Benchmarking the PSA-CMA-ES on the BBOB Noiseless Testbed

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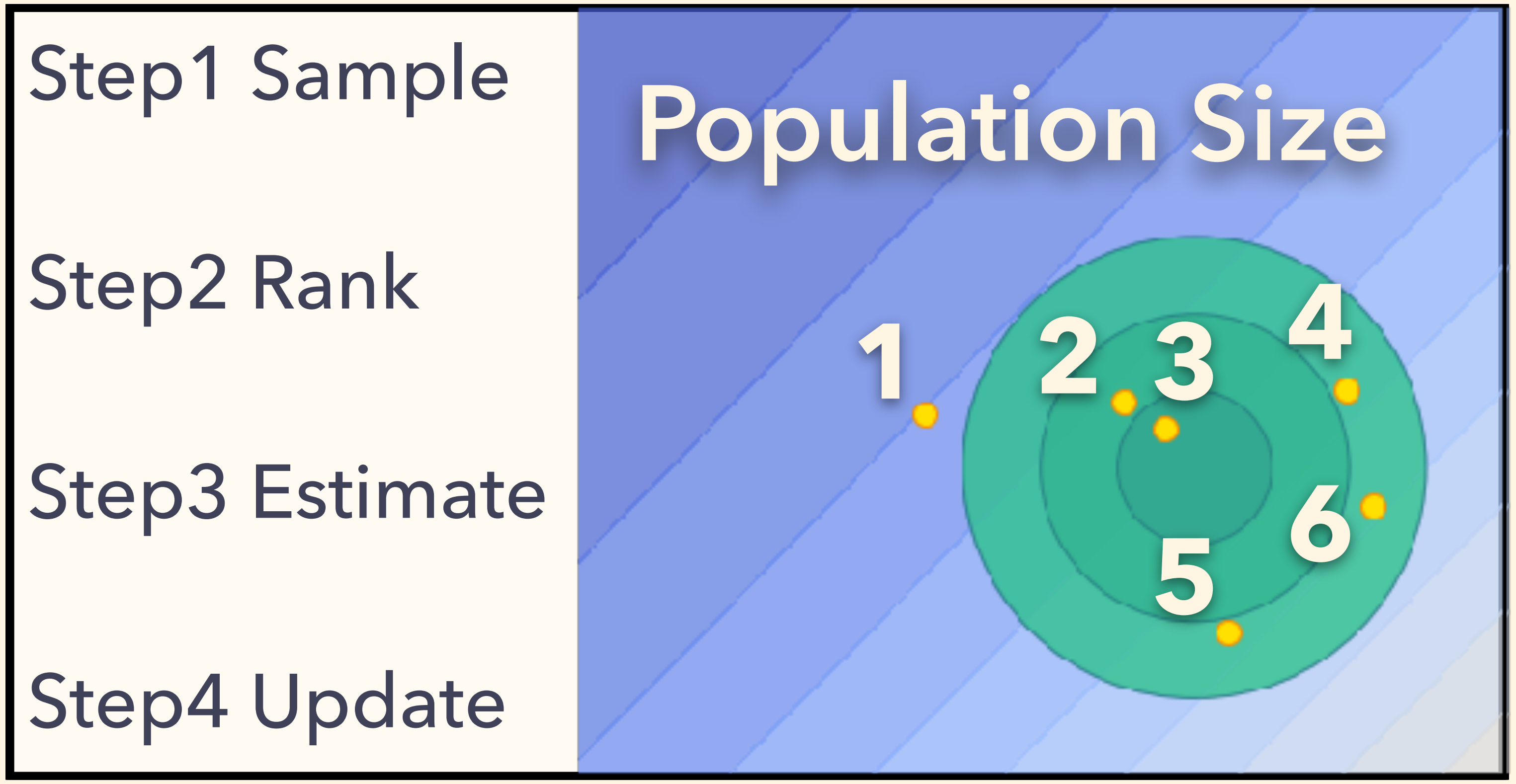
CMA-ES

- It maintains a multivariate normal distribution $\mathcal{N}(m, \Sigma)$



$$\Sigma = \sigma^2 C$$

m: mean vector
σ : step-size
C: covariance matrix

- All of its hyper-parameters have their default values
  i.e. the learning rate, the population size
- The population size needs tuning
  if the objective function is a noisy or multimodal function
  [Hansen 2004]

CMA-ES: Population Size Tuning

Approach to Avoid Tuning by Users

- To utilize a multi-run strategy with different population sizes
- To adapt the population size

BIPOP-CMA-ES

First run: CMA-ES with the default population size

→ unimodal functions

Additional runs:

- CMA-ES with an increased population size
  → well-structured multimodal or noisy functions

- CMA-ES with a relatively small step-size and population size
  → weakly-structured multimodal functions

CMA-ES: Population Size Tuning

Approach to Avoid Tuning by Users

- To utilize a multi-run strategy with different population sizes
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PSA-CMA-ES [Nishida2018, Thursday 19, ENUM4]

- Based on tendency of the parameter update

Key Observation
On multimodal functions and noisy functions, the parameter update has less tendency than on noiseless unimodal functions.

