Evolution Strategies: Principles and Practical Issues

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Outline

- Introduction to Natural Evolution Strategies (NES)
  - Stochastic optimization framework that uses natural gradient
  - NES is similar to CMA-ES
- Practical Issues for Difficult Problems (e.g. Multimodal and Noisy)
  - Hyperparameter tuning is required
  - Learning rate adaptation (Nomura+, GECCO'23 Best Paper Nominated)

Black-Box Optimization on Continuous Domain

Goal of continuous black-box optimization (BBO):

$$x^* = \underset{x \in \mathcal{X}}{\operatorname{argmax}}\ f(x)$$

- X is continuous space

- Objective function is "**<u>black-box</u>**"
  - Not assume availability of gradient
  - We only use function evaluation value

Stochastic Relaxation for BBO [WSG+14]

- We want to optimize f(x), but the gradient wrt. x is not available
- Instead of directly finding x*, NES searches distribution parameter θ*:

$$x^* = \underset{x \in \mathcal{X}}{\operatorname{argmax}}\ f(x)$$

$$\Big\Downarrow \quad \textbf{Stochastic Relaxation}$$

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}}\ \mathbb{E}_{x \sim p(x;\theta)}[f(x)] =: J(\theta)$$

Gradient for Distribution Parameter [WSG+14]

- Suppose we can find $\nabla_\theta \log p(x;\theta)$
- By using the so-called 'log-likelihood trick':

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \int f(x)p(x;\theta)dx \\
&= \int f(x)\nabla p(x;\theta)dx \\
&= \int f(x)\nabla \log p(x;\theta)p(x;\theta)dx \\
&= \mathbb{E}_{x\sim p(x;\theta)}[f(x)\nabla_\theta \log p(x;\theta)] \approx \frac{1}{\lambda}\sum_{i=1}^{\lambda} f(x_i)\nabla_\theta \log p(x_i;\theta)
\end{aligned}
$$

- Update the distribution parameter via gradient ascent

$$\theta \leftarrow \theta + \eta \cdot \nabla_\theta J(\theta)$$

Multivariate Gaussian Distribution

- One can use any distribution whose derivative of log-likelihood is obtained
- Most widely used one: multivariate Gaussian distribution (MGD)
- Distribution parameters:
  - Mean vector : $m \in \mathbb{R}^d$
  - Covariance matrix: $\Sigma \in \mathbb{R}^{d \times d}$
- Density of the distribution:

$$p(x;\theta) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \cdot \exp\left(-\frac{1}{2}(x-m)^\top \Sigma^{-1}(x-m)\right)$$

Vanilla gradient for Multivariate Gaussian Distribution

- We first calculate the log-likelihood for estimating gradient:

$$\log p(x;\theta) = -\frac{d}{2}\log(2\pi) - \frac{1}{2}\log\det(\Sigma) - \frac{1}{2}(x-m)^\top \Sigma^{-1}(x-m)$$

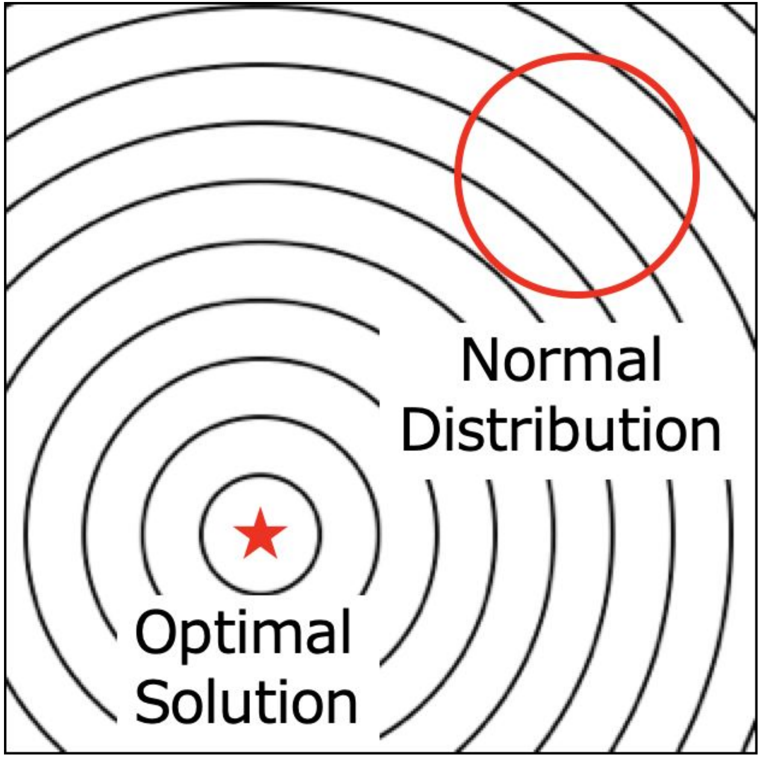
- (Vanilla) gradient for the log-likelihood:

$$\nabla_m \log p(x;\theta) = \Sigma^{-1}(x-m)$$

$$\nabla_\Sigma \log p(x;\theta) = \frac{1}{2}\Sigma^{-1}(x-m)(x-m)^\top - \frac{1}{2}\Sigma^{-1}$$

