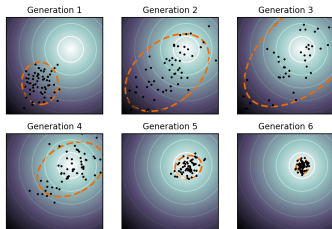


# Optimization in Machine Learning

## CMA-ES Algorithm

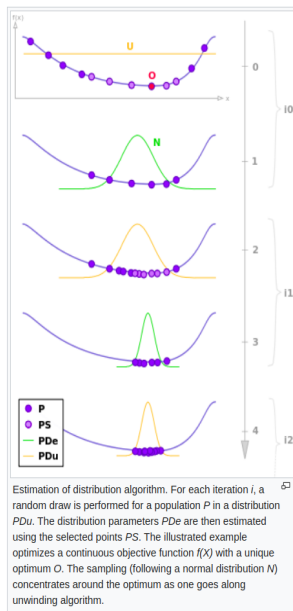


### Learning goals

- CMA-ES strategy
- Estimation of distribution
- Step size control

# ESTIMATION OF DISTRIBUTION ALGORITHM

- Instead of population, maintain distribution to sample offspring from
- 1 Draw  $\lambda$  offsprings  $\mathbf{x}^{(i)}$  from  $p(\cdot|\theta^{[t]})$
  - 2 Evaluate fitness  $f(\mathbf{x}^{(i)})$
  - 3 Update  $\theta^{[t+1]}$  with  $\mu$  best offsprings

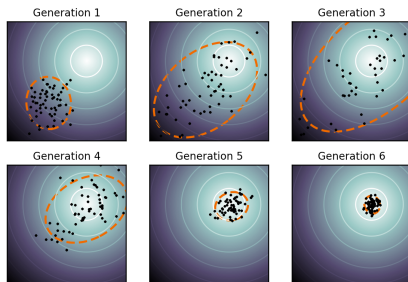


# COVARIANCE MATRIX ADAPTATION

Sample distribution is multivariate Gaussian

$$\mathbf{x}^{[t+1](i)} \sim \mathbf{m}^{[t]} + \sigma^{[t]} \mathcal{N}(\mathbf{0}, \mathbf{C}^{[t]}) \quad \text{for } i = 1, \dots, \lambda$$

- $\mathbf{x}^{[t+1](i)} \in \mathbb{R}^d$   $i$ -th offspring;  $\lambda \geq 2$  number of offspring
- $\mathbf{m}^{[t]} \in \mathbb{R}^d$  mean value and  $\mathbf{C}^{[t]} \in \mathbb{R}^{d \times d}$  covariance matrix
- $\sigma^{[t]} \in \mathbb{R}_+$  “overall” standard deviation/step size



**Question:** How to adapt  $\mathbf{m}^{[t+1]}$ ,  $\mathbf{C}^{[t+1]}$ ,  $\sigma^{[t+1]}$  for next generation  $t + 1$ ?

# CMA-ES: BASIC METHOD - ITERATION 1

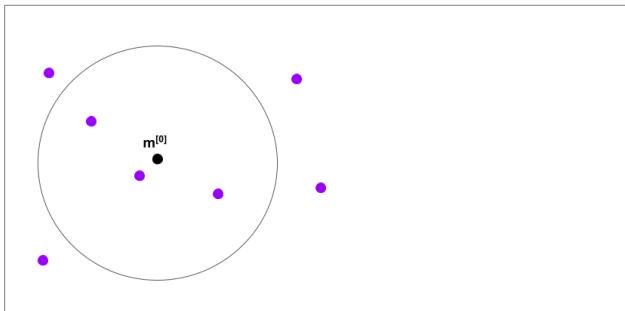
- 0 Initialize  $\mathbf{m}^{[0]}$ ,  $\sigma^{[0]}$  problem-dependent and  $\mathbf{C}^{[0]} = \mathbf{I}_d$



# CMA-ES: BASIC METHOD - ITERATION 1

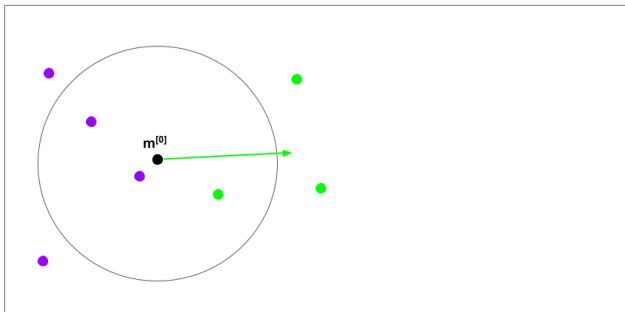
- 1 **Sample**  $\lambda$  offsprings from distribution

$$\mathbf{x}^{[1](i)} = \mathbf{m}^{[0]} + \sigma^{[0]} \mathcal{N}(\mathbf{0}, \mathbf{C}^{[0]})$$