Population Size Adaptation

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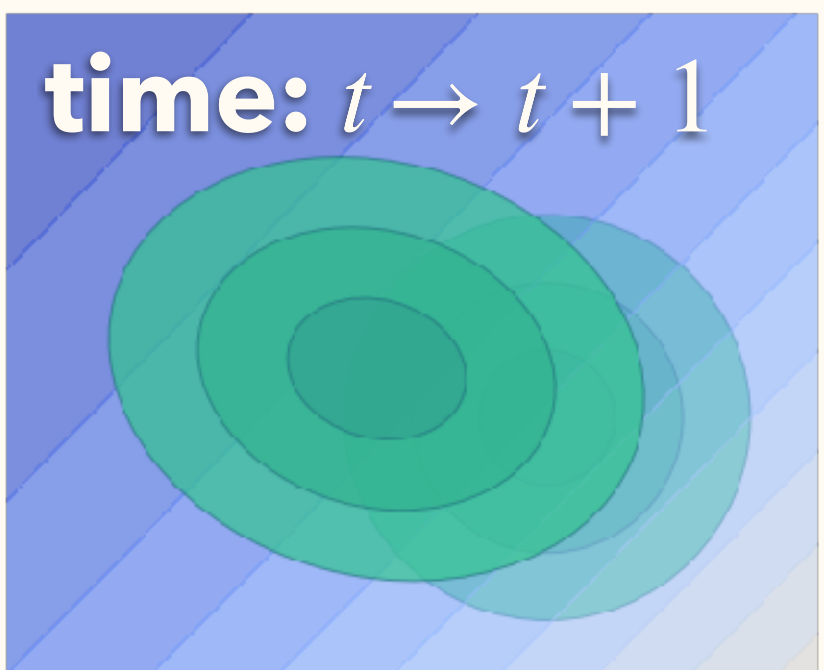
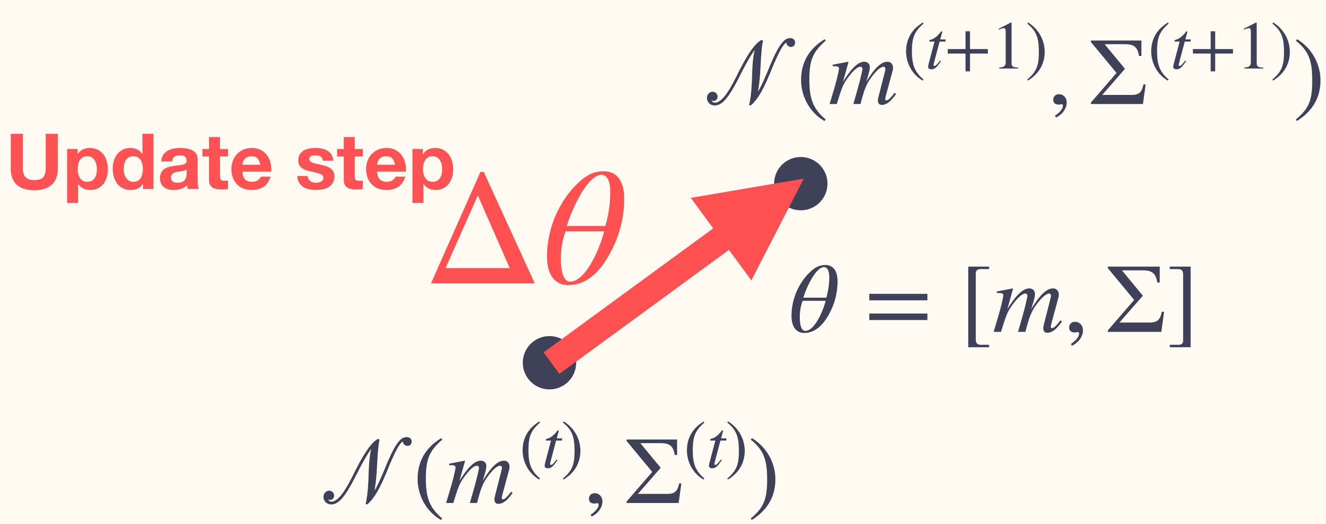
In the parameter space of the sampling distribution…





Population Size Adaptation

- Based on tendency of the parameter update

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In the parameter space of the sampling distribution…

On
- noiseless unimodal function

Population Size Adaptation

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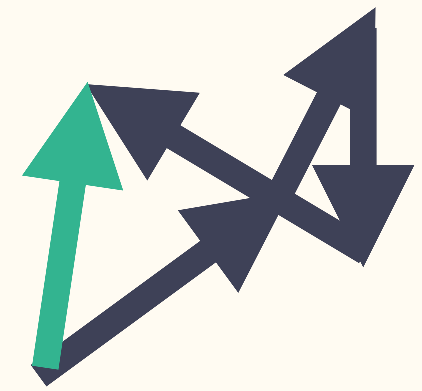
In the parameter space of the sampling distribution…

On
- multimodal functions
- noisy functions



PSA: Evolution Path

- It accumulates steps in the parameter space

$$p_\theta^{(t+1)} \leftarrow (1-\beta)\, p_\theta^{(t)} + \sqrt{\beta(2-\beta)} \frac{\mathcal{I}_{\theta^{(t)}}^{\frac{1}{2}} \Delta\theta^{(t+1)}}{\sqrt{\mathbb{E}[\|\mathcal{I}_{\theta^{(t)}}^{\frac{1}{2}} \Delta\theta^{(t+1)}\|^2]}}$$

β : cumulation factor

$\mathcal{I}_\theta$: Fisher information matrix under θ

$\mathbb{E}[\,\cdot\,]$: expectation under a random function $f(x) = \epsilon$

normalization factor

→ To absorb the effect of…

- Parameterization of the sampling distribution
- Change of the population size

under a random function

$$\|p_\theta\|^2 \approx 1$$

when λ is too large

$$\|p_\theta\|^2 \gg 1$$

λ: population size

PSA: Population Size Update

$$\lambda^{(t+1)} \leftarrow \lambda^{(t)} \exp\left(\beta\left(\gamma^{(t+1)} - \frac{\|p_\theta^{(t+1)}\|^2}{\alpha}\right)\right)$$

α : threshold

$\gamma^{(t)}$: normalization factor $\approx 1 \ (t \gg 1)$

$$\gamma^{(t+1)} \leftarrow (1-\beta)^2\gamma^{(t)} + \beta(2-\beta)$$

$\|p_\theta\|^2 < \alpha \Rightarrow$ The population size increases

$\|p_\theta\|^2 > \alpha \Rightarrow$ The population size decreases

→ the population size is adapted so that the parameter update has sufficient tendency

PSA: Step-size Correction

- Based on the quality gain analysis [Akimoto 2017]
  ⟶ The optimal step-size depends on the population size
- A practical step-size adaptation in the CMA-ES usually well follows the optimal value [Krause 2017]
- It implies that the step-size is increased when the population size increases, and vice versa.
- The step-size adaptation is corrupted by the population size adaptation.