Illustrative Behavior with Multivariate Gaussian (MGD)

1. Generates solutions from the MGD
2. Evaluates solutions and estimates gradient
3. Updates the parameters
4. Repeats until the criterion is met



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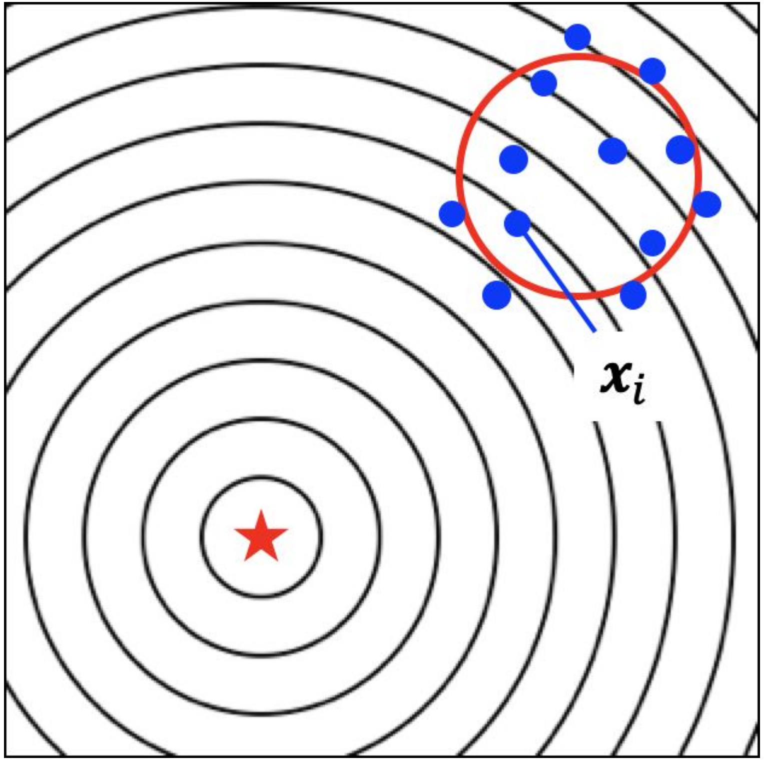

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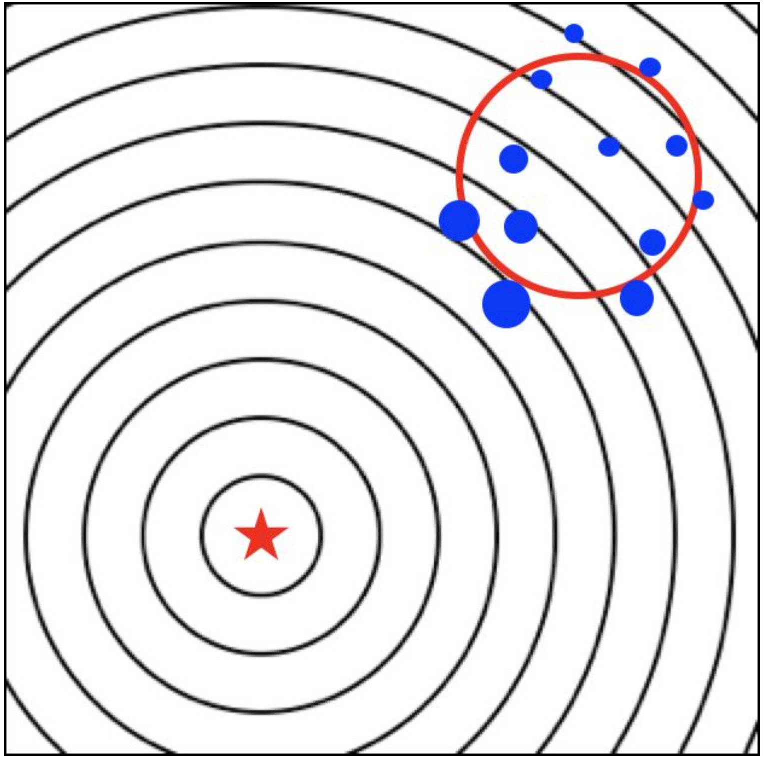

