

CMA-ES with Learning Rate Adaptation: Can CMA-ES with Default Population Size Solve Multimodal and Noisy Problems?



GECCO'23

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Outline

1. CMA-ES and Its Issues for difficult (multimodal and/or noisy) problems

Users need expensive hyperparameter tuning (e.g. population size)

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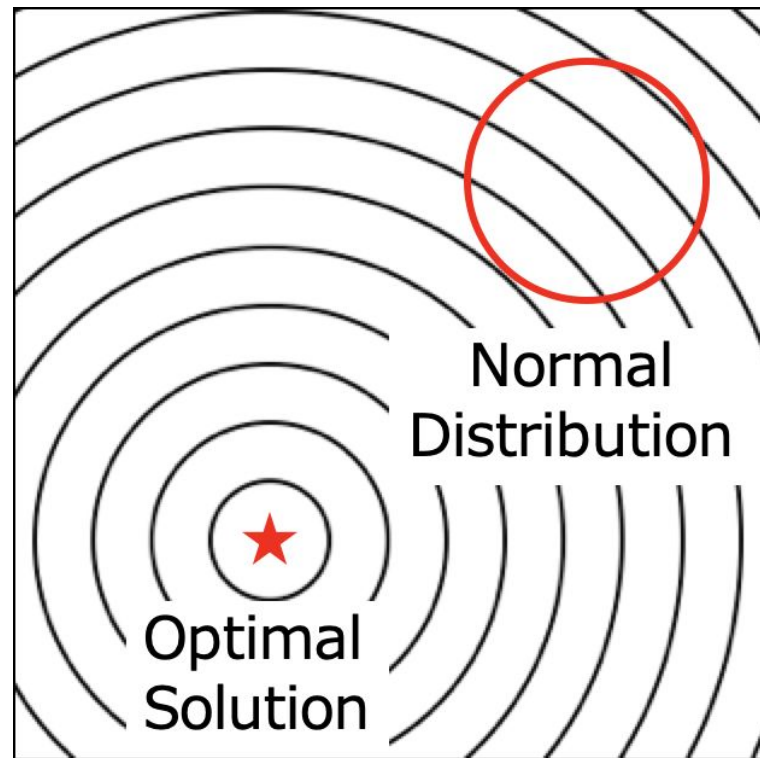
Can the CMA-ES with default population size (λ) solve multimodal and noisy problems?

3. Experimental Results

With LRA, CMA with default λ (e.g. $\lambda=15$ for $d=40$) can succeed on Rastrigin

CMA-ES [HMK03,Han16]

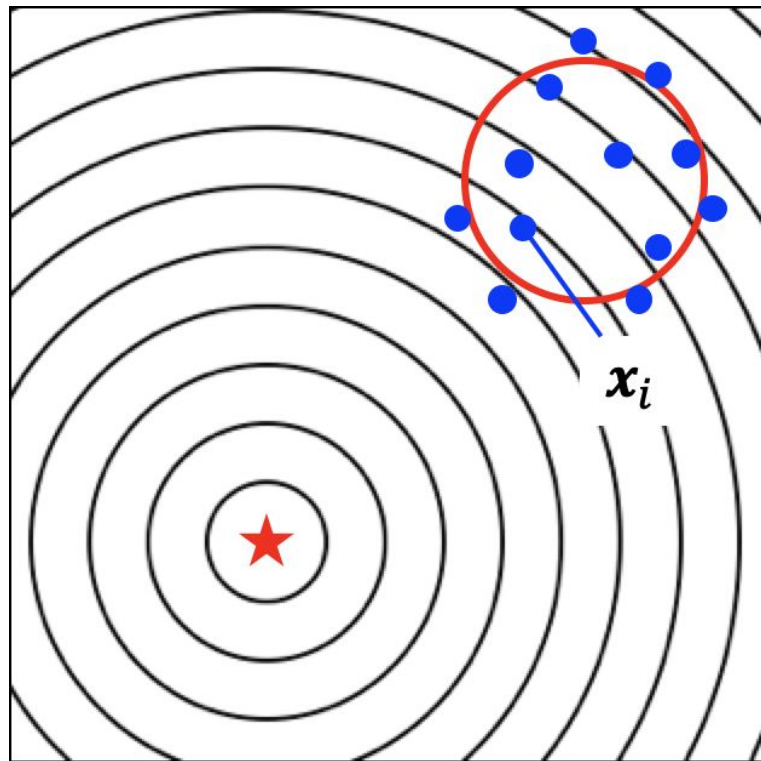
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- multivariate Gaussian distribution (MGD)
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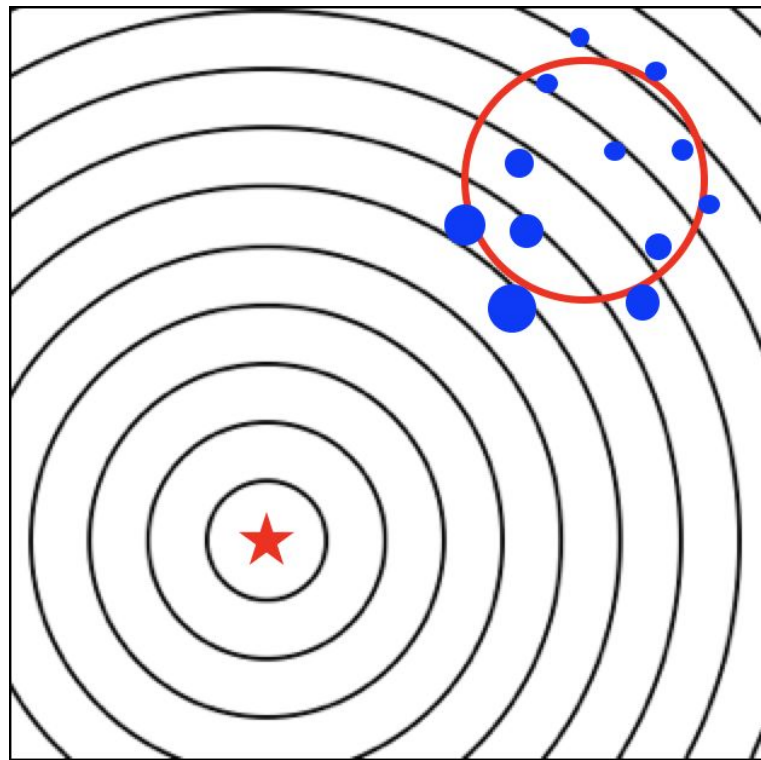
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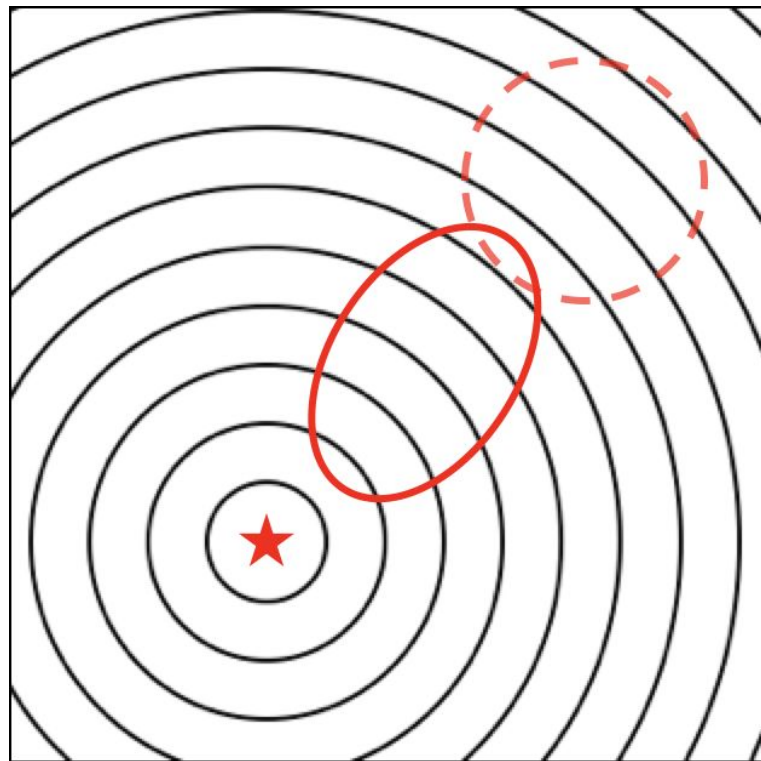
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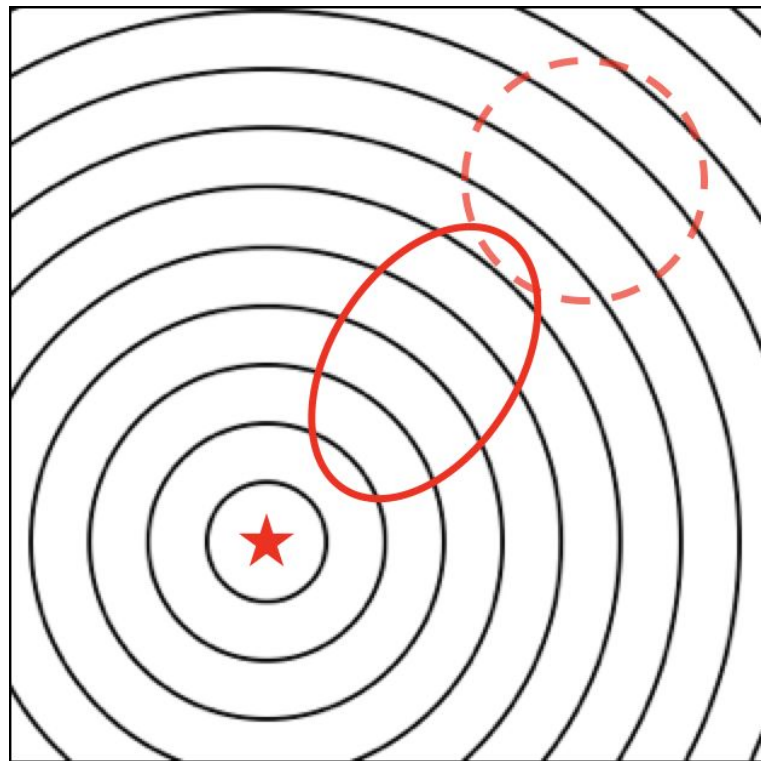
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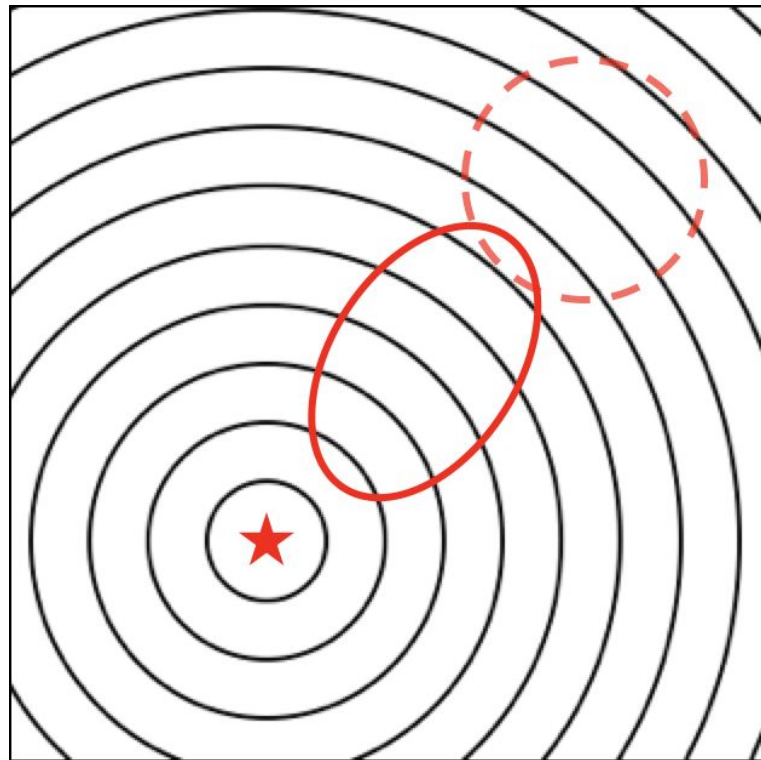
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We consider the most commonly used CMA-ES