After updating the population size...

$$\sigma^{(t+1)} \leftarrow \sigma^{(t+1)} \cdot \frac{\sigma^*(\lambda^{(t+1)})}{\sigma^*(\lambda^{(t)})}$$

$$\sigma^*(\lambda) = \frac{c(\lambda) \cdot n \cdot \mu_w(\lambda)}{n - 1 + c(\lambda)^2 \cdot \mu_w(\lambda)}$$

$$c(\lambda) = -\sum_{i=1}^{\lambda} \mathbb{E}[\mathcal{N}_{i:\lambda}]$$

PSA-CMA-ES

1. An iteration of CMA-ES

   A step in the parameter space

$$\Delta\theta = [\Delta m, \Delta\Sigma]$$

$$\Delta m = m^{(t+1)} - m^{(t)}$$

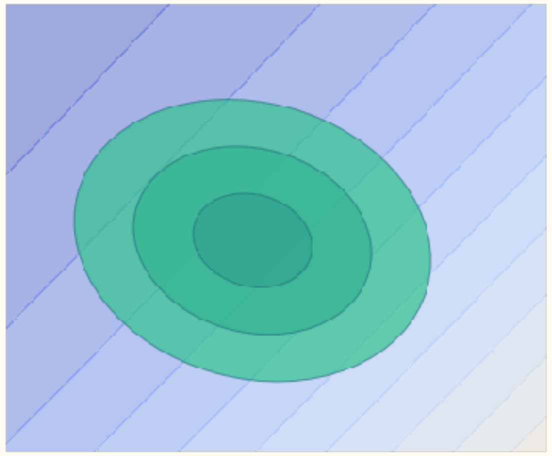
$$\Delta\Sigma = (\sigma^{(t+1)})^2 C^{(t+1)} - (\sigma^{(t)})^2 C^{(t)}$$

Step1 Sample

Step2 Rank

Step3 Estimate

Step4 Update



$$\mathcal{N}(m^{(t)}, (\sigma^{(t)})^2 C^{(t)})$$

$$\Downarrow$$

$$\mathcal{N}(m^{(t+1)}, (\sigma^{(t+1)})^2 C^{(t+1)})$$

2. Update the evolution path

   and the population size

$$p_\theta^{(t+1)} \leftarrow (1-\beta)\, p_\theta^{(t)} + \sqrt{\beta(2-\beta)} \frac{\mathcal{I}^{\frac{1}{2}}_{\theta^{(t)}} \Delta\theta^{(t+1)}}{\sqrt{\mathbb{E}[\| \mathcal{I}^{\frac{1}{2}}_{\theta^{(t)}} \Delta\theta^{(t+1)} \|^2]}}$$

$$\lambda^{(t+1)} \leftarrow \lambda^{(t)} \exp\left(\beta\left(\gamma^{(t+1)} - \frac{\|p_\theta^{(t+1)}\|^2}{\alpha}\right)\right)$$

3. Correct the step-size

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

Restart Strategy for PSA-CMA-ES

First run: CMA-ES with the default population size $(\sigma^{(0)} = 2)$

→ unimodal functions

Second run: PSA-CMA-ES $(\sigma^{(0)} = 2)$

→ well-structured multimodal

Max population size

$$\lambda_{\max} = 2^9 \cdot \lambda_{\mathrm{def}}$$

Additional runs:

PSA-CMA-ES with a relatively small step-size

$$\sigma^{(0)} = 2 \cdot 10^{-2 \cdot \mathcal{U}[0,1]}$$

→ weakly-structured multimodal functions

Simple Restart

All runs: PSA-CMA-ES $(\sigma^{(0)} = 2, \lambda_{\max} = \infty)$

Simulation

Common Setting

- Initialization: $m^{(0)} \sim \mathcal{U}[4,4)^D \quad (D\text{: problem dimension})$
- Termination:
  - The target function value is reached
  - The number of evaluation is over $10^6 \cdot D$
  - One of the termination conditions [Hansen 2009] is satisfied