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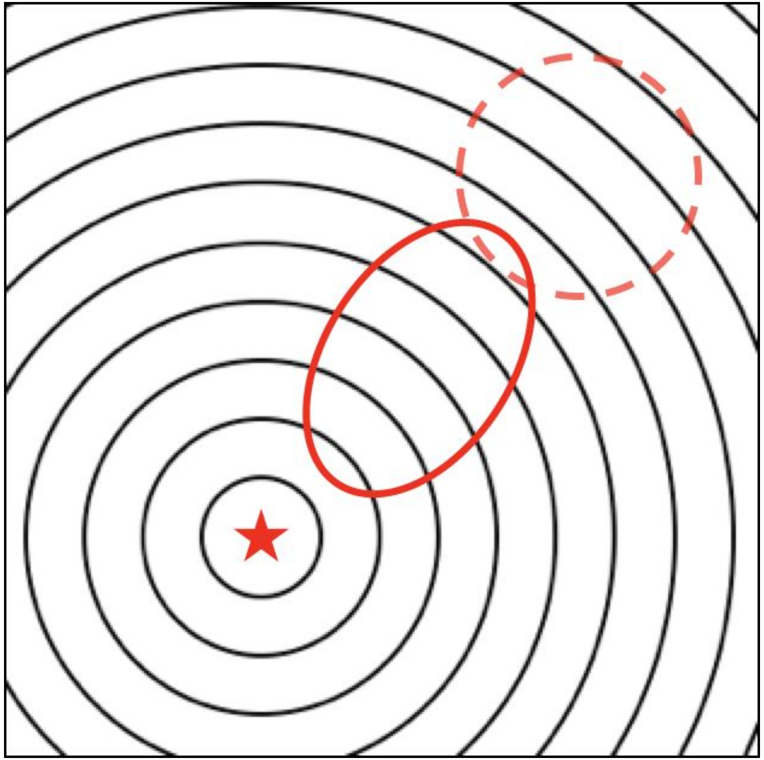

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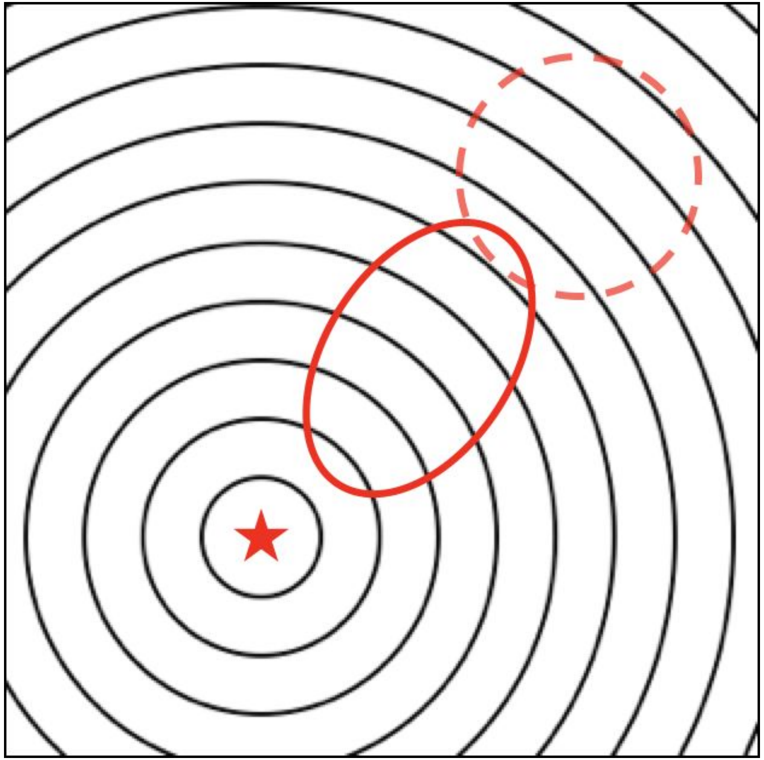


Rethinking Vanilla Gradient and Natural Gradient

- The vanilla gradient can be characterized as the steepest ascent within the small Euclidean distance in the parameter space
  - The update depends on the choice of parameterization
  - The vanilla gradient can show unstable and unsatisfying performance
- Natural gradient: steepest ascent direction within the small KL divergence
  - Let F be Fisher information matrix,

$$\tilde{\nabla}_\theta J(\theta) = F^{-1} \nabla_\theta J(\theta)$$

Fitness Shaping [GSY+10]

