Accelerating Derivative-Free Simulation Optimization

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Simulation Optimization: Problem Statement

Problem:

$$\min_{x \in \mathbb{R}^d} f(x) := \mathbb{E}[F(x,\xi)],$$

- $f: \mathbb{R}^d \to \mathbb{R}$ is smooth and bounded from below;
- f estimated by $\bar{F}(x,n) = n^{-1}\sum_{j=1}^{n} F(x,\xi_j)$;
- derivative information is not directly available.

Challenges:

- Need to approximate gradient (biased gradients).
- Simulation oracle call typically takes quite a while.

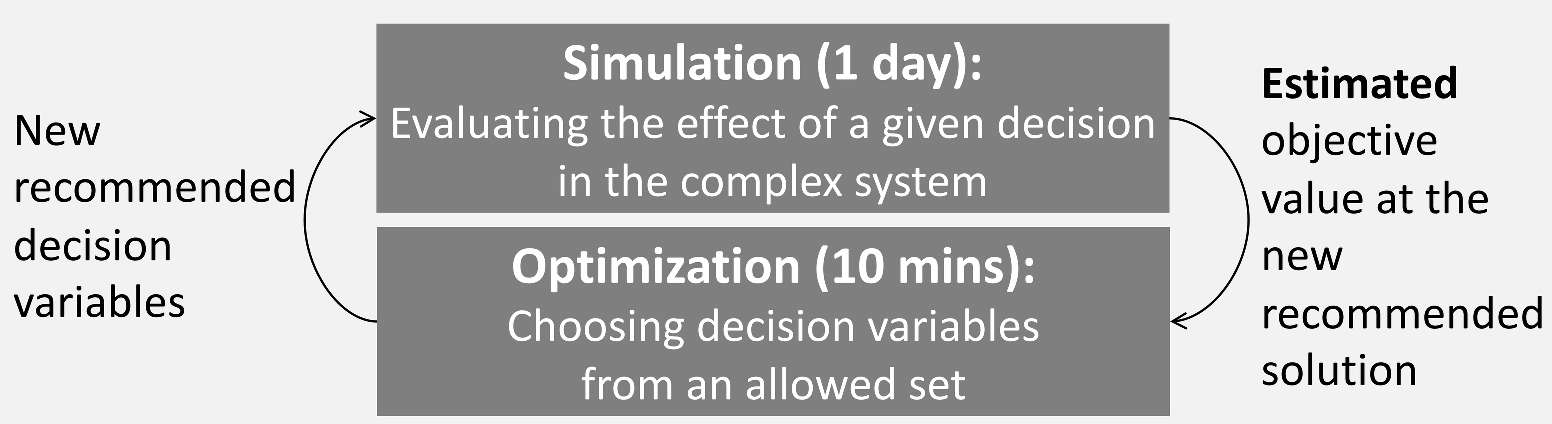


Fig 1. An iteration within a simulation optimization framework

"For efficiency, we want to minimize the number of simulation oracle calls during optimization"

Adaptive Sampling and Trust Region (TR)

Adaptive sampling:

- Simulation effort $N(x)$ is a stopping time determined by
  $N(x) = \min\{n: \widehat{SE}(x,n) \le \text{optimality gap at } x\}$.

Stochastic trust-region method:

- Optimization evolves through minimizing local models within a region of radius Δ.
- TR is a robust solution method in derivative-free settings and in the presence of noise.

