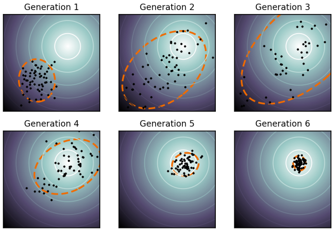
Optimization in Machine Learning

Evolutionary Algorithms
CMA-ES Algorithm



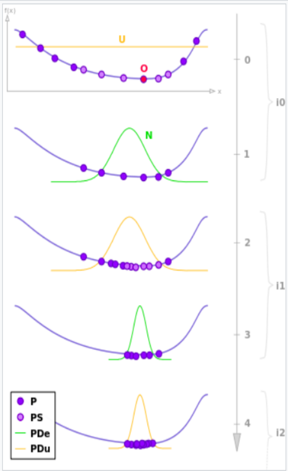
Learning goals

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

ESTIMATION OF DISTRIBUTION ALGORITHM

- Instead of population, maintain distribution to sample offspring from

1. Draw λ offsprings $\mathbf{x}^{(i)}$ from $p(\cdot|\boldsymbol{\theta}^{[t]})$
2. Evaluate fitness $f(\mathbf{x}^{(i)})$
3. Update $\boldsymbol{\theta}^{[t+1]}$ with μ best offsprings



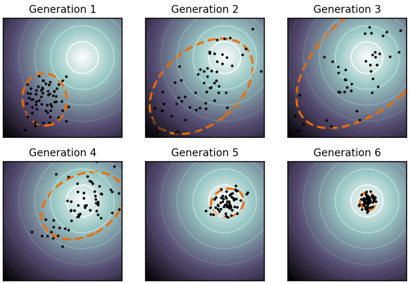
Estimation of distribution algorithm. For each iteration *i*, a random draw is performed for a population *P* in a distribution *PDu*. The distribution parameters *PDe* are then estimated using the selected points *PS*. The illustrated example optimizes a continuous objective function *f(X)* with a unique optimum *O*. The sampling (following a normal distribution *N*) concentrates around the optimum as one goes along unwinding algorithm.

COVARIANCE MATRIX ADAPTATION

Sample distribution is multivariate Gaussian

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

- $\mathbf{x}^{[t+1](i)} \in \mathbb{R}^d$ 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

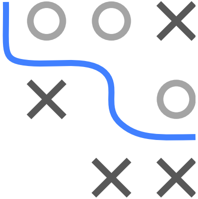


Question: How to adapt $\mathbf{m}^{[t+1]}$, $\mathbf{C}^{[t+1]}$, $\sigma^{[t+1]}$ for next generation $t+1$?

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 / 2

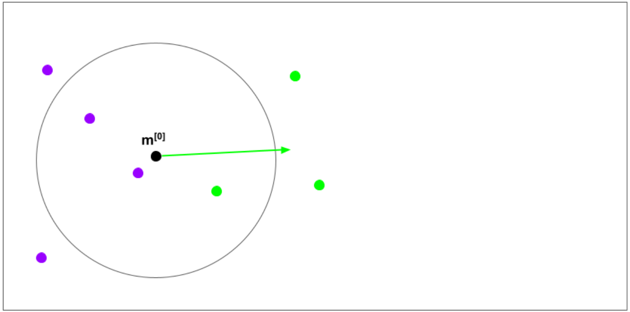


1. **Sample** λ offsprings from distribution

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

CMA-ES: BASIC METHOD - ITERATION 1 / 3

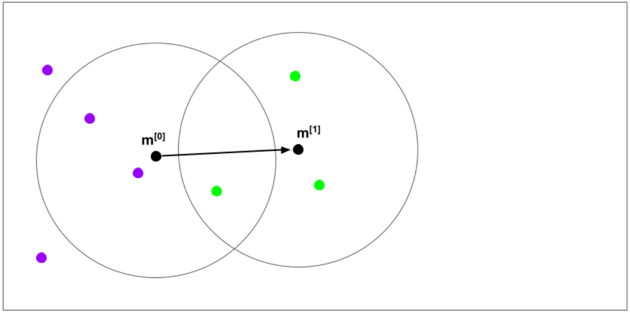
❷ **Selection and recombination** of $\mu < \lambda$ best-performing offspring using fixed weights $w_1 \geq \ldots \geq w_\mu > 0, \sum_{i=1}^{\mu} w_i = 1$.
$\mathbf{x}_{i:\lambda}$ is i-th ranked solution, ranked by $f(\mathbf{x}_{i:\lambda})$.