CMA-ES and Its Dependence on Hyperparameters

- CMA-ES is a quasi-hyperparameter-free method
 - Hyperparameter values are automatically computed from:
 - (1) dimensionality, (2) population size λ ; by default, $\lambda = 4 + \lfloor 3 \ln d \rfloor$
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- Possible approach: online λ adaptation [NA16,NA18]

Our Approach: Learning Rate Adaptation

- Important observation [MA17]:
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- **Learning rate adaptation** vs. **population size adaptation**
 - Learning rate adaptation is more practically useful
 - E.g. parallel implementation (may be population size = # of workers)

Learning Rate Adaptation: Setup

- Notations :

vectorization operator, $\Sigma = \sigma^2 C$

- distribution parameters : $\theta_m = m, \theta_\Sigma = \text{vec}(\Sigma)$
- original updates : $\Delta_m^{(t)} = m^{(t+1)} - m^{(t)}, \Delta_\Sigma^{(t)} = \text{vec}(\Sigma^{(t+1)} - \Sigma^{(t)})$
- learning rate factors : $\eta_m^{(t)}, \eta_\Delta^{(t)}$

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- Modified updates :

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How to adapt these learning rate?

Why We Use SNR for Learning Rate Adaptation?

- We adapt the learning rate based on the signal-to-noise ratio (SNR):

$$\text{SNR} := \frac{\|\mathbb{E}[\Delta]\|_F^2}{\text{Tr}(F \text{Cov}[\Delta])} = \frac{\|\mathbb{E}[\Delta]\|_F^2}{\mathbb{E}[\|\Delta\|_F^2] - \|\mathbb{E}[\Delta]\|_F^2}$$

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F : Fisher information matrix

- Noisy problems: $\text{SNR} \rightarrow 0$ when noise becomes dominant
 - To improve function value, maintaining a positive SNR is crucial
 - We apply similar arguments to multimodal problems

SNR-Based Learning Rate Adaptation

- Assume LR is small over n iterations \Leftrightarrow updates are i.i.d

- n steps update:

$$\begin{aligned}\theta^{(t+n)} &= \theta^{(t)} + \eta \sum_{k=0}^{n-1} \Delta^{(t+k)} \\ &\approx \theta^{(t)} + \mathcal{D} \left(n\eta \mathbb{E}[\Delta], n\eta^2 \text{Cov}[\Delta] \right)\end{aligned}$$

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- $n = 1/\eta \Rightarrow \mathcal{D} \left(\mathbb{E}[\Delta], \eta \text{Cov}[\Delta] \right)$
 - By taking small η , we can obtain more concentrated update
- SNR over n iterations: $\frac{\|\mathbb{E}[\Delta]\|_F^2}{\eta \text{Tr}(F \text{Cov}[\Delta])} = \frac{1}{\eta} \text{SNR}$
- **Our method**: keep SNR over $n(=1/\eta)$ itr. as (positive) constant
 - $\text{SNR} = \alpha\eta \quad (\alpha > 0)$

SNR Estimation with Moving Averages

- We introduce moving averages for each m and Σ

$$\mathcal{E}^{(t+1)} = (1 - \beta)\mathcal{E}^{(t)} + \beta \tilde{\Delta}^{(t)},$$

$$\mathcal{V}^{(t+1)} = (1 - \beta)\mathcal{V}^{(t)} + \beta \|\tilde{\Delta}^{(t)}\|_2^2$$

local coordinate

$$\tilde{\Delta}_m = \sqrt{\Sigma}^{-1} \Delta_m$$

$$\tilde{\Delta}_\Sigma = 2^{-\frac{1}{2}} \text{vec}(\sqrt{\Sigma}^{-1} \text{vec}^{-1}(\Delta_\Sigma) \sqrt{\Sigma}^{-1})$$

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$$\begin{aligned} \text{SNR} &:= \frac{\mathbb{E}[\tilde{\Delta}]^2}{\text{Tr}(\text{Cov}[\tilde{\Delta}])} = \frac{\mathbb{E}[\tilde{\Delta}]^2}{\mathbb{E}[\|\tilde{\Delta}\|^2] - \|\mathbb{E}[\tilde{\Delta}]\|^2}, \\ &\approx \frac{\|\mathcal{E}\|_2^2 - \frac{\beta}{2-\beta} \mathcal{V}}{\mathcal{V} - \|\mathcal{E}\|_2^2} =: \widehat{\text{SNR}} \end{aligned}$$

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Approximation!
(See paper for details)

$$\approx \frac{\|\mathcal{E}\|_2^2 - \frac{\beta}{2-\beta} \mathcal{V}}{\mathcal{V} - \|\mathcal{E}\|_2^2} =: \widehat{\text{SNR}}$$

Update Equation of Learning Rate Adaptation

Adapting learning rate by:

$$\eta \leftarrow \eta \cdot \exp \left(\min(\gamma\eta, \beta) \Pi_{[-1,1]} \left(\frac{\widehat{\text{SNR}}}{\alpha\eta} - 1 \right) \right)$$

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bring SNR closer to $\alpha\eta$

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prevent η to change more than the factor of $\exp(y)$ or $\exp(-y)$ in $1/\eta$ iterations

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Adapting learning rate by: projection onto $[-1, 1]$ bring SNR closer to $\alpha\eta$

$$\eta \leftarrow \eta \cdot \exp \left(\min(\underbrace{\gamma\eta}_{\text{red}}, \underbrace{\beta}_{\text{blue}}) \underbrace{\Pi_{[-1,1]}}_{\text{green}} \left(\boxed{\frac{\widehat{\text{SNR}}}{\alpha\eta} - 1} \right) \right)$$

wait for the effect of the change of previous η

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$$\eta \leftarrow \min(\eta, \underline{1})$$

upper bound

prevent η to change more than the factor of $\exp(y)$ or $\exp(-y)$ in $1/\eta$ iterations