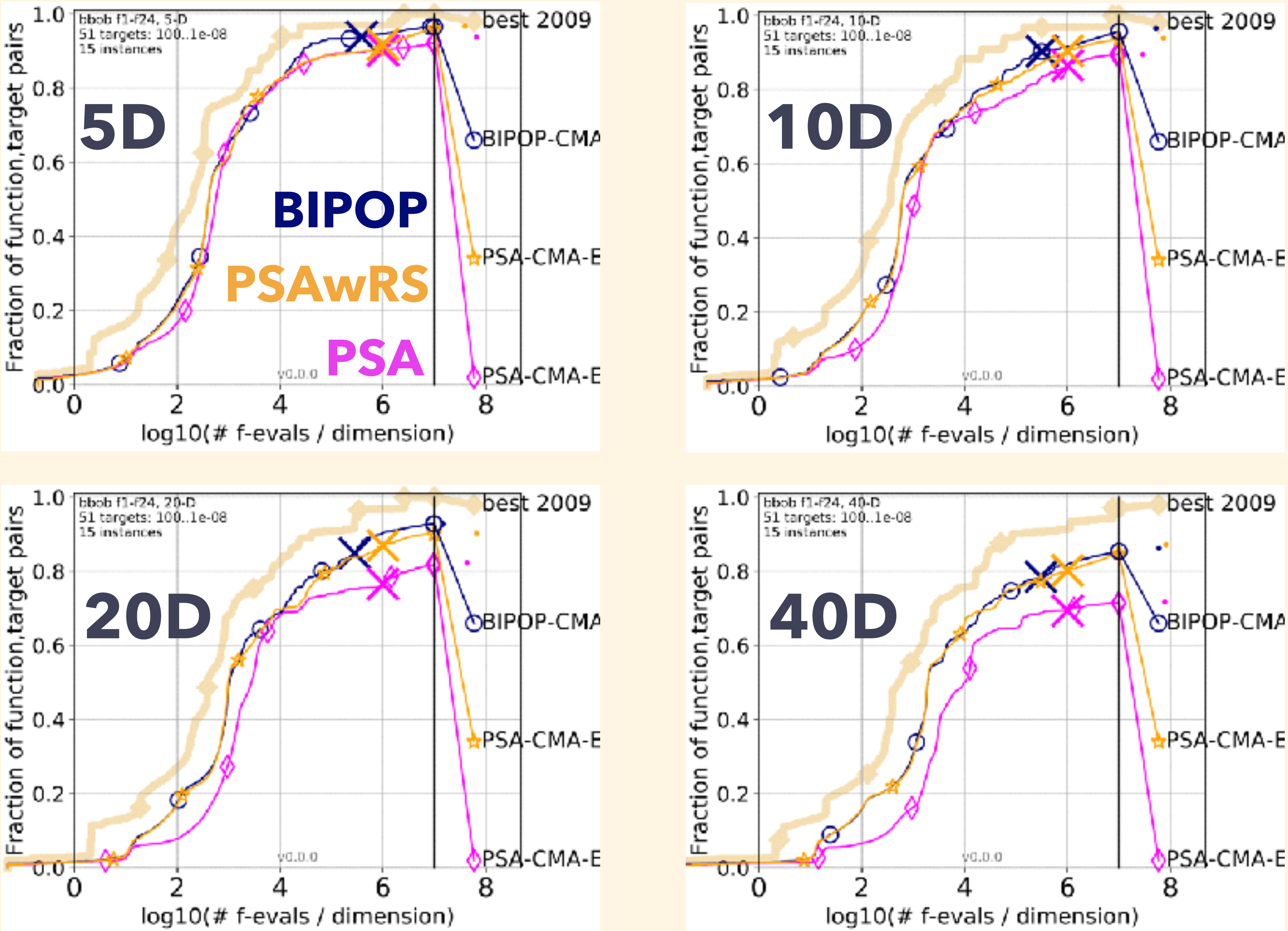
Algorithm Variants

PSA: PSA-CMA-ES with the simple restart

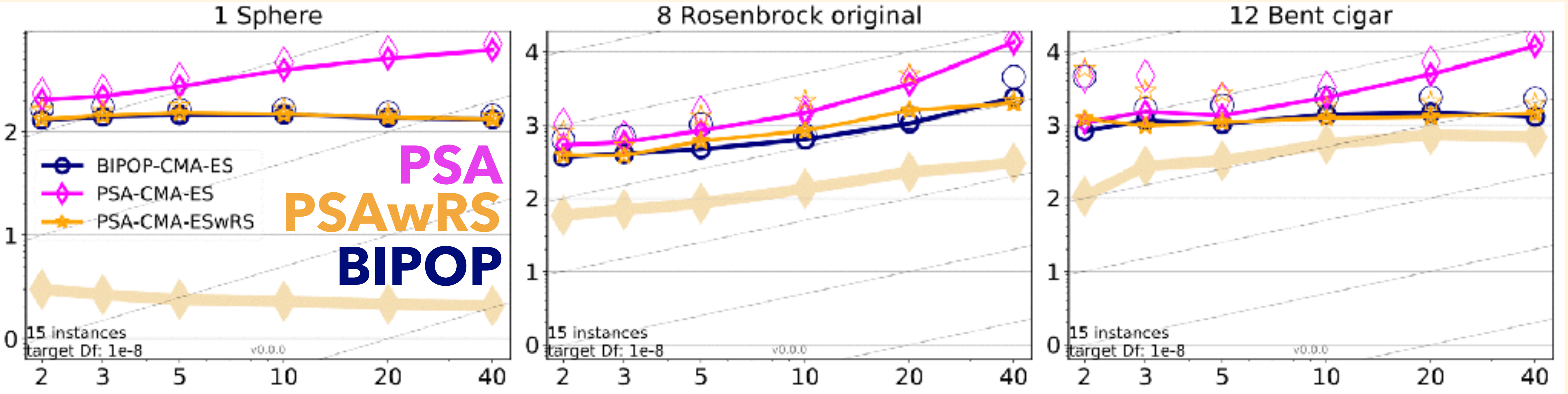
PSAwRS: PSA-CMA-ES with the proposed restart strategy

BIPOP: BIPOP-CMA-ES [Hansen 2009]

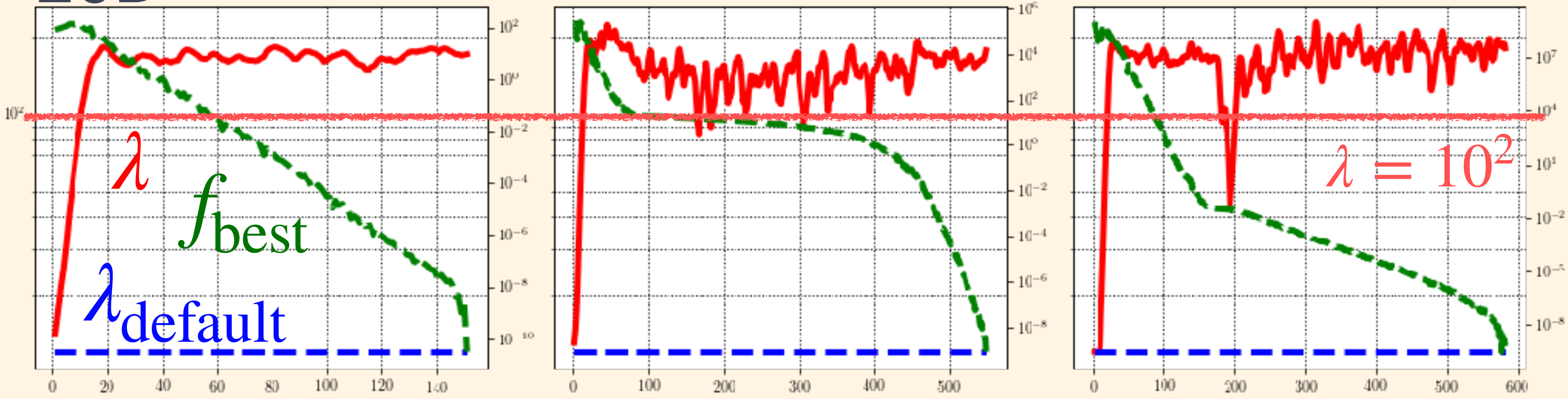
Overall Performance (f1-f24)