- Fitness shaping: replace function values with ***weights*** $(w_1 \geq \cdots \geq w_\lambda)$

$$F^{-1}\nabla_\theta J(\theta) \approx \frac{1}{\lambda}\sum_{i=1}^{\lambda} f(x_i) F^{-1}\nabla_\theta \log p(x_i;\theta)$$

Fitness Shaping

$$\sum_{i=1}^{\lambda} w_i F^{-1}\nabla_\theta \log p(x_{i:\lambda};\theta)$$

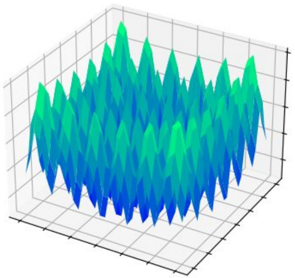
$x_{i:\lambda}$: *i*-th best solution

NES uses only ranking rather than function value itself

- Invariant under monotonically increasing transformation of *f*
- NES = Natural Gradient + Fitness Shaping
  - CMA-ES = NES + additional operations (CSA & rank-one update)

Practical Issues of ES for Difficult Problems

- Why does ES fail for Difficult Problems?
  - Noisy case: update does not proceed at certain situations
  - Multimodal problems are similar to noisy problems



- Naive approach: Sample size tuning
  - Larger sample size can be helpful for difficult problems
  - Knowing good value is challenging ⇒ expensive tuning is required
- Promising approach: Learning rate adaptation
  - Increasing sample size has effect similar to decreasing learning rate
  - Learning rate adaptation is more practically useful

Learning Rate Adaptation: Setup

vectorization operator, Σ = σ^2 C

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

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- Modified updates :
  - $\theta_m^{(t+1)} = \theta_m^{(t)} + \eta_m^{(t)} \Delta_m^{(t)}$
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original updates can be recovered with η =1

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How to adapt these learning rate?

Learning Rate Adaptation: Main Idea

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

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

F: Fisher information matrix

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F: Fisher information matrix

- ***Noisy problems***: ***SNR $\to$ 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 ⇔ updates are i.i.d
- *n* steps update:

$$\theta^{(t+n)} = \theta^{(t)} + \eta \sum_{k=0}^{n-1} \Delta^{(t+k)}$$

$$\approx \theta^{(t)} + \mathcal{D}\left(n\eta\mathbb{E}[\Delta], n\eta^2\mathrm{Cov}[\Delta]\right)$$

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- $n = 1/\eta \Rightarrow \mathcal{D}\left(\mathbb{E}[\Delta], \eta\mathrm{Cov}[\Delta]\right)$
  - By taking small η, we can obtain [more concentrated update]()

SNR-Based Learning Rate Adaptation

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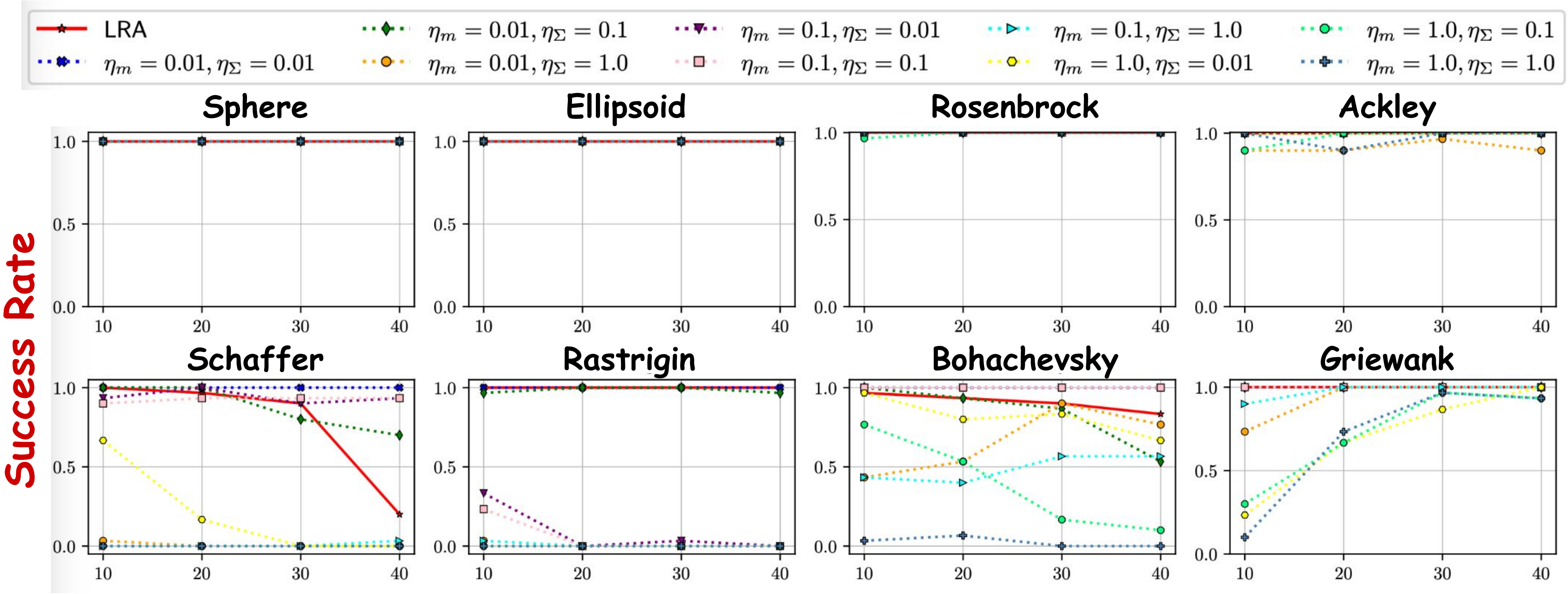
- *n = 1/η* ⇒ $\mathcal{D}\left(\mathbb{E}[\Delta], \eta\mathrm{Cov}[\Delta]\right)$
  - By taking small *η*, we can obtain *more concentrated update*
- SNR over *n* iterations: $\dfrac{\|\mathbb{E}[\Delta]\|_F^2}{\eta\,\mathrm{Tr}(F\,\mathrm{Cov}[\Delta])} = \dfrac{1}{\eta}\mathrm{SNR}$
- **Our method**: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