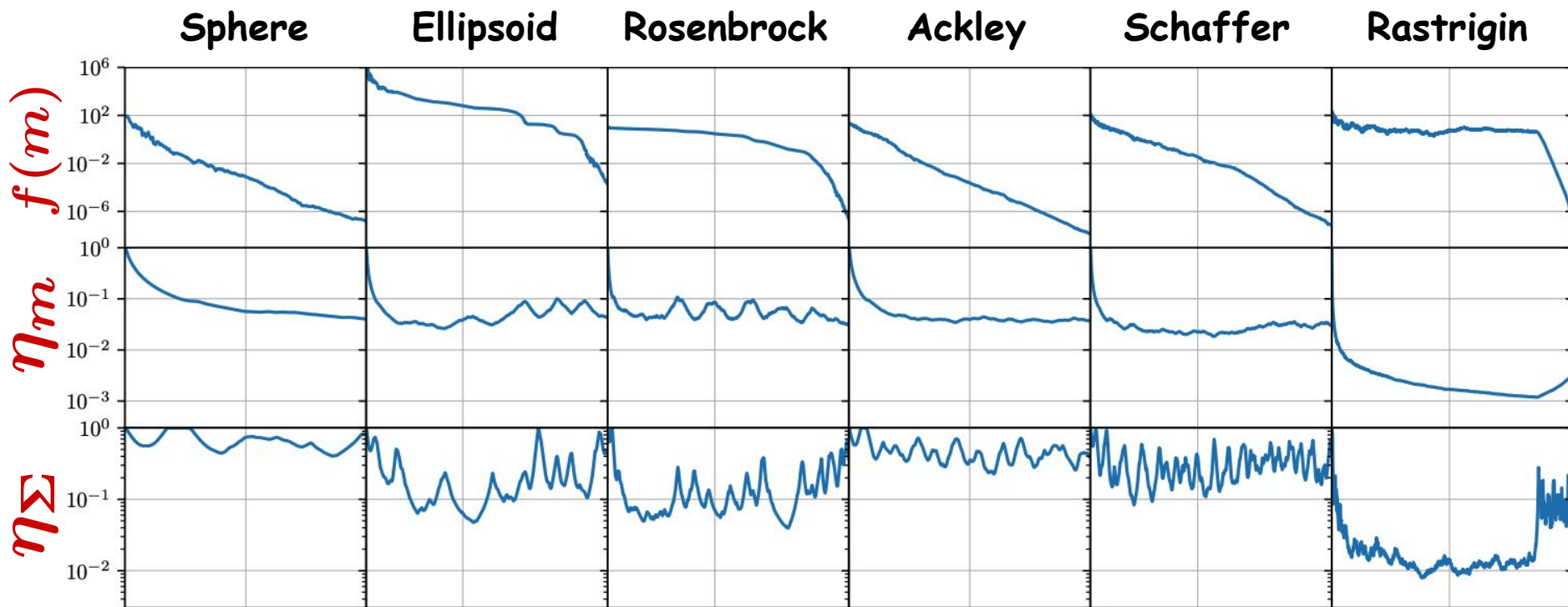
Experiments: Research Questions and Setups

- RQ1. Does the learning rate adaptation (LRA) behave appropriately depending on search situations?
- RQ2. Can LRA-CMA (CMA-ES with LRA) with default λ solve multimodal and/or noisy problems?
- (See paper for RQ3. Hyperparameter Sensitivity)

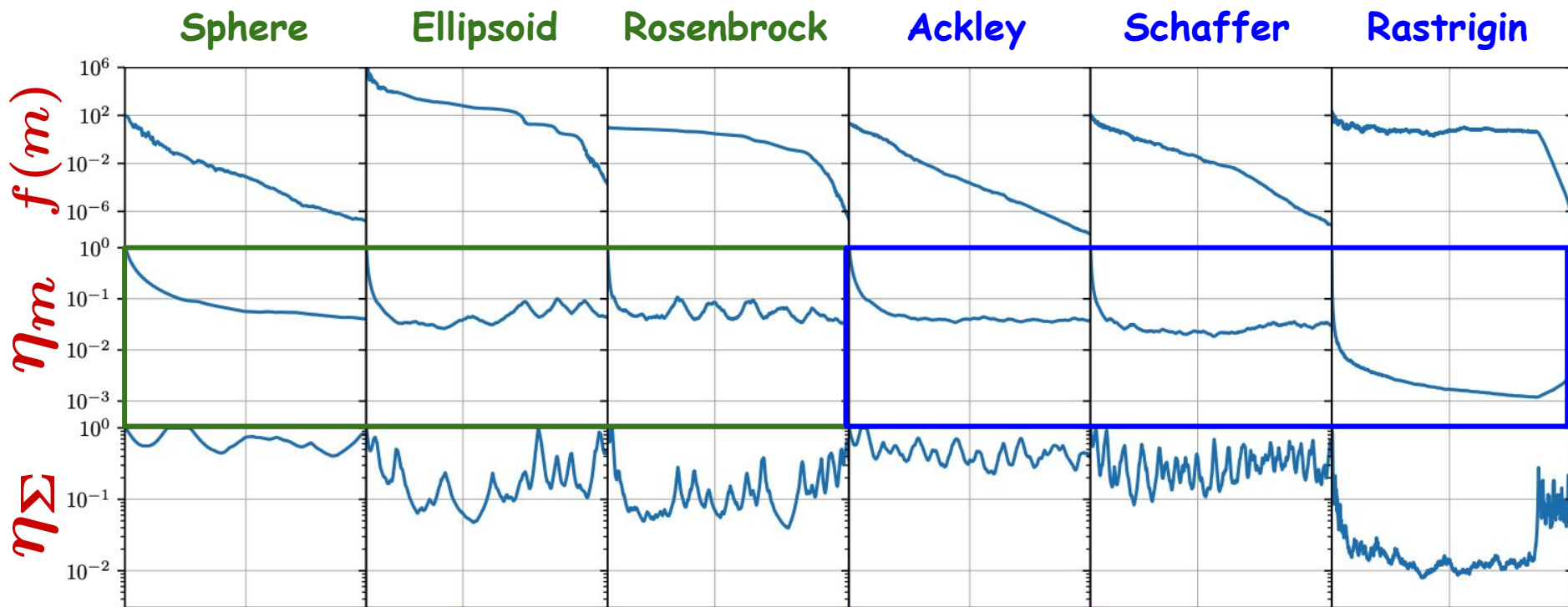
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- Benchmark problems
 - 3 unimodal functions & 5 multimodal functions
Sphere, Ellipsoid, Rosenbrock Ackley, Schaffer, Rastrigin, Bohachevsky, Griewank
 - In noisy problems, we considered additive Gaussian noise