Unimodal Functions

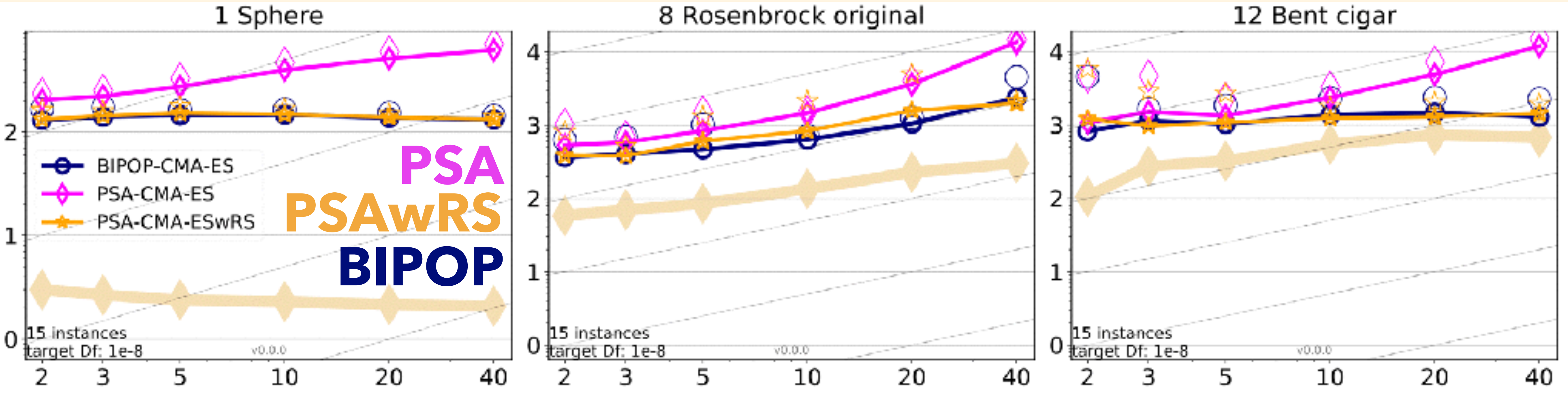


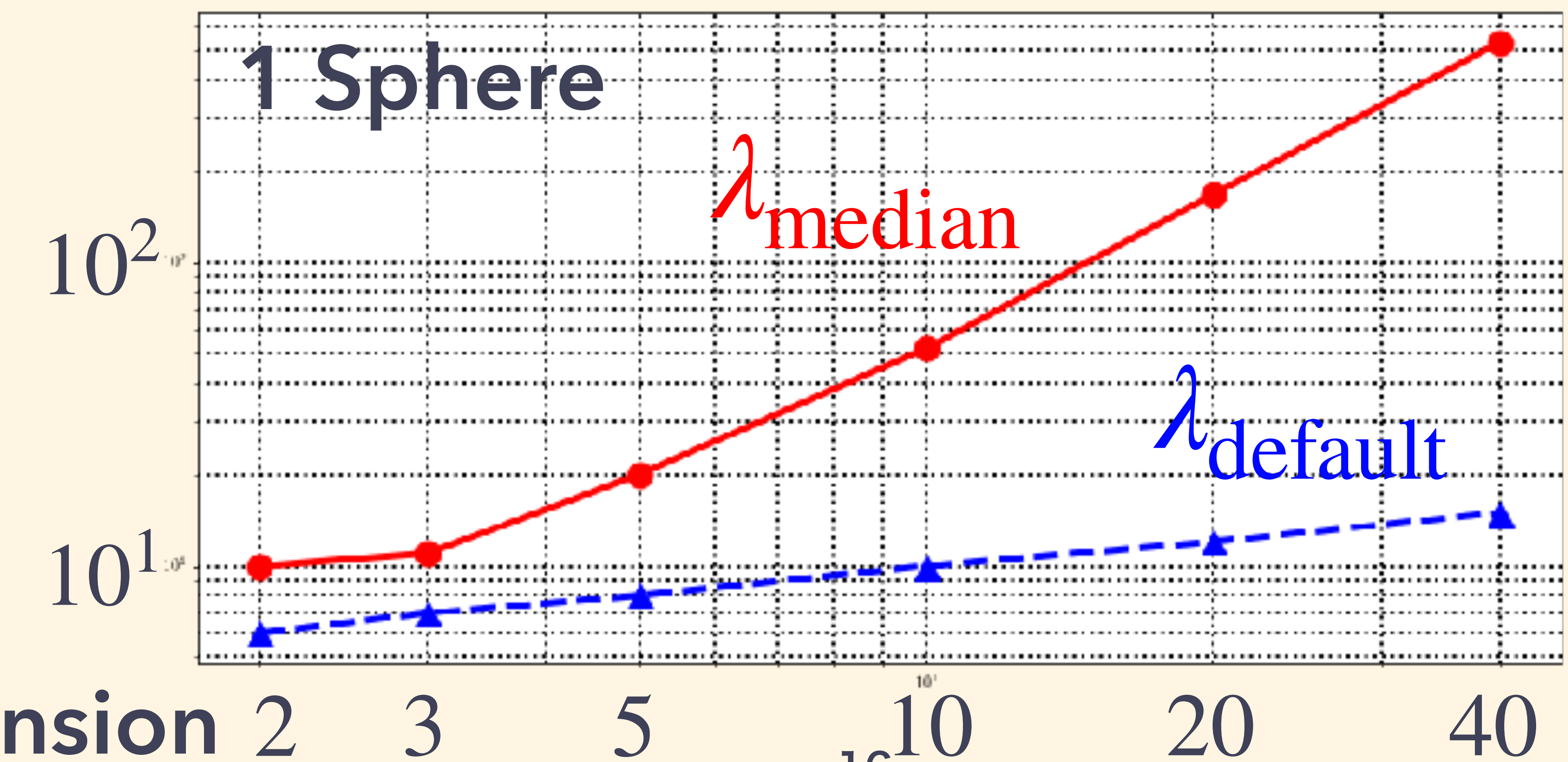
20D



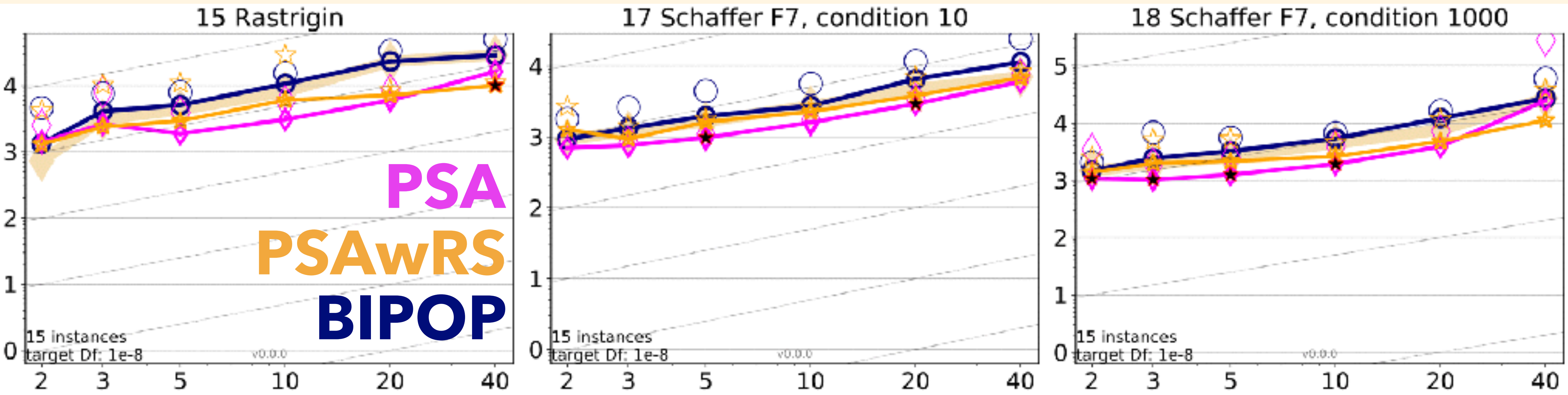
Number of Iteration

Unimodal Functions

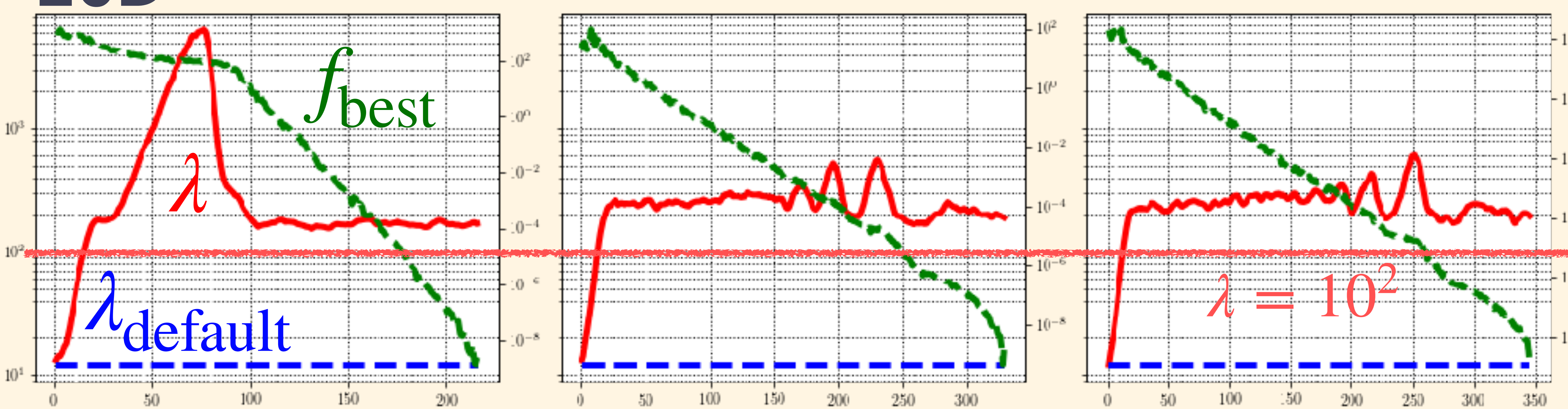