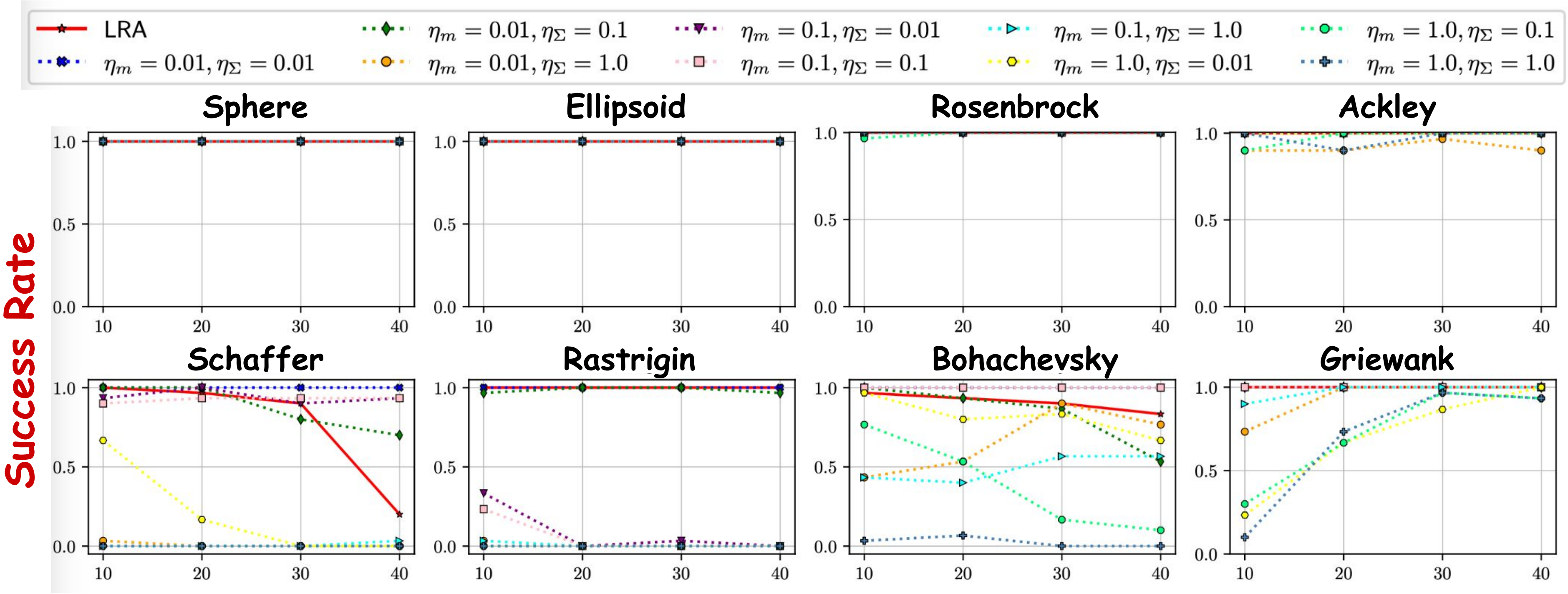
Success Rate versus (10-40)Dim. (Noiseless Problems)