Typical LRA-CMA behavior on 10-D noiseless problems

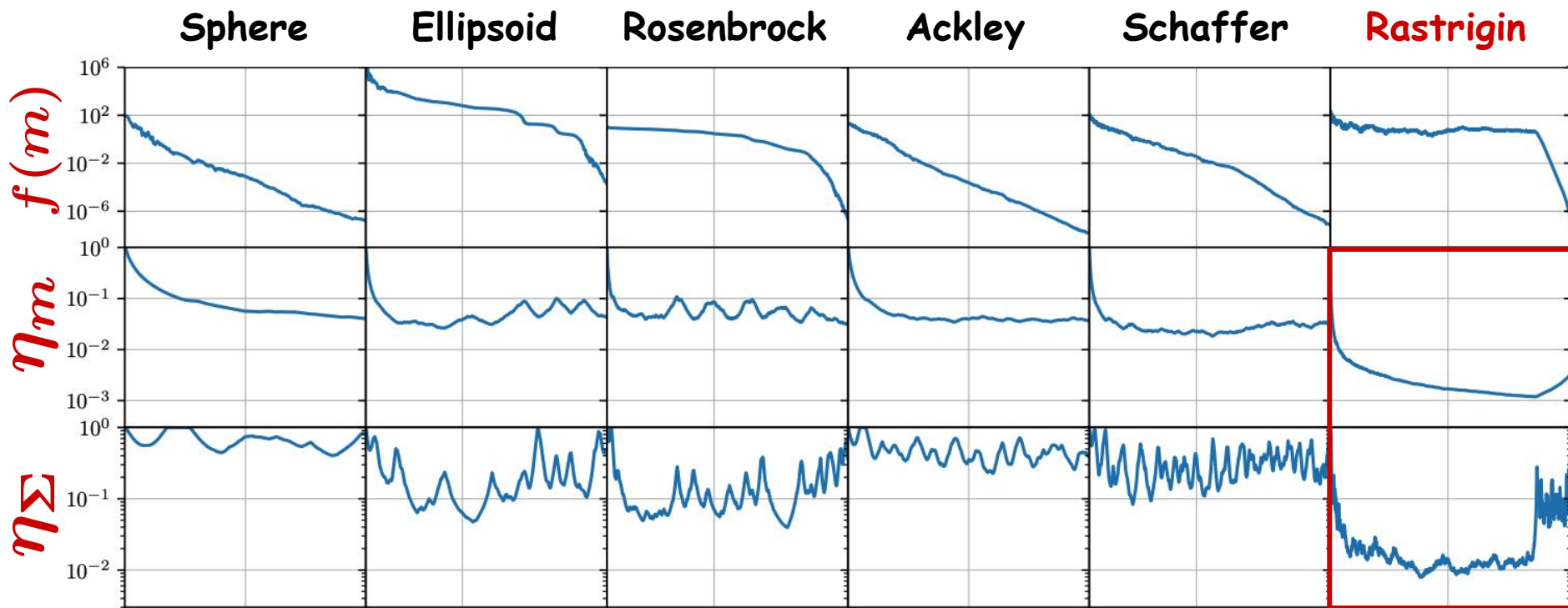


Typical LRA-CMA behavior on 10-D noiseless problems



η_m was slightly smaller on multimodal problems than on unimodal problems

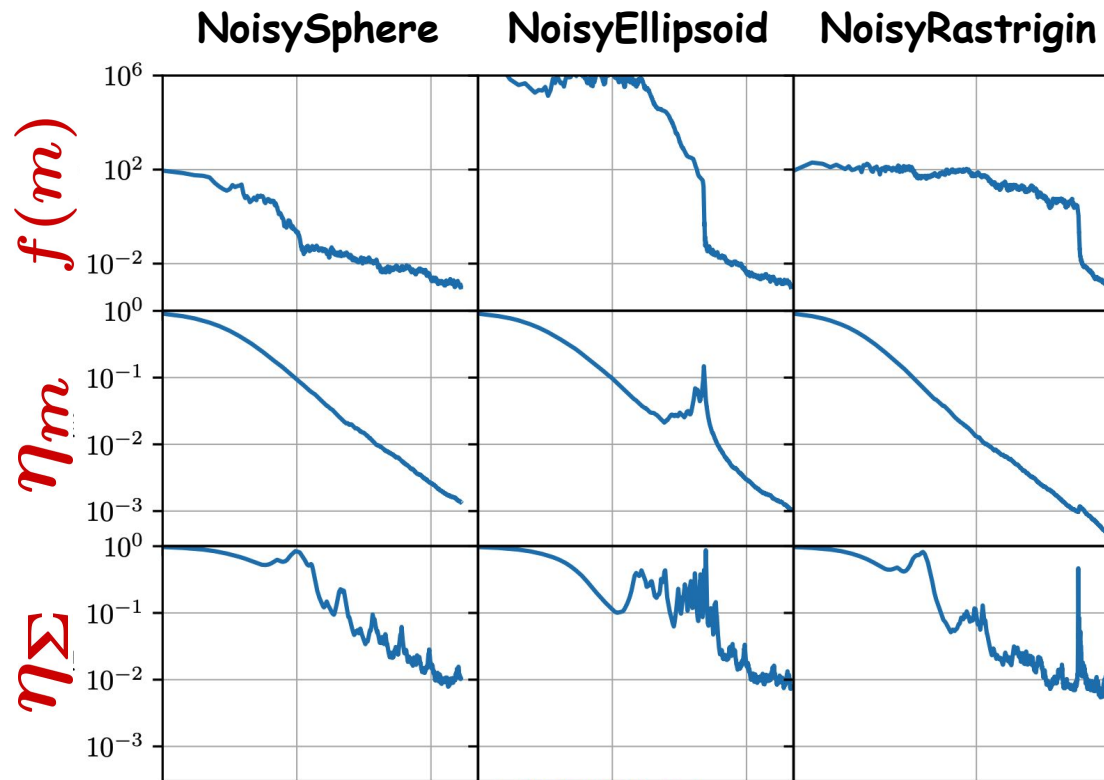
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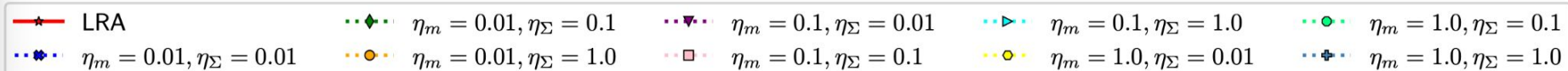
η_m and η_Σ clearly decreased at the beginning
⇒ learning rates are adapted according to difficulty of search situations

Typical LRA-CMA behavior on 10-D noisy problems

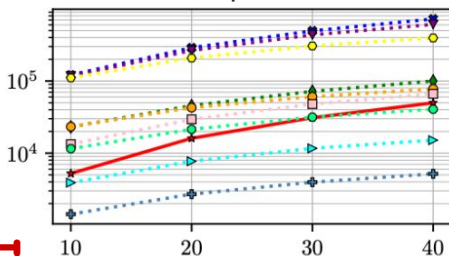
- Noise:
 - Early: negligible behavior is similar to noiseless
 - After: critical fvalue approached noise scale
 - η decreased



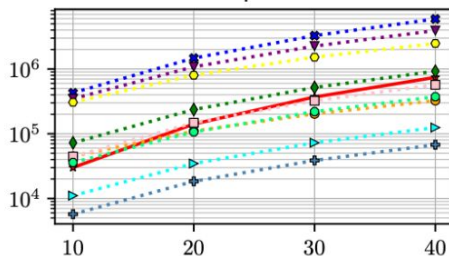
SP1 versus (10-40)Dim. (Noiseless Problems)



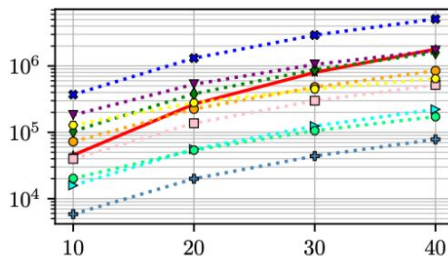
Sphere



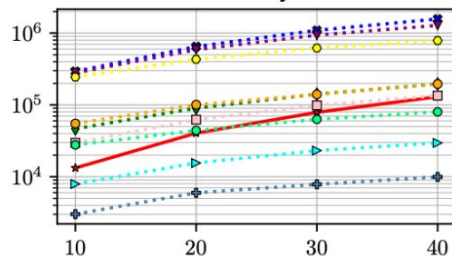
Ellipsoid



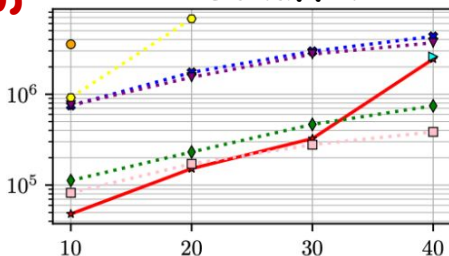
Rosenbrock



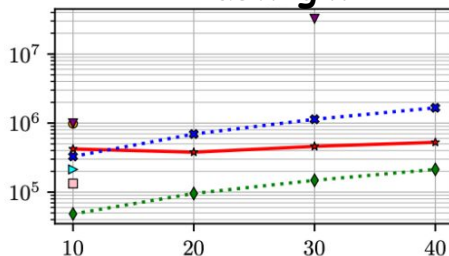
Ackley



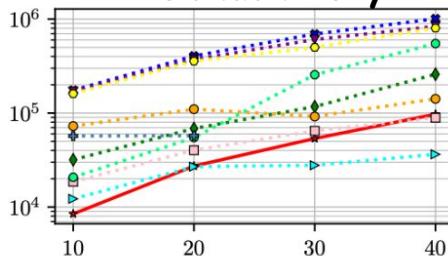
Schaffer



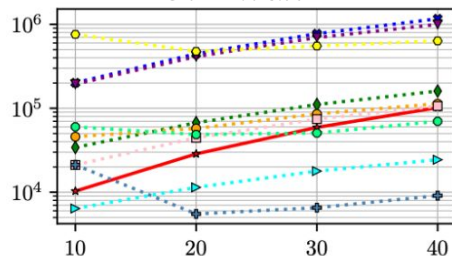
Rastrigin



Bohachevsky

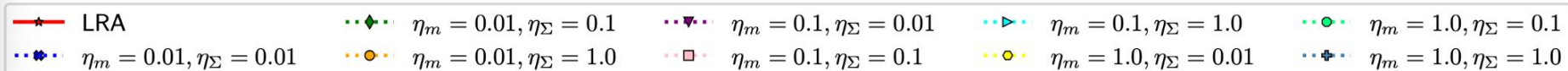


Griewank

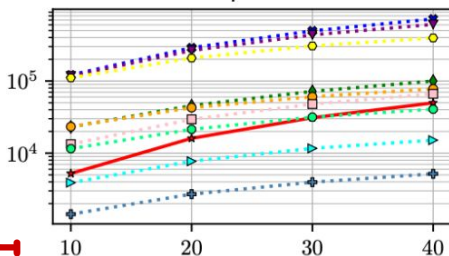


with high $\eta \Rightarrow$ worse on multimodal, with small $\eta \Rightarrow$ slow on unimodal
Clear trade-off in efficiency exists depending on η

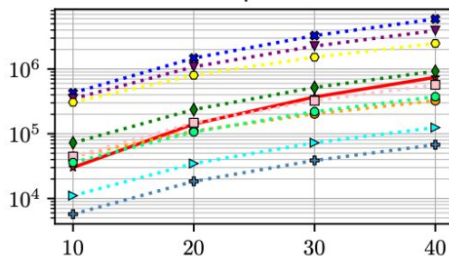
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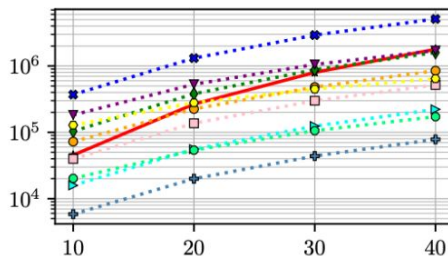
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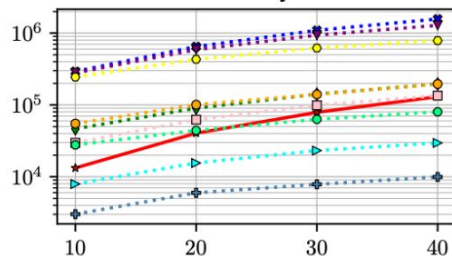
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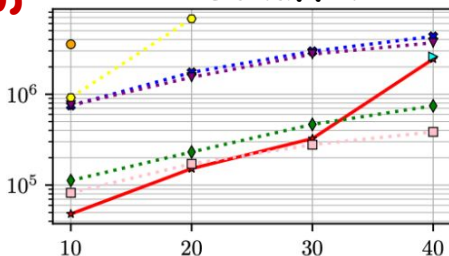
Rosenbrock