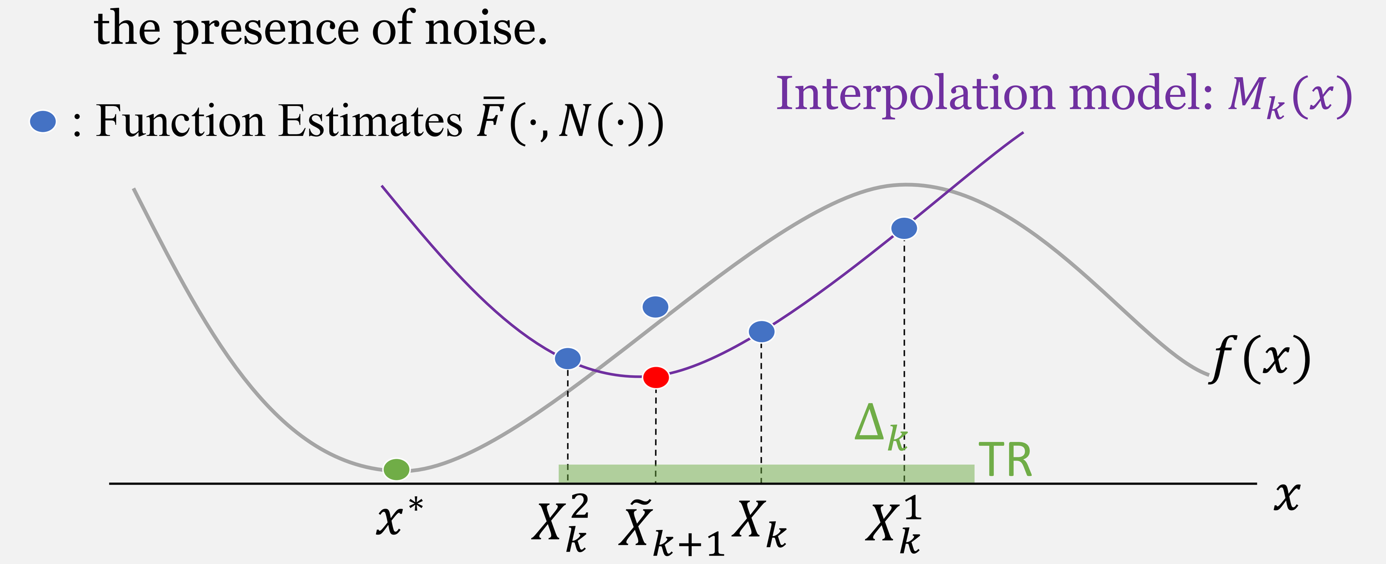


Fig 2. An iteration of the adaptive sampling trust-region method

"How do we handle high-dimensional problems with the adaptive sampling trust-region method (ASTRO-DF)?"

Accelerating ASTRO-DF

Acceleration by reusing the previous simulation results:

- Use a rotated coordinate basis so that the required number of design point becomes from $\mathcal{O}(d^2)$ to $\mathcal{O}(d)$.
- Reuse two design points and their replications.