For multimodal, CMA with high η often *failed*, but with small η had a high SR

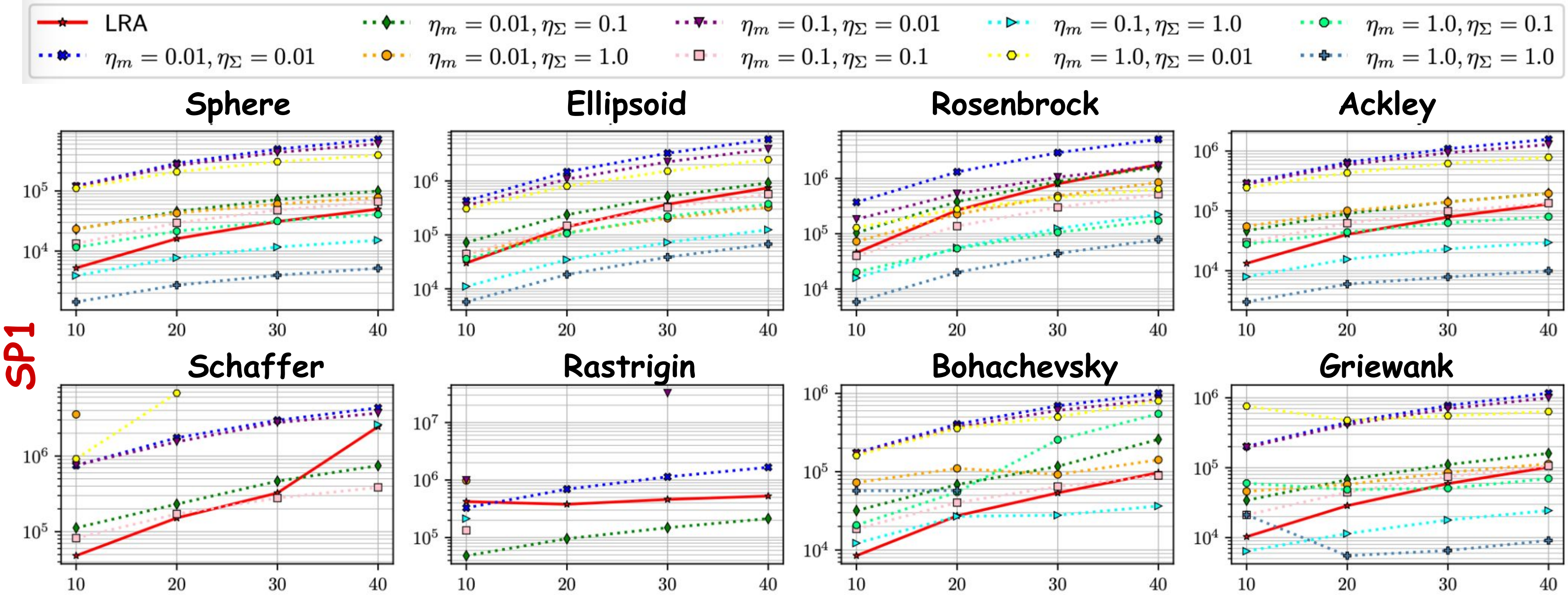
Success is highly dependent on the η setting