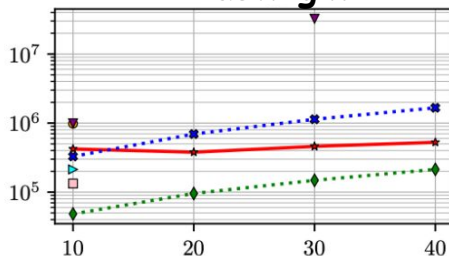
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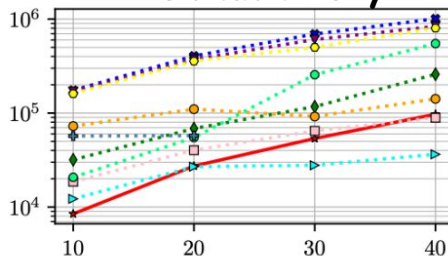
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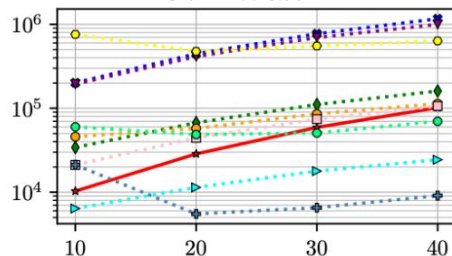
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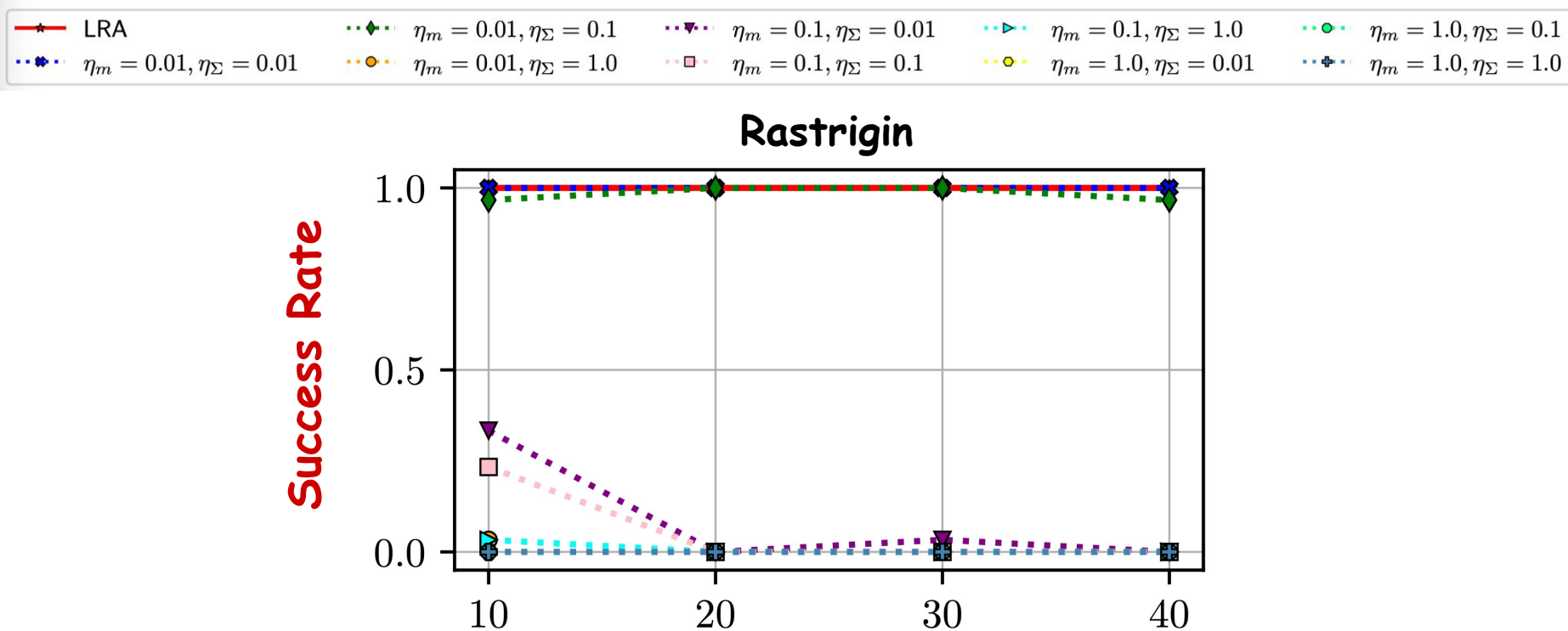


Griewank



LRA shows stable and relatively good performance without expensive tuning

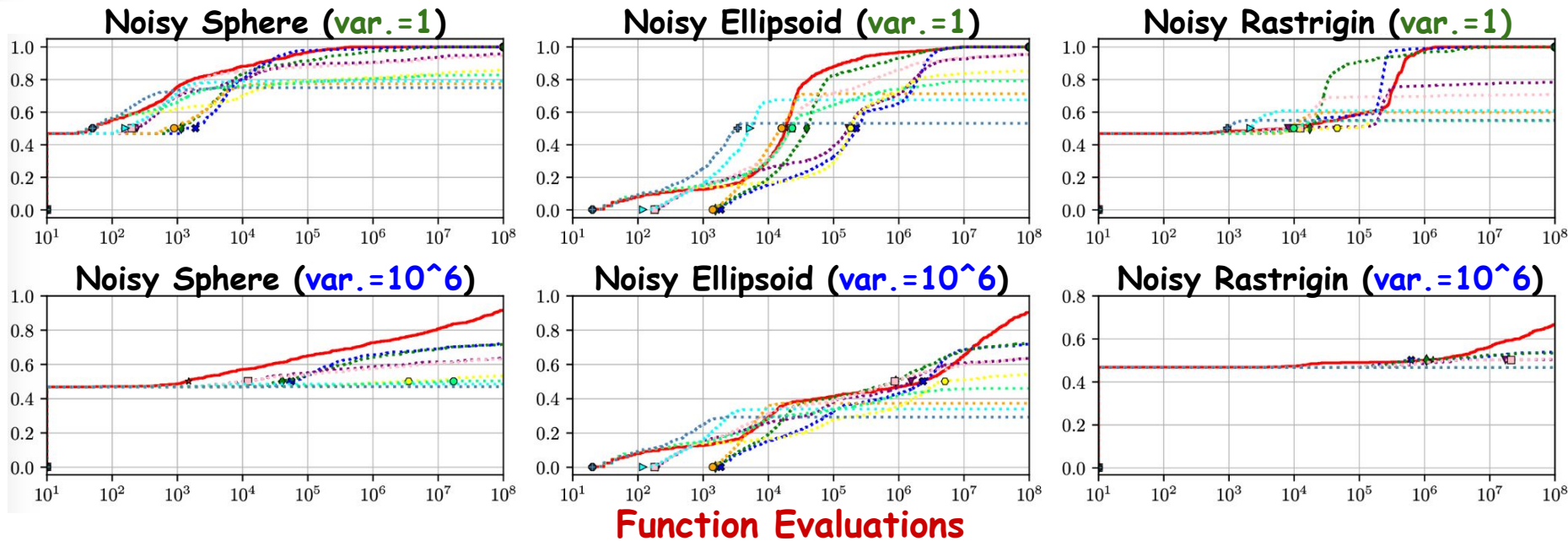
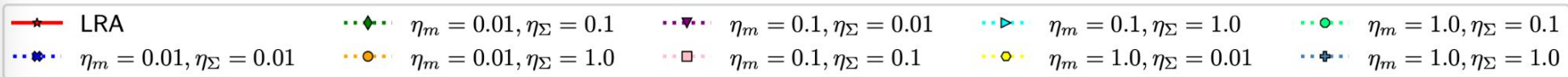
Success Rate on Rastrigin Function



LRA with default λ (e.g. $\lambda=15$ for $d=40$) succeeded in all($n=30$) trials on Rastrigin

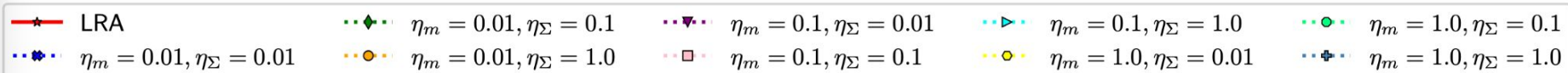
Empirical cumulative density function on noisy problems