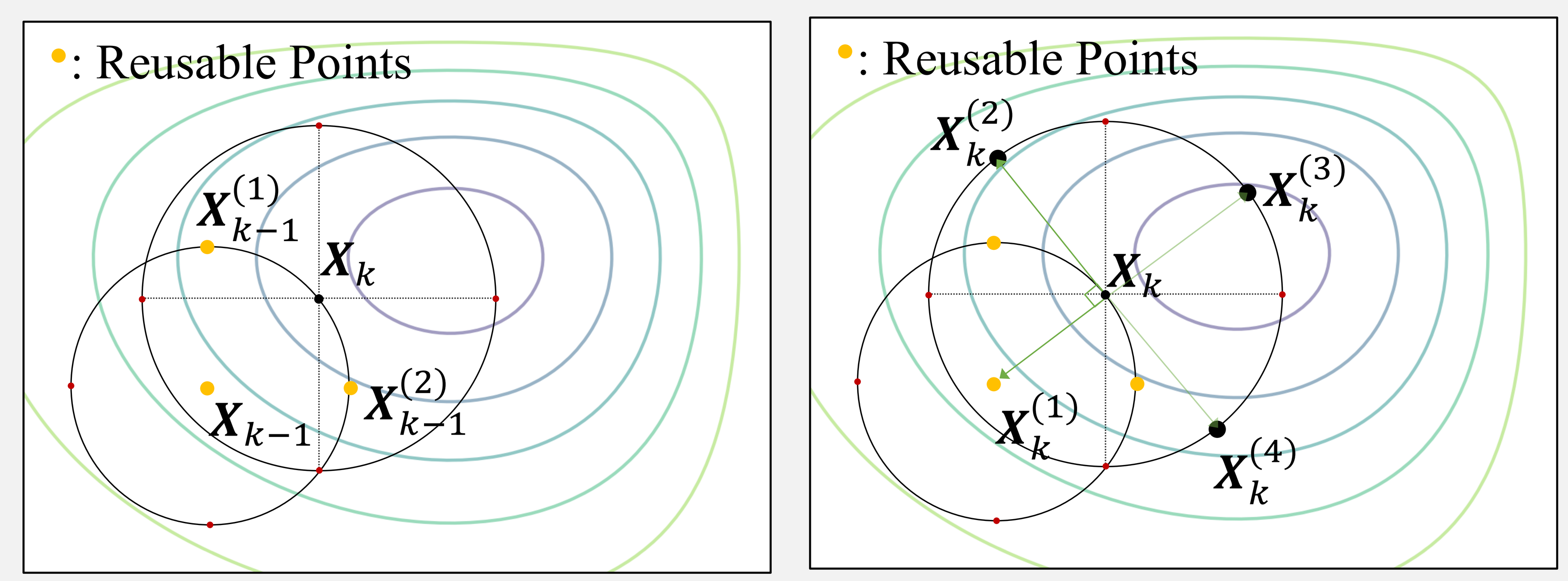
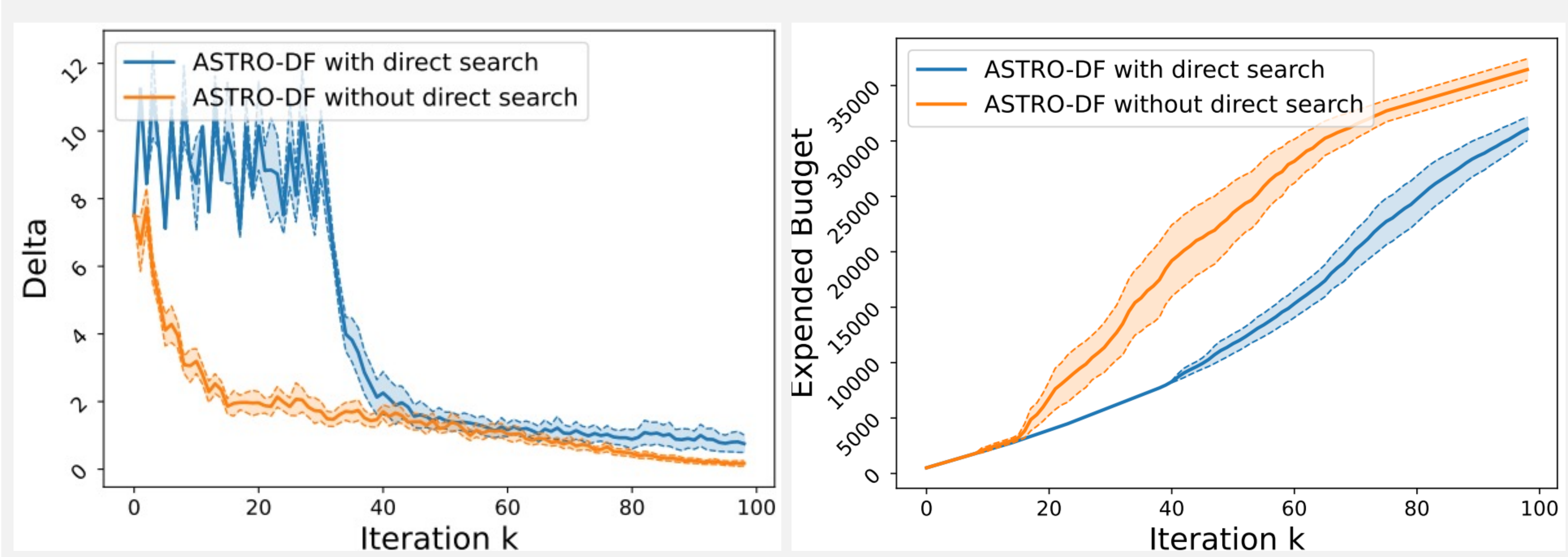