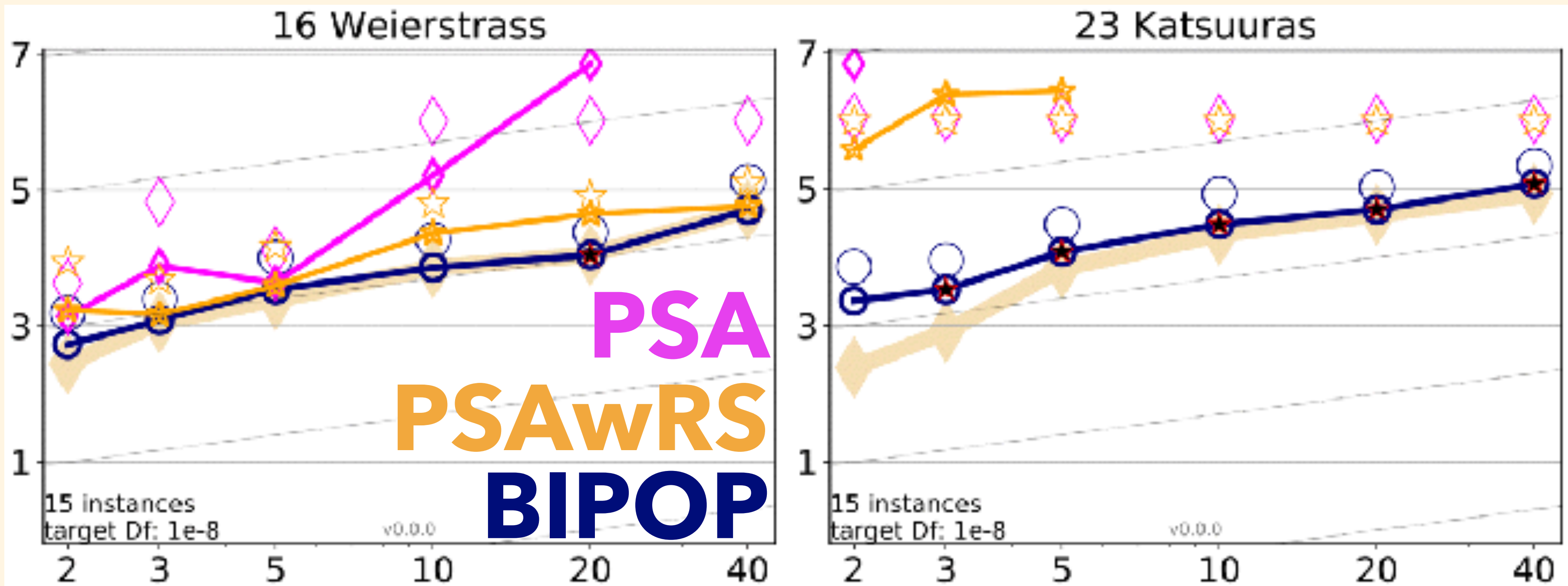
Well-structured Multimodal Functions



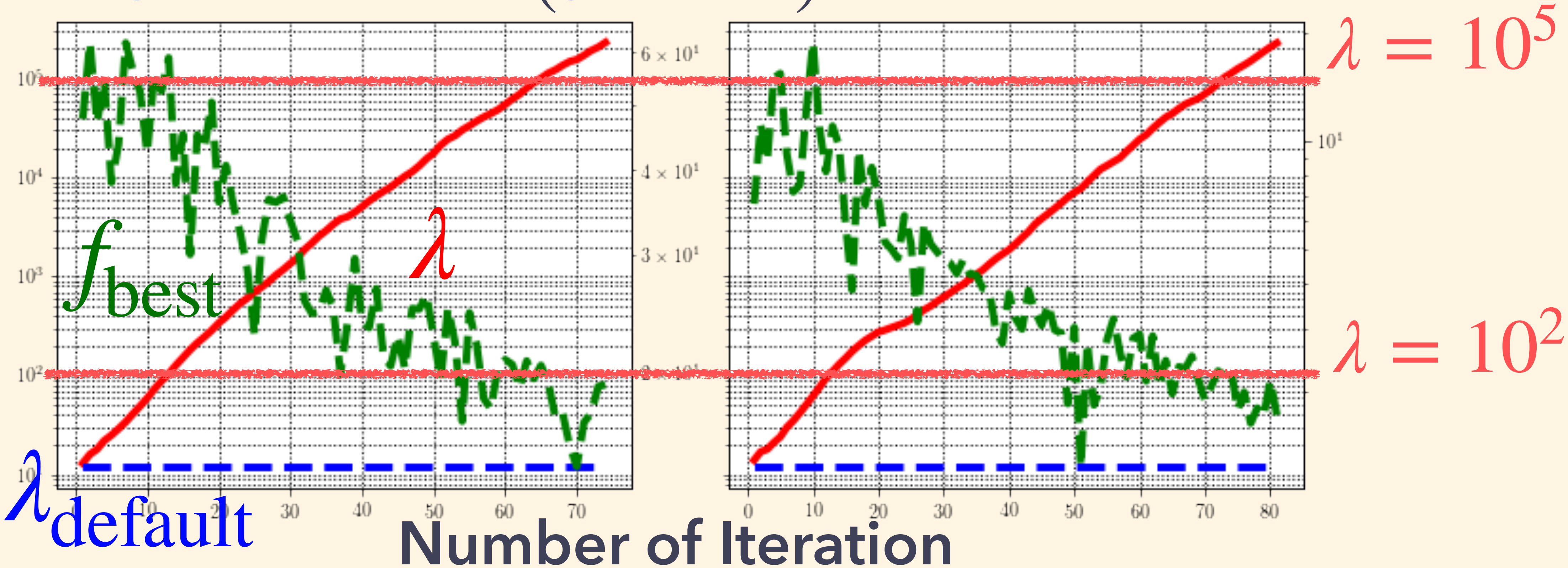
20D



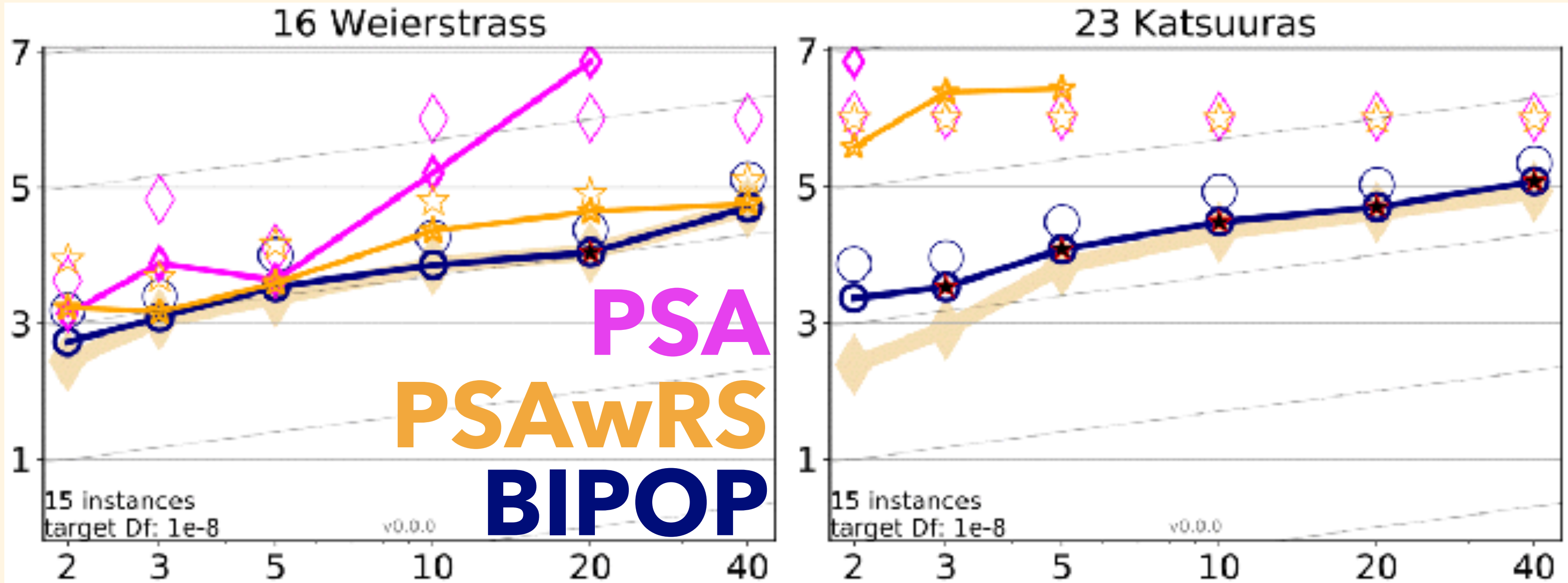
Repetitive Multimodal Functions



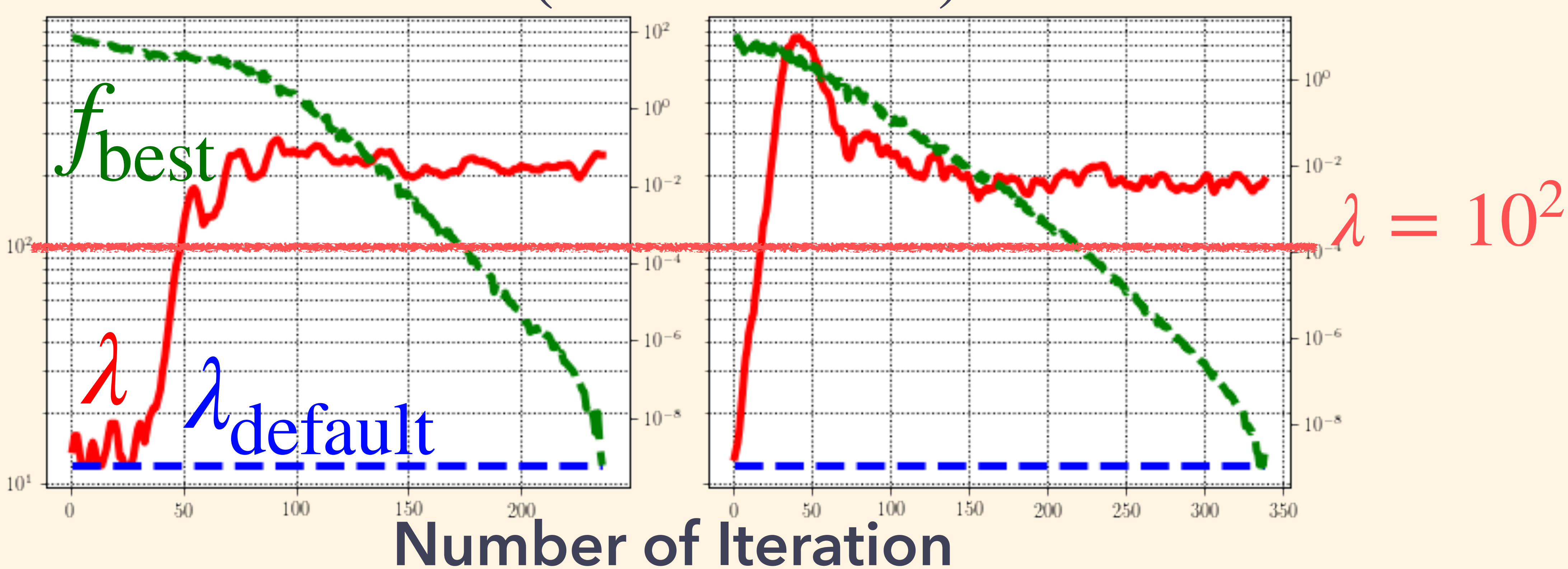
20D $(\sigma^{(0)} = 2)$



Repetitive Multimodal Functions



20D $(\sigma^{(0)} = 2/100)$



Summary

- PSA-CMA-ESwRS is comparable with BIPOP-CMA-ES.

On unimodal functions

- PSA-CMA-ES performs worse as dimension gets greater.

On well-structured multimodal functions

- PSA-CMA-ES works better than BIPOP-CMA-ES.

On repetitive multimodal functions

- An initial step-size is important to avoid inefficient increase of the population size.

Future Work

- To investigate the hyper-parameter setting