Prop. of reached targets

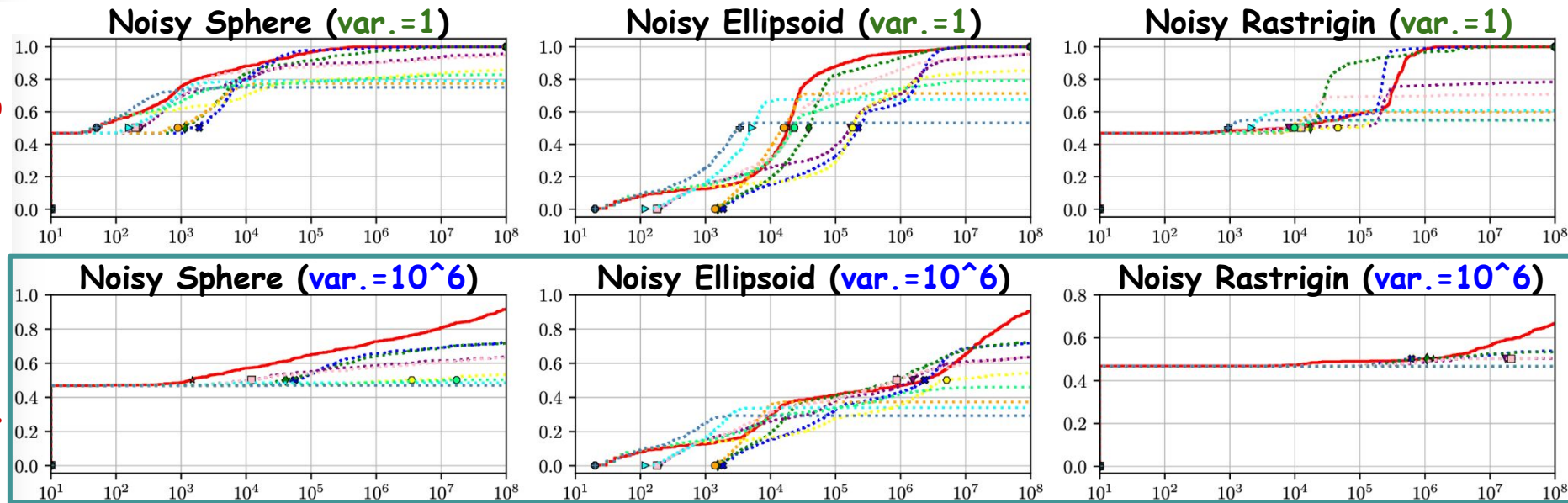


CMA with fixed η had stopped improving the function value
 In contrast, LRA continued to improve it even in strong noise

Empirical cumulative density function on noisy problems



Prop. of reached targets



Function Evaluations

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In contrast, LRA continued to improve it even in strong noise

Use of LRA-CMA with Python

- Available from [CyberAgentAILab/cmaes](#) (#star=233)

```
optimizer = CMA(mean=np.ones(10) * 3, sigma=2.0, lr_adapt=True)
```

Please create issues if you have any problems!

- (Scheduled for next month) Available from [optuna](#) (#star=8.4k)
private communication w/ optuna team
 - optuna:
 - popular BBO/HPO software (300k downloads/week)

A wider audience can use LRA-CMA!

Conclusion

- Ultimate goal:
 - Hyperparameter-Free CMA-ES even for difficult problems
- Approach: LRA-CMA
 - Learning rate is adapted to maintain a positive constant SNR
- Evaluation:
 - LRA-CMA with default population size works well without tuning
- Future work:
 - Comparison against population size adaptation

Please feel free to contact masahironomura5325@gmail.com
if you have any questions!

References & Appendix

References

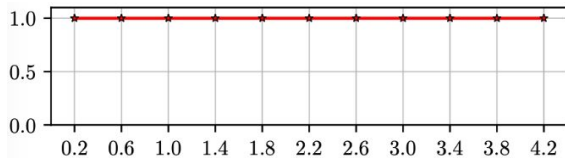
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- [NA16] Kouhei Nishida and Youhei Akimoto. [Population Size Adaptation for the CMA-ES Based on the Estimation Accuracy of the Natural Gradient](#). In *Proceedings of the Genetic and Evolutionary Computation*, page 237–244, 2016.
- [NA18] Kouhei Nishida and Youhei Akimoto. [PSA-CMA-ES: CMA-ES with Population Size Adaptation](#). In *Proceedings of the Genetic and Evolutionary Computation Conference*, page 865–872, 2018.

Appendix: Effects of Hyperparameters (1)

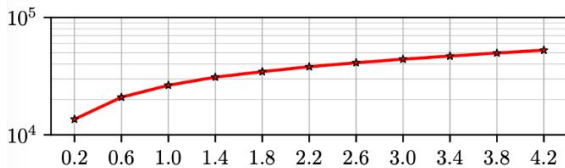
a effect: success rate and SP1 on 30-D noiseless problems (30 trials)

Sphere

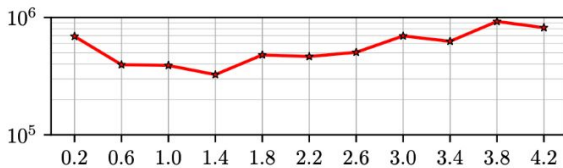
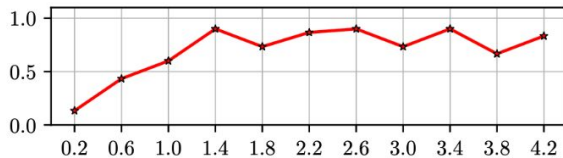
Success
Rate



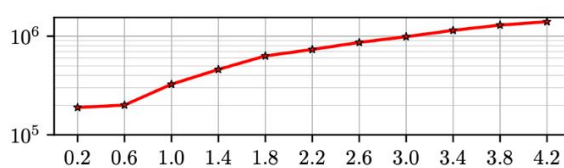
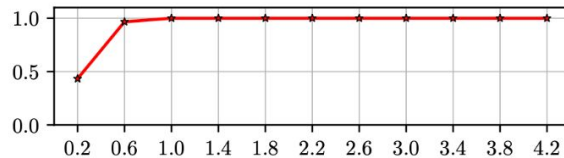
SP1



Schaffer

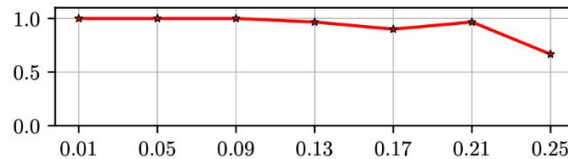
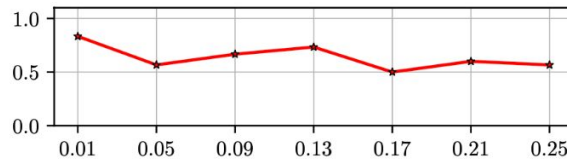
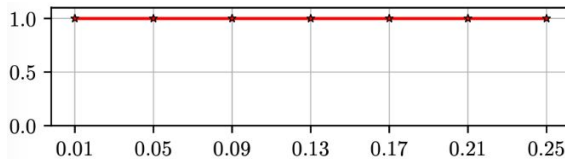


Rastrigin

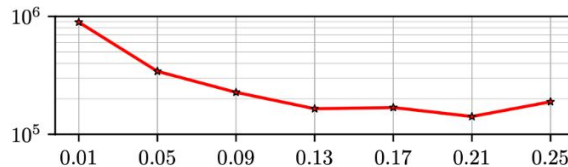
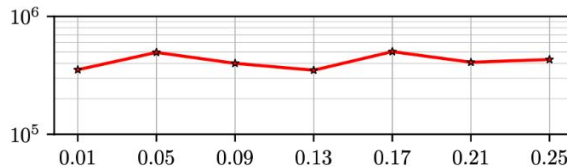
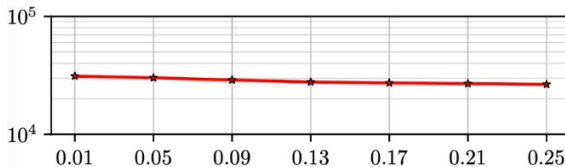


β_Σ effect: success rate and SP1 on 30-D noiseless problems (30 trials)

Success
Rate

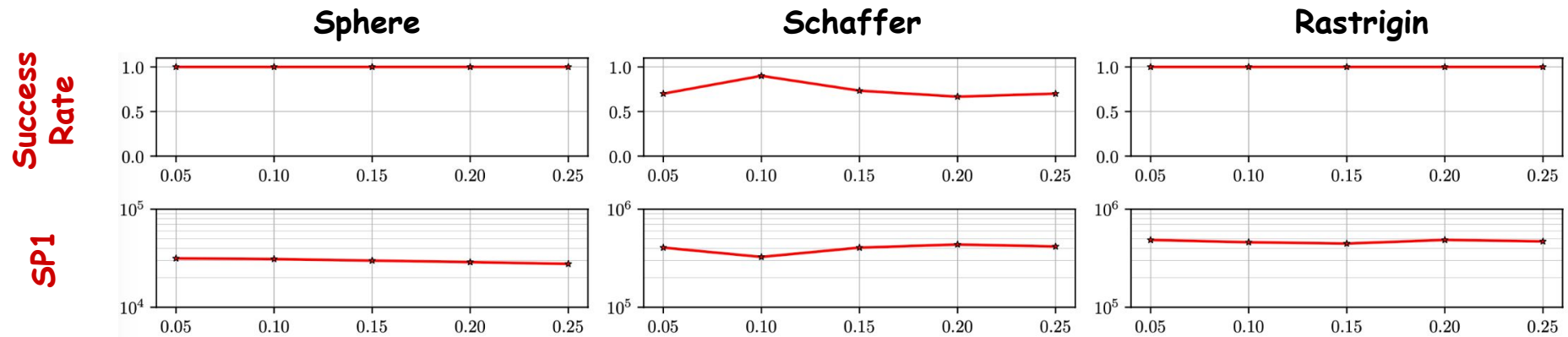


SP1

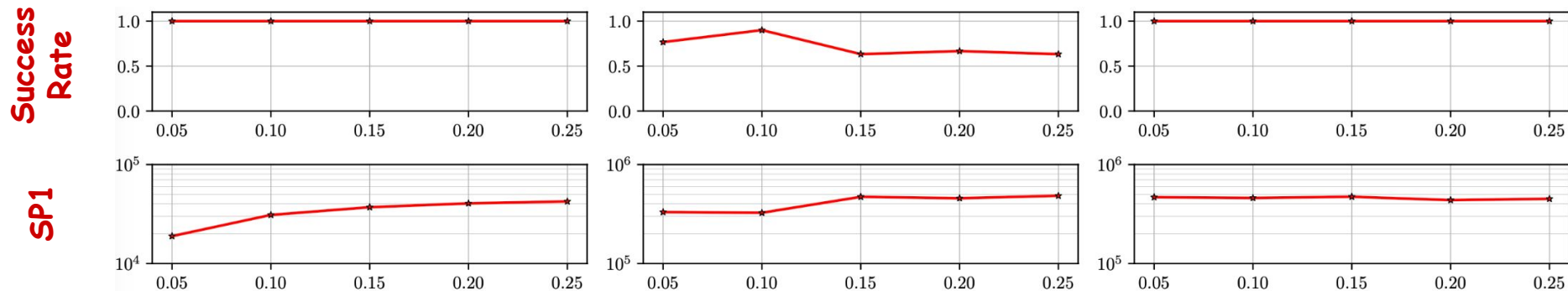


Appendix: Effects of Hyperparameters (2)