Fig 3. The design point X_{k-1}, being the farthest from X_k among the reusable design points, is reused as $X_k^{(1)}$

Acceleration with a direct search:

- When an interpolation point has a lower function estimate, it uses that as the candidate point instead of the point suggested by the model.



(a) Trust-region radius (Δ_k) (b) Expended budget

Fig 4. Using the direct search increases the chances of accepting a new incumbent and prevents step size from shrinking too quickly during the early stages of the search

Acceleration with Common Random Numbers:

- Querying the oracle with the same random number.
- Preserving structure inherent to function sample-paths.

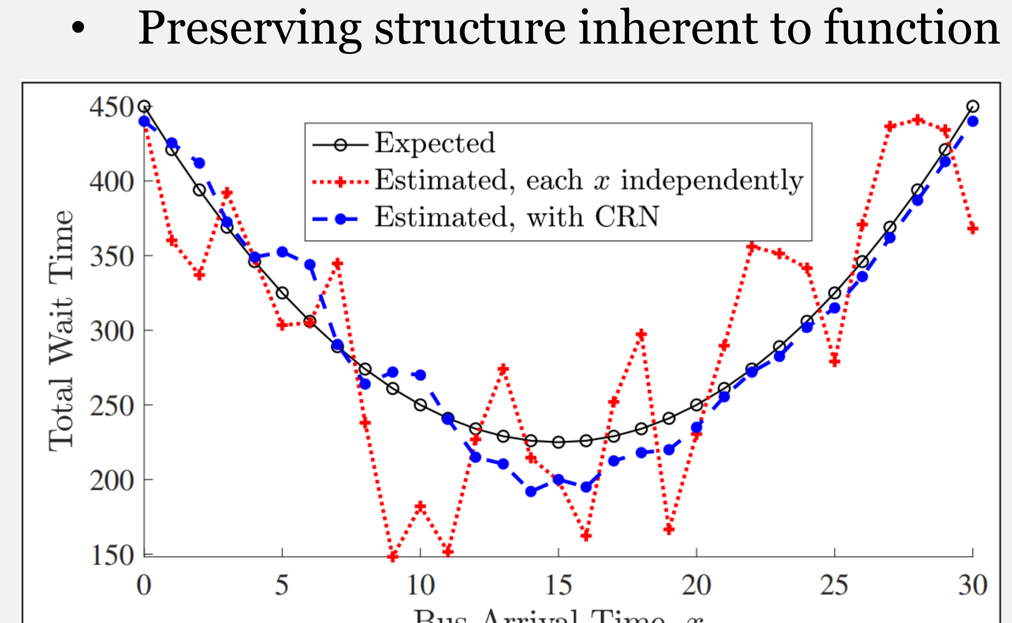


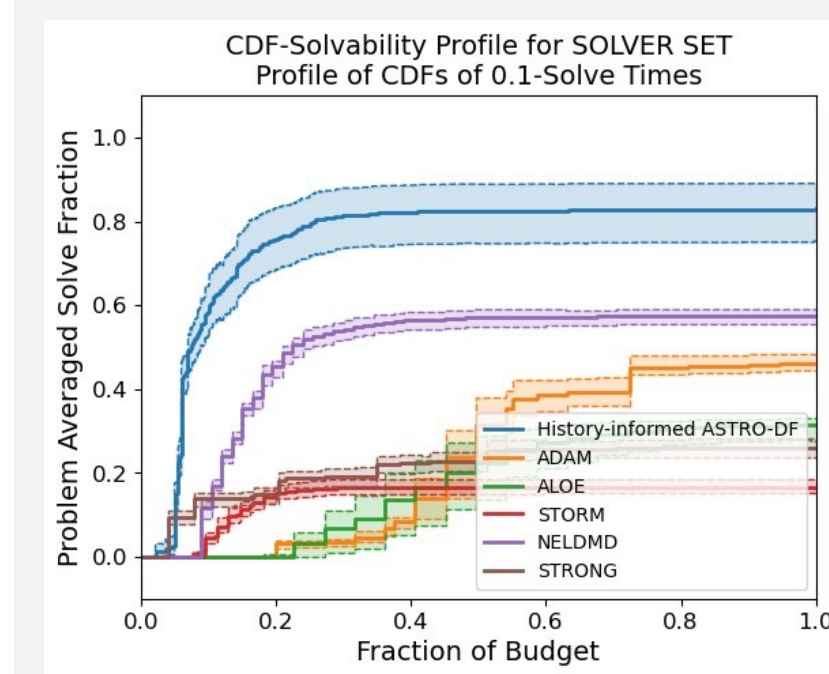
Fig 5. The black curve is the true function f, the blue curve is f's estimate constructed with CRN, and the red curve is f's estimate constructed with independent sampling.

ASTRO-DF vs Accelerated ASTRO-DF:

	ASTRO-DF	Accelerated ASTRO-DF
Interpolation set selection	Random	Rotated Coordinate Basis
Interpolation set	(d+1)(d+2)/2	2d+1
Candidate point by	Model	Model + Direct Search
# of reusing points	≥ 0	2

Results

Numerical Results:



Methods:

1. Direct search method
   - Nelder-Mead
2. Model-based methods
   - STORM
   - STRONG
3. Gradient-based methods
   - ALOE
   - ADAM

Fig 6. The fraction of the "solved" problems on 60 problems in SimOpt library

Theoretical Results:

- Most existing stochastic TR for derivative free optimization does not have guarantees on the complexity.

Method	Iteration complexity	Sample complexity
VNSP[1]	-	-
LB[2]	-	-
STR[3]	-	-
STORM[4]	$\mathcal{O}(\epsilon^{-2})$	$\tilde{\mathcal{O}}(\epsilon^{-6})$
ASTRO-DF	$\mathcal{O}(\epsilon^{-2})$	$\tilde{\mathcal{O}}(\epsilon^{-6})$
ASTRO-DF with CRN	$\mathcal{O}(\epsilon^{-2})$	$\tilde{\mathcal{O}}(\epsilon^{-4})$

1 Deng and Ferris (2009)
2 Larson and Billups (2016)
3 Rinaldi et al (2023)
4 Chen et al (2018), Blanchet et al (2019), Jin et al (2023)

Conclusion

- ASTRO-DF is a prominent algorithm for derivative-free problems that adaptively allocates simulation budget for efficiency but lacks flexibility in higher dimension.
- We accelerate ASTRO-DF using three key ideas:
  + 1) Reuse strategy and 2) CRN for saving budget per iteration,
  + 3) Direct search for a slower convergence rate of step size.
- CRN improves the sample complexity of ASTRO-DF from $\tilde{\mathcal{O}}(\epsilon^{-6})$ to $\tilde{\mathcal{O}}(\epsilon^{-4})$, outperforming the existing results.

References

- Shashaani, S., F. Hashemi, and R. Pasupathy. 2018. "ASTRO-DF: A class of adaptive sampling trust-region algorithms for derivative-free stochastic optimization". SIAM Journal on Optimization28(4):3145–3176
- Ha, Yunsoo, Sara Shashaani, and Raghu Pasupathy. 2023. "On Common-Random-Numbers and The Complexity of Adaptive Sampling Trust-Region Methods". https://optimization-online.org/wp-content/uploads/2023/08/astrodf-complexity-online-version.pdf.