# CMA-ES: BASIC METHOD - ITERATION 1

- ② **Selection and recombination** of  $\mu < \lambda$  best-performing offspring using fixed weights  $w_1 \geq \dots \geq w_\mu > 0, \sum_{i=1}^{\mu} w_i = 1$ .  
 $\mathbf{x}_{i:\lambda}$  is  $i$ -th ranked solution, ranked by  $f(\mathbf{x}_{i:\lambda})$ .

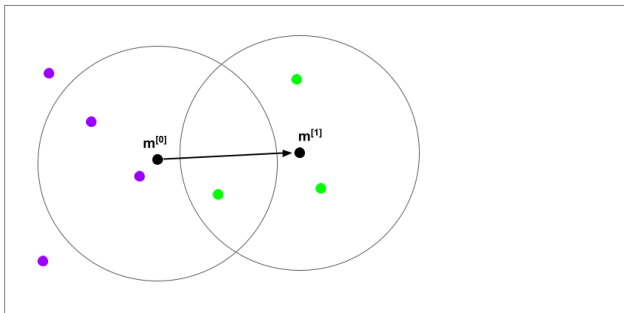


Calculation of auxiliary variables ( $\mu = 3$  points)

$$\mathbf{y}_w^{[1]} := \sum_{i=1}^{\mu} w_i (\mathbf{x}_{i:\lambda}^{[1]} - \mathbf{m}^{[0]}) / \sigma^{[0]} := \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}^{[1]}$$

# CMA-ES: BASIC METHOD - ITERATION 1

## ③ Update mean



Movement towards the new distribution with mean

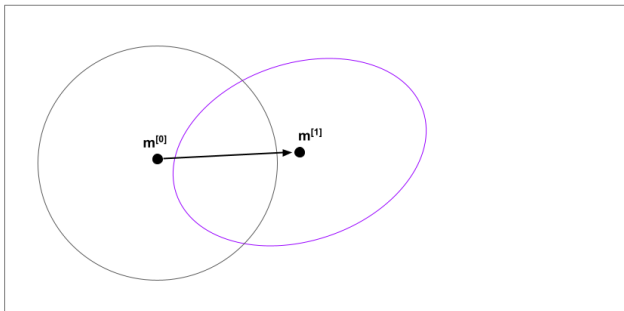
$$\mathbf{m}^{[1]} = \mathbf{m}^{[0]} + \sigma^{[0]} \mathbf{y}_w^{[1]}.$$

# CMA-ES: BASIC METHOD - ITERATION 1

## 4 Update covariance matrix

Roughly: elongate density ellipsoid in direction of successful steps.

$\mathbf{C}^{[1]}$  reproduces successful points with higher probability than  $\mathbf{C}^{[0]}$ .



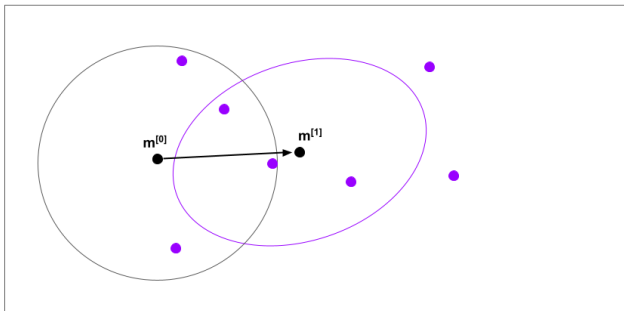
Update  $\mathbf{C}^{[0]}$  using sum of outer products and parameter  $c_\mu$ :

$$\mathbf{C}^{[1]} = (1 - c_\mu)\mathbf{C}^{[0]} + c_\mu \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}^{[1]} (\mathbf{y}_{i:\lambda}^{[1]})^\top \text{ (rank-}\mu \text{ update).}$$