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



LRA-CMA had a relatively *good success rate without η tuning*

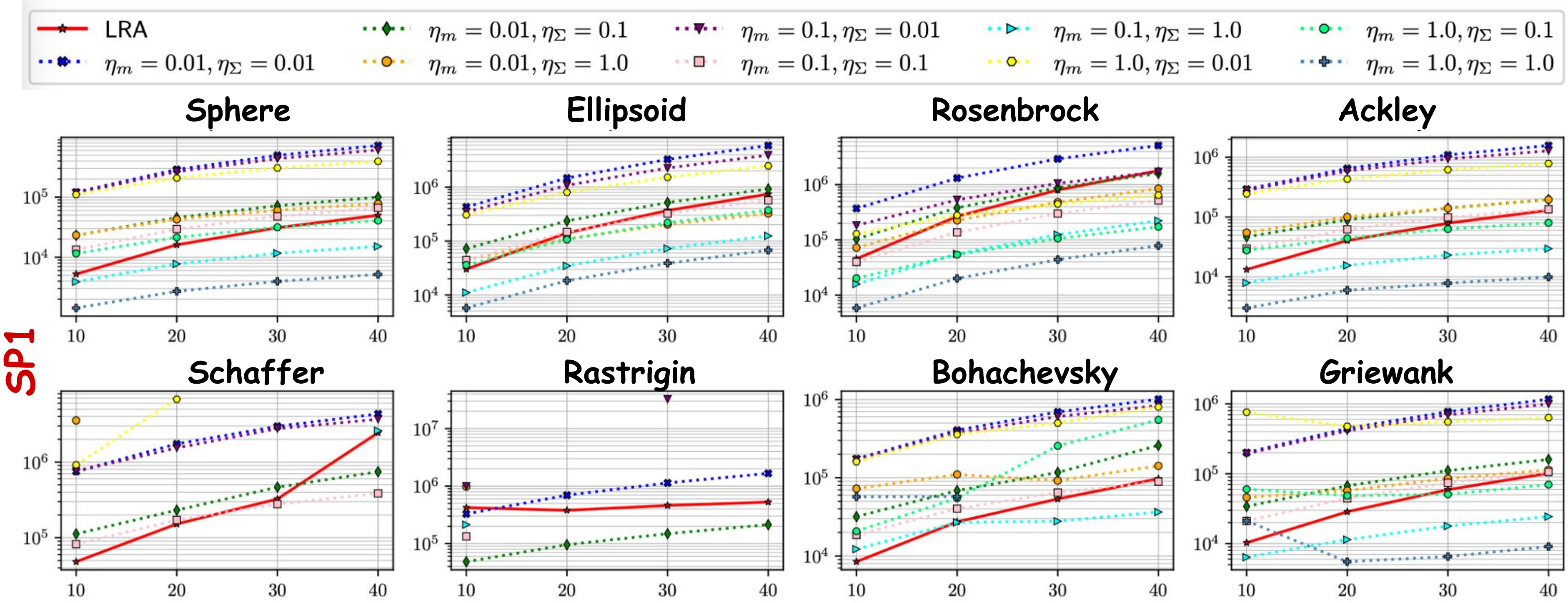
SP1 versus (10-40)Dim. (Noiseless Problems)



with high $\eta \Rightarrow$ worse on multimodal, with small $\eta \Rightarrow$ slow on unimodal

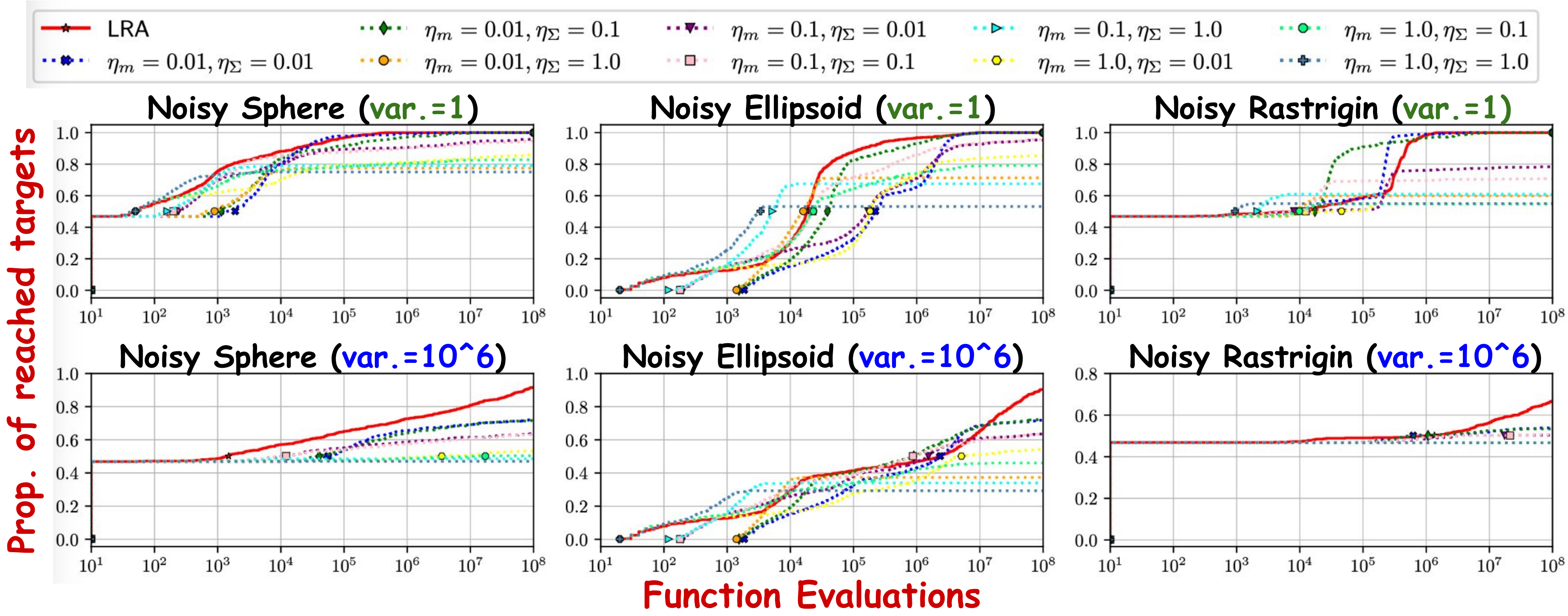
Clear trade-off in efficiency exists depending on η