β_m effect: success rate and SP1 on 30-D noiseless problems (30 trials)



γ effect: success rate and SP1 on 30-D noiseless problems (30 trials)



Appendix: Effects of Hyperparameters (3)

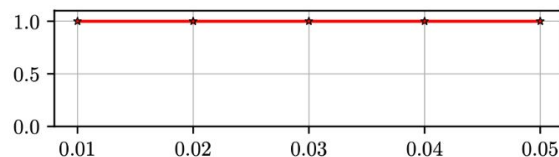
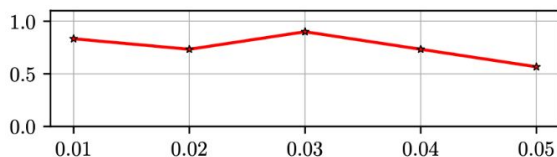
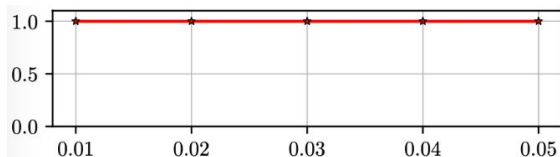
β_Σ effect (refined): success rate and SP1 on 30-D noiseless problems (30 trials)

Sphere

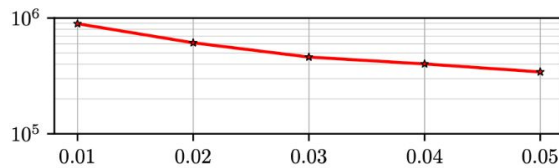
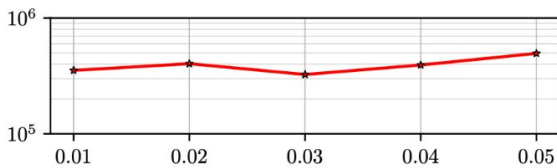
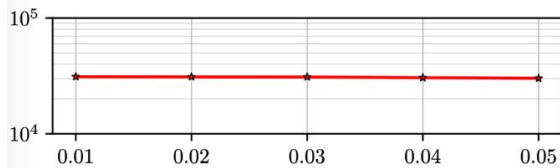
Schaffer

Rastrigin

Success
Rate



SP1

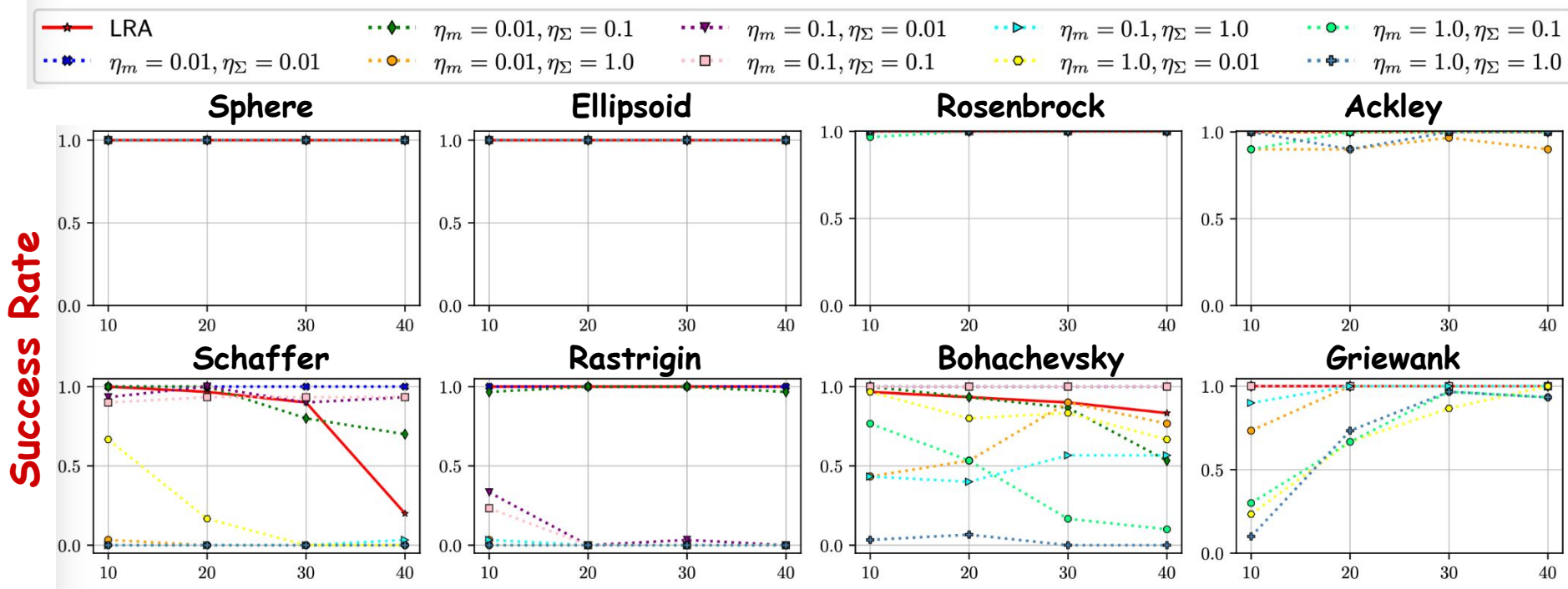


Appendix: Benchmark Problems and Initial Distributions

Definitions	Initial Distributions
$f_{\text{Sphere}}(\mathbf{x}) = \sum_{i=1}^d x_i^2$	$\mathbf{m}^{(0)} = [3, \dots, 3], \sigma^{(0)} = 2$
$f_{\text{Ellipsoid}}(\mathbf{x}) = \sum_{i=1}^d (1000^{\frac{i-1}{d-1}} x_i)^2$	$\mathbf{m}^{(0)} = [3, \dots, 3], \sigma^{(0)} = 2$
$f_{\text{Rosenbrock}}(\mathbf{x}) = \sum_{i=1}^{d-1} (100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2)$	$\mathbf{m}^{(0)} = [0, \dots, 0], \sigma^{(0)} = 0.1$
$f_{\text{Ackley}}(\mathbf{x}) = 20 - 20 \cdot \exp(-0.2 \sqrt{\frac{1}{d} \sum_{i=1}^d x_i^2}) + e - \exp(\frac{1}{d} \sum_{i=1}^d \cos(2\pi x_i))$	$\mathbf{m}^{(0)} = [15.5, \dots, 15.5], \sigma^{(0)} = 14.5$
$f_{\text{Schaffer}}(\mathbf{x}) = \sum_{i=1}^{d-1} (x_i^2 + x_{i+1}^2)^{0.25} \cdot [\sin^2(50 \cdot (x_i^2 + x_{i+1}^2)^{0.1}) + 1]$	$\mathbf{m}^{(0)} = [55, \dots, 55], \sigma^{(0)} = 45$
$f_{\text{Rastrigin}}(\mathbf{x}) = 10d + \sum_{i=1}^d (x_i^2 - 10 \cos(2\pi x_i))$	$\mathbf{m}^{(0)} = [3, \dots, 3], \sigma^{(0)} = 2$
$f_{\text{Bohachevsky}}(\mathbf{x}) = \sum_{i=1}^{d-1} (x_i^2 + 2x_{i+1}^2 - 0.3 \cos(3\pi x_i) - 0.4 \cos(4\pi x_{i+1}) + 0.7)$	$\mathbf{m}^{(0)} = [8, \dots, 8], \sigma^{(0)} = 7$
$f_{\text{Griewank}}(\mathbf{x}) = \frac{1}{4000} \sum_{i=1}^d x_i^2 - \prod_{i=1}^d \cos(x_i / \sqrt{i}) + 1$	$\mathbf{m}^{(0)} = [305, \dots, 305], \sigma^{(0)} = 295$