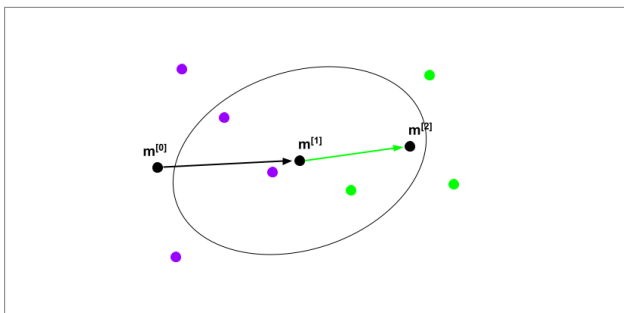
# CMA-ES: BASIC METHOD - ITERATION 2

- 1 **Sample** from distribution for new generation



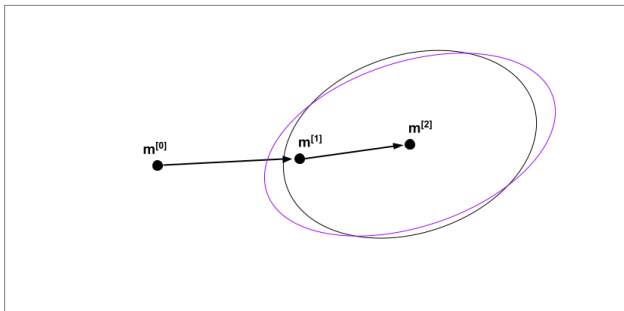
# CMA-ES: BASIC METHOD - ITERATION 2

- ② Selection and recombination of  $\mu < \lambda$  best-performing offspring
- ③ Update mean



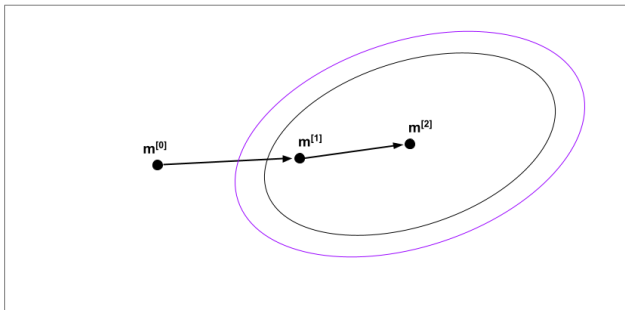
# CMA-ES: BASIC METHOD - ITERATION 2

## ④ Update covariance matrix



# CMA-ES: BASIC METHOD - ITERATION 2

- ⑤ **Update step-size** exploiting correlation in history of steps.  
steps point in similar direction  $\implies$  increase step-size  
steps cancel out  $\implies$  decrease step-size



# UPDATING $\mathbf{C}$ : FULL UPDATE

Full CMA update of  $\mathbf{C}$  combines rank- $\mu$  update with a rank-1 update using exponentially smoothed evolution path  $\mathbf{p}_c \in \mathbb{R}^d$  of successive steps and learning rate  $c_1$ :

$$\mathbf{p}_c^{[0]} = \mathbf{0}, \quad \mathbf{p}_c^{[t+1]} = (1 - c_1)\mathbf{p}_c^{[t]} + \sqrt{\frac{c_1(2 - c_1)}{\sum_{i=1}^{\mu} w_i^2}} \mathbf{y}_w$$

Final update of  $\mathbf{C}$  is

$$\mathbf{C}^{[t+1]} = (1 - c_1 - c_{\mu} \sum_j w_j) \mathbf{C}^{[t]} + \underbrace{c_1 \mathbf{p}_c^{[t+1]} (\mathbf{p}_c^{[t+1]})^{\top}}_{\text{rank-1}} + \underbrace{c_{\mu} \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}^{[t+1]} (\mathbf{y}_{i:\lambda}^{[t+1]})^{\top}}_{\text{rank-}\mu}$$

- Correlation between generations used in rank-1 update
- Information from entire population is used in rank- $\mu$  update

# UPDATING $\sigma$ : METHODS STEP-SIZE CONTROL

- **1/5-th success rule**: increases the step-size if more than 20 % of the new solutions are successful, decrease otherwise
- **$\sigma$ -self-adaptation**: mutation is applied to the step-size and the better - according to the objective function value - is selected
- **Path length control via cumulative step-size adaptation (CSA)**

Intuition:

- Short cumulative step-size  $\triangleq$  steps cancel  $\rightarrow$  decrease  $\sigma^{[t+1]}$
- Long cumulative step-size  $\triangleq$  corr. steps  $\rightarrow$  increase  $\sigma^{[t+1]}$