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



LRA shows stable and relatively good performance <u>without expensive tuning</u>

Empirical cumulative density function on noisy problems



CMA with fixed η had stopped improving the function value

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

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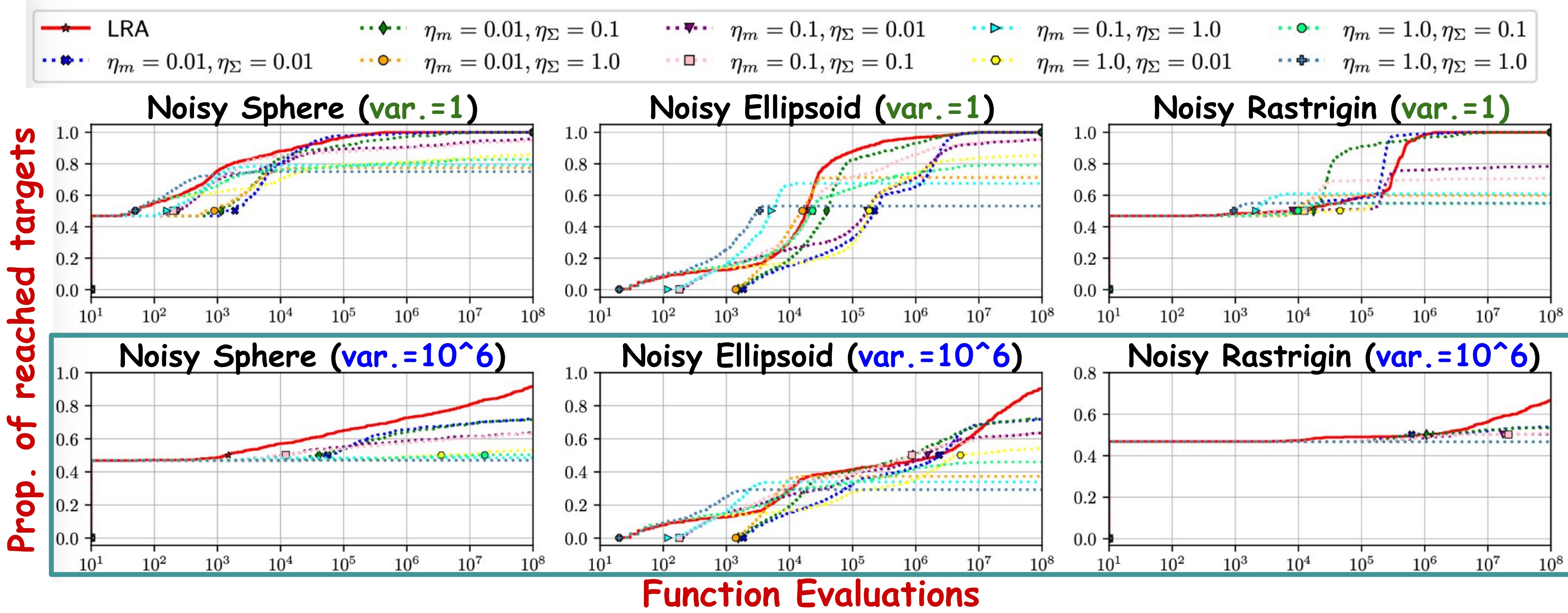

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Use of LRA-CMA with Python

- 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!

- Available from optuna (#star=8.4k)
    - optuna:
        - popular BBO/HPO software (300k downloads/week)

A wider audience can use LRA-CMA!

Summary

- Natural ES (NES) and CMA-ES
  - Popular class of ES that is based on natural gradient
- Practical Issues for Difficult Problems
  - Hyperparameter (e.g. sample size) tuning is required
- Learning Rate Adaptation:
  - LRA-CMA with default sample size works well without tuning
- Ultimate Goal for Future:
  - Developing Completely Hyperparameter-Free ES

Appendix

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

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

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

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- The SNR is estimated as:

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

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Approximation!
(See paper for details)

Update Equation of Learning Rate Adaptation

Adapting learning rate by:

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

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Adapting learning rate by:

bring SNR closer to $\alpha\eta$

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wait for the effect of the change of previous η

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

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projection onto [-1, 1]

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$$\eta \leftarrow \min(\eta, 1)$$

upper bound