2 - \hat{d}_{kj}^2)^2$$

Experiments in Large Problems: SNL

- ZO-Adam, ZO-SGD, ZO-RBCD-DRSOM and ZO-RMP-DRSOM are tested in a 500-sensor SNL problem.
- ZO-RMP-DRSOM again outperforms others.



Advantage of SOLNP+

- Able to make use of dual information.
- Provide estimation of both primal and dual solutions.
- It seems Faster in speed.
- It seems Robust under noise.

Thank you!