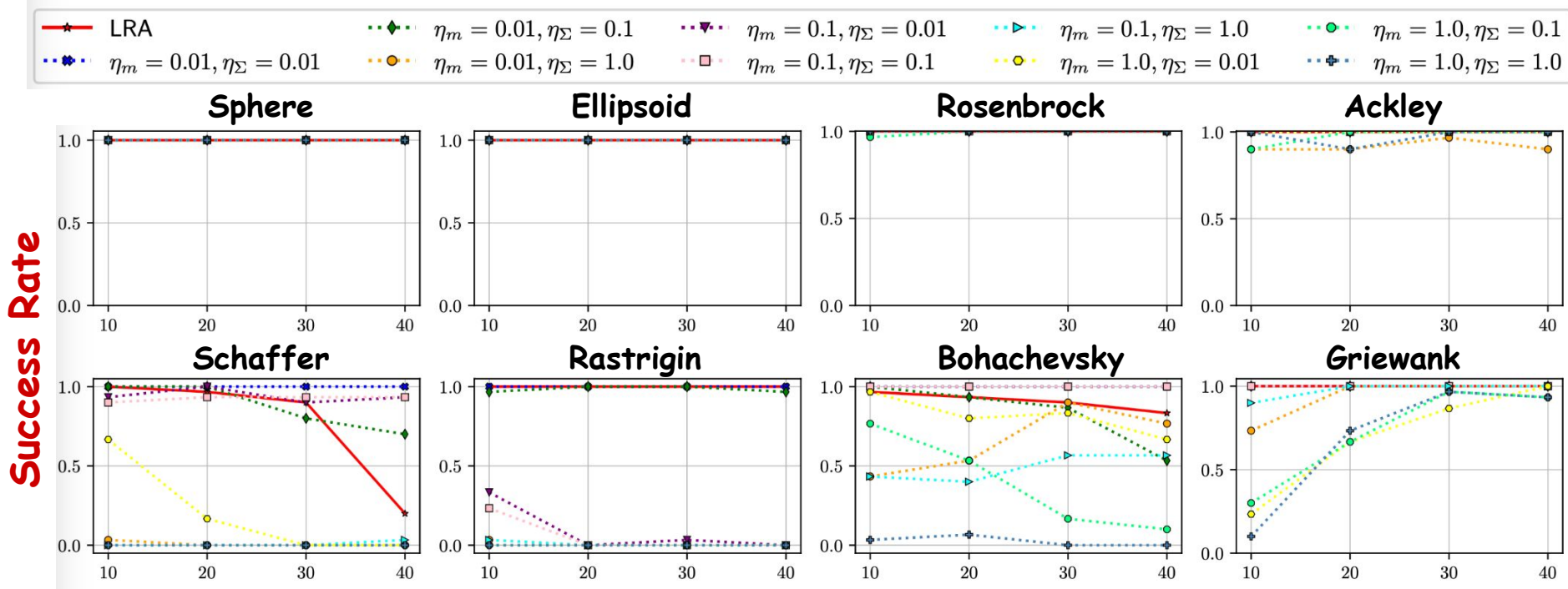
Although the Rosenbrock function has local minima,
in our setting, it could be regarded as an almost unimodal problem

Success Rate versus (10-40)Dim. (Noiseless Problems)



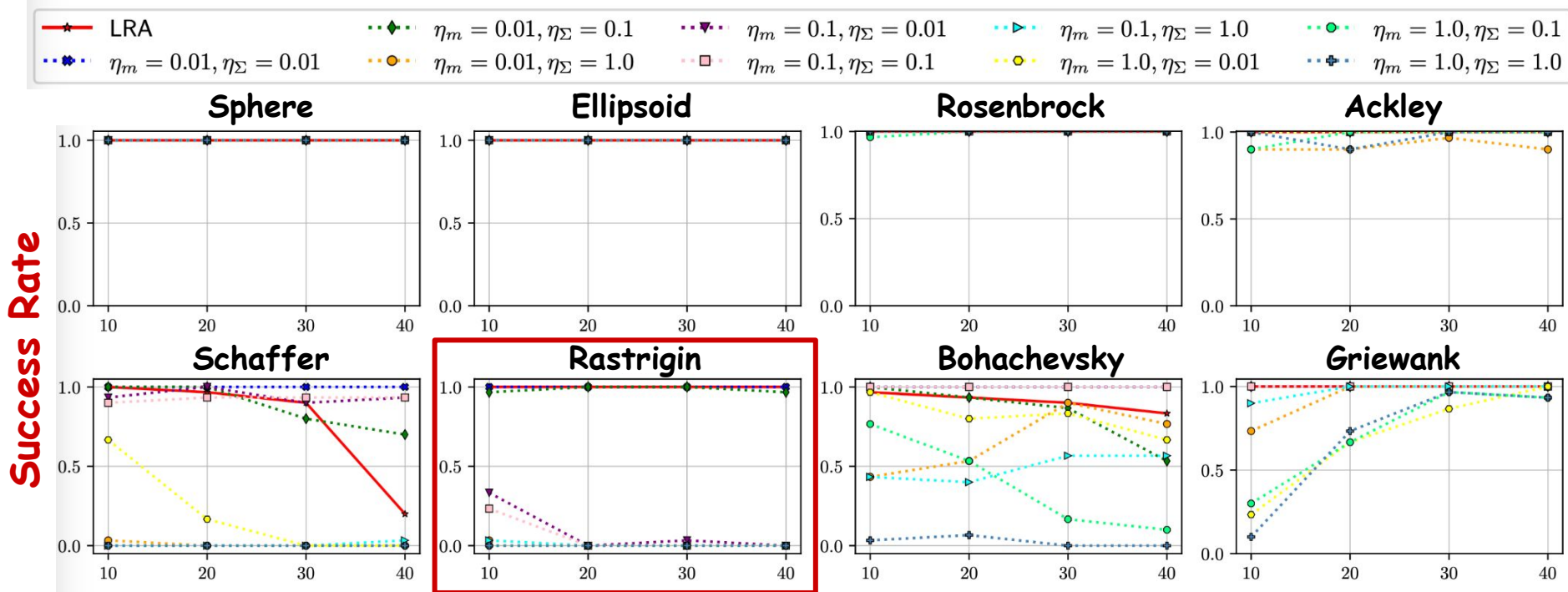
For multimodal, CMA with high η often failed, but with small η had a high SR
Success is highly dependent on the η setting

Success Rate versus (10-40)Dim. (Noiseless Problems)



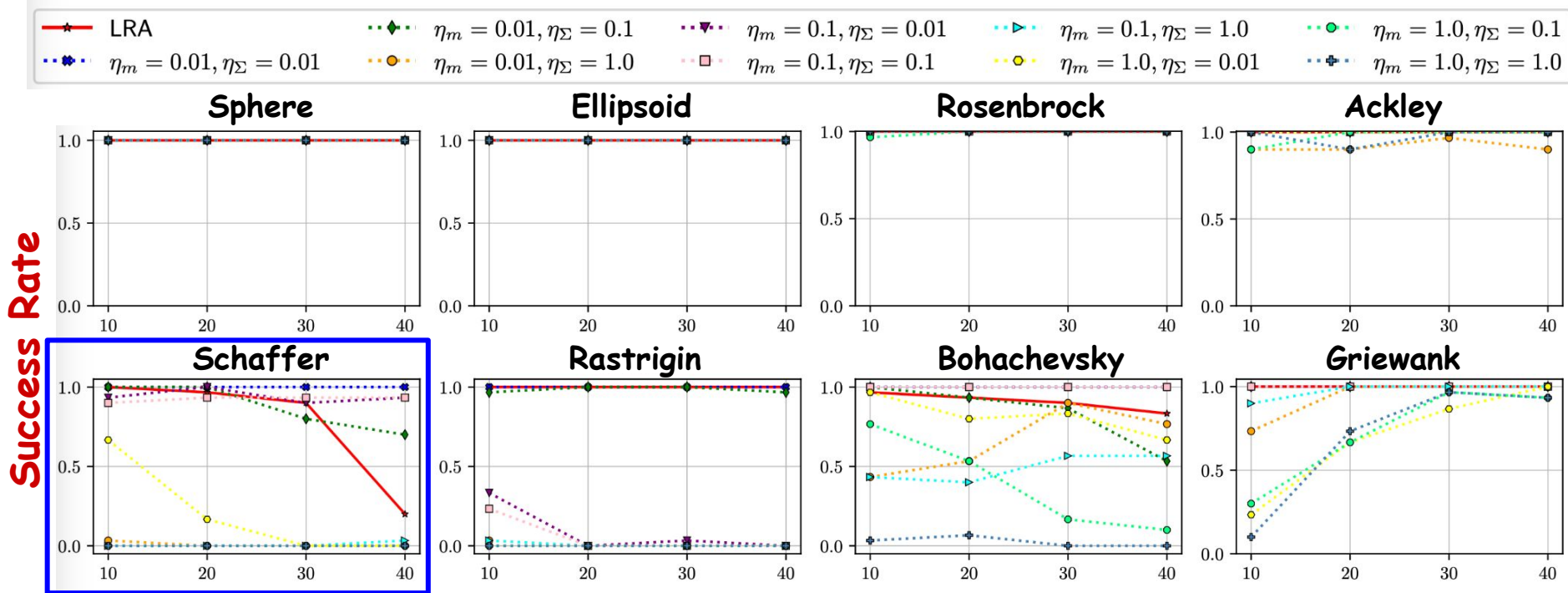
LRA-CMA had a relatively good Success Rate without η tuning

Success Rate versus (10-40)Dim. (Noiseless Problems)



LRA with default λ (e.g. $\lambda=15$ for $d=40$) succeeded in all trials on Rastrigin

Success Rate versus (10-40)Dim. (Noiseless Problems)



LRA performance degrades on Schaffer with d=40 \Rightarrow future work

Appendix: Step-Size Correction

- When the learning rate for m is updated, appropriate step-size changes
- Quality gain analysis for optimal step-size:

$$\sigma^* \propto 1/\eta_m \quad \text{on (infinite-dim) convex quadratic functions}$$

- To maintain the optimal step-size, we perform step-size correction:

$$\sigma^{(t+1)} \leftarrow \frac{\eta_m^{(t)}}{\eta_m^{(t+1)}} \sigma^{(t+1)}$$