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 / 4

❸ Update mean

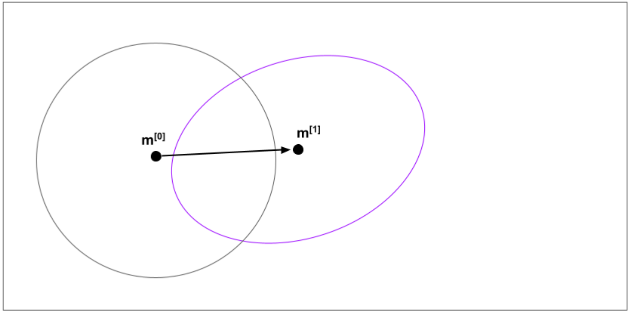


Movement towards the new distribution with mean $\mathbf{m}^{[1]} = \mathbf{m}^{[0]} + \sigma^{[0]}\mathbf{y}_w^{[1]}$.

CMA-ES: BASIC METHOD - ITERATION 1 / 5

❹ **Update covariance matrix**

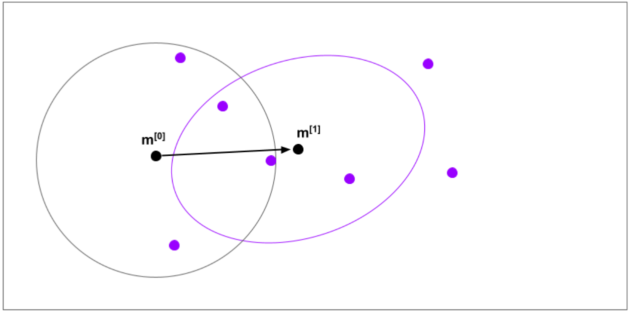
Roughly: elongate density ellipsoid in direction of successful steps.
$\mathbf{C}^{[1]}$ reproduces successful points with higher probability than $\mathbf{C}^{[0]}$.



Update $\mathbf{C}^{[0]}$ using sum of outer products and parameter c_μ:
$\mathbf{C}^{[1]} = (1 - c_\mu)\mathbf{C}^{[0]} + c_\mu \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}^{[1]} (\mathbf{y}_{i:\lambda}^{[1]})^\top$ (rank-μ update).

CMA-ES: BASIC METHOD - ITERATION 2

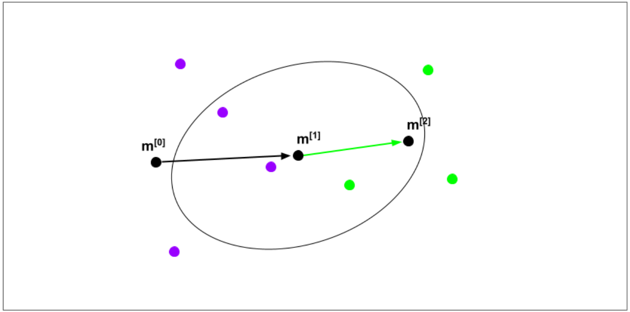
1. **Sample** from distribution for new generation



CMA-ES: BASIC METHOD - ITERATION 2 / 2

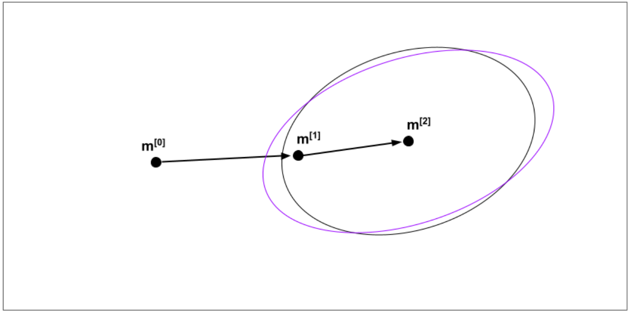
❷ **Selection and recombination** of $\mu < \lambda$ best-performing offspring

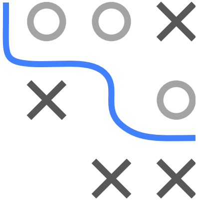
❸ **Update mean**



CMA-ES: BASIC METHOD - ITERATION 2 / 3

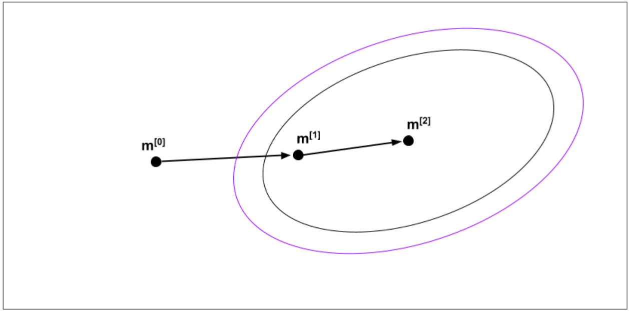
❹ **Update covariance matrix**





CMA-ES: BASIC METHOD - ITERATION 2 / 4

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 C: FULL UPDATE

Full CMA update of **C** combines rank-μ 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 **C** is

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

- Correlation between generations used in rank-1 update
- Information from entire population is used in rank-μ update

UPDATING σ: 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

- σ**-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 $\sigma^{[t+